

Collaborative Research Centre 1261

**Magnetoelectric Sensors: From Composite Materials to
Biomagnetic Diagnostics**

Christian-Albrechts-Universität zu Kiel

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1 General information

1.1 Key data

1.1.1 Governing bodies of the Collaborative Research Centre

Spokesperson:	Prof. Dr.-Ing. Eckhard Quandt
Representative Spokespersons:	Prof. Dr. med. Günther Deuschl Prof. Dr. Martina Gerken
Steering Committee:	Prof. Dr. med. Günther Deuschl Prof. Dr. Franz Faupel Prof. Dr. Martina Gerken Prof. Dr.-Ing. Eckhard Quandt Prof. Dr.-Ing. Gerhard Schmidt PD Dr. Bridget Murphy

1.1.2 Project leaders

Project leaders	Year of birth	Doctorate obtained in:	Home institution, location	Project
Adelung, Rainer, Prof. Dr.	1971	2000	IMS	A2, A5
Bahr, Andreas, Prof. Dr.-Ing.	1979	2017	EEIT	B1
Deuschl, Günther, Prof. Dr. Dr. h.c.	1950	1980	Neuro	T1
Enzingmüller, Carolin, Dr.	1984	2017	IPN	SOP
Faupel, Franz, Prof. Dr.	1957	1985	IMS	A2, A4, B7
Frey, Norbert, Prof. Dr.	1966	1994	Cardio	B10
Gerken, Martina, Prof. Dr.	1973	2003	EEIT	A8, IRTG
Helmers, Ann-Kristin, Dr.	1987	2015	Neurosurg	T1
Höft, Michael, Prof. Dr.-Ing.	1972	2002	EEIT	B1, T1, Z2
Kienle, Lorenz, Prof. Dr.	1967	1998	IMS	A6
Lofink, Fabian, Dr.	1977	2014	ISIT	A9
Maetzler, Walter, Prof. Dr.	1971	2002	Neuro	B9, IRTG
McCord, Jeffrey, Prof. Dr.-Ing.	1965	1997	IMS	A1, A10, IRTG
Meyners, Dirk, Dr.	1973	2006	IMS	A1, Z1
Murphy, Bridget, PD Dr.	1969	2004	IEAP	A6
Niekiel, Florian, Dr.-Ing.	1987	2017	ISIT	Z1
Parchmann, Ilka, Prof. Dr.	1969	1997	IPN	SOP
Quandt, Eckhard, Prof. Dr.-Ing.	1960	1990	IMS	A7, A9, Z3
Rieger, Robert, Prof. Dr.	1975	2004	EEIT	A4
Schmidt, Gerhard, Prof. Dr.-Ing.	1971	2001	EEIT	B2, B9, B10, Z2
Selhuber-Unkel, Christine, Prof. Dr.	1980	2006	IMS	B7
Wulfinghoff, Stephan, Prof. Dr.-Ing.	1982	2014	IMS	A10

1.1.3 Participating institutions

Kiel University (CAU)

Faculty of Engineering

Institute of Electrical Engineering and Information Technology (EEIT)

Institute for Materials Science (IMS)

Faculty of Mathematics and Natural Sciences

Institute of Experimental and Applied Physics (IEAP)

Faculty of Medicine

University Hospital Schleswig-Holstein, Campus Kiel (UKSH)

Department for Internal Medicine III, Cardiology and Angiology (Cardio)

Department for Neurology (Neuro)

Department for Neurosurgery (Neurosurg)

Leibniz-Institute for Science and Mathematics Education, Kiel (IPN)

Fraunhofer Institute for Silicon Technology, Itzehoe (ISIT)

Boston Scientific Medizintechnik GmbH, Neuromodulation, Ratingen

1.1.4 Project groups and projects

Project	Status	Title	Research area	Project leaders, institutions, locations
Project Area A: Sensor Technology				
A1		Magnetostrictive Multilayers for Magnetoelectric Sensors	Magnetic Materials Functional Materials	McCord (IMS) Meyners (IMS)
A2		Hybrid Magnetoelectric Sensors based on Mechanically Soft Composite Materials	Nano Materials Material Compounds	Adelung (IMS) Faupel (IMS)
A3	E	Resonant Magnetoelectric Sensors	Functional Materials Micro Systems Technology	Quandt (IMS) Wagner (ISIT)
A4		ΔE -Effect Sensors	Material Compounds Electronic Systems	Faupel (IMS) Rieger (EEIT)
A5		Piezotronic Magnetoelectric Composites	Nano Materials	Adelung (IMS)
A6		Microstructure and Structural Change of Magnetoelectric and Piezotronic Sensors	Solid State Physics Electron Microscopy	Murphy (IEAP) Kienle (IMS)
A7		Electrically Modulated Magnetoelectric Sensors	Functional Materials	Quandt (IMS)
A8		Modelling of Magnetoelectric Sensors	Theoretical Electrical Eng.	Gerken (EEIT)
A9	N	Surface Acoustic Wave Magnetic Field Sensors	Functional Materials Micro Systems Technology	Quandt (IMS) Lofink (ISIT)
A10	N	Magnetic Noise of Magnetoelectric Sensors	Magnetic Materials Computational Materials	McCord (IMS) Wulfinghoff (IMS)
Project area B: Magnetoelectric Sensor Systems for Medical Applications				
B1		Sensor Noise Performance and Analogue System Design	Microwave Engineering Sensor Systems	Höft (EEIT) Bahr (EEIT)
B2		Digital Signal Processing	System Theory	Schmidt (EEIT)
B3	E	Inverse Solutions for Localization of Biomagnetic Activity in Heart and Brain	Medical Psychology Neuropediatrics	Siniatchkin (IMPS) Stephani (Pedneuro)
B5	E	Individualized Deep Brain Stimulation	Neurology Microwave Engineering	Deuschl (Neuro) Höft (EEIT)
B6	E	Multimodal Mapping of Nerve Pathology with Magnetoelectric Sensors	Neurology System Theory	Laufs (Neuro) Schmidt (EEIT)

B7		3D-Imaging of Magnetically Labelled Cells	Material Compounds Biomaterials	Faupel (IMS) Selhuber-Unkel (IMS)
B9	N	Magnetoelectric Sensors for Movement Detection and Analysis	Neurology System Theory	Maetzler (Neuro) Schmidt (EIT)
B10	N	Magnetoelectric Sensor Systems for Cardiac Applications	Cardiology System Theory	Frey (Cardio) Schmidt (EIT)
T1	N	Transfer project – Individualized Deep Brain Stimulation	Microwave Engineering Neurology Neurosurgery	Höft (EIT) Deuschl (Neuro) Helmers (Neurosurg)
Central Projects				
Z1		MEMS Magnetoelectric Sensor Fabrication	Functional Materials Micro Systems Technology	Meyners (IMS) Niekiel (ISIT)
Z2		Magnetoelectric Sensor Characterization	Microwave Engineering System Theory	Höft (EIT) Schmidt (EIT)
IRTG		Integrated Research Training Group	Theoretical Electrical Eng. Neurology Magnetic Materials	Gerken (EIT) Maetzler (Neuro) McCord (IMS)
SOP		Scientific Outreach Project	Science and Mathematics Education	Enzengmüller (IPN) Parchmann (IPN)
Z3		Central tasks of the Collaborative Research Center	Functional Materials	Quandt (IMS)

1.2 Research profile of the Collaborative Research Centre

1.2.1 Summary of the research programme

The detection of magnetic field distributions in the head or torso makes powerful diagnostics of functions of the brain (magnetoencephalography MEG) or heart (magnetocardiography MCG) possible. Additionally, the detection of artificial weak magnetic fields, e.g., for deep brain stimulation, of magnetically labelled cells in scaffolds or for movement analysis offers attractive new biomagnetic applications. Systems used as routine diagnostic tools need to be easy-to-handle and cost-effective, thus, operation at room temperature is essential. In the first funding period, uncooled magnetoelectric (ME) magnetic field sensors have revealed their potential to detect weak magnetic fields at low frequencies, as required for those applications. These ME sensors are based on ME composites, i.e. composites consisting of at least one magnetostrictive and one piezoelectric constituent, which were fabricated using micro-electro-mechanical systems (MEMS) technology.

The general objectives of the Collaborative Research Centre CRC 1261 are investigations of different ME sensor approaches with a special focus on high sensitivity at biomagnetic frequencies (project area **A**) and their evaluation and utilization in medically relevant questions (project area **B**). The research program to pursue these goals requires intensive interdisciplinary collaboration between materials scientists, electrical engineers and physicians (neurology and cardiology). Project area **A**, entitled “Sensor Technology”, covers research from new materials (**A1**, **A2**) to the investigation of different ME sensor approaches [ΔE -effect (**A4**), piezotronic readout (**A5**, **A6**), electrically modulated sensors (**A7**) and surface acoustic wave sensors (**A9**)]. All projects that focus on improving the detection limit at biomagnetically relevant frequencies will be supported by modelling (**A8**, **A10**) and advanced characterization (**A6**, **A10**). These modelling projects are linked closely to the modelling activities in project area **B**. This area **B**, entitled “Magnetoelectric Sensor Systems for Medical Applications”, includes signal processing (**B1**, **B2**) and selected application areas in cardiology, neurology and life sciences, which have different detection requirements in magnetic field strength, frequency and spatial resolution (**B7**, **B9**, **B10** and **T1**). Further collaborations of the two project areas **A** and **B** and the two service projects are fostered by six focus groups which are dedicated to organizing the work on the overarching topics “Magnetic Layers” (Focus Group **F1**), “Modelling” (Focus Group **F2**), “Comparison of Sensor Concepts” (Focus Group **F3**), “ME Sensors” (Focus Group **F4**), “Concepts based on ΔE -effect” (Focus Group **F5**) and “Biomedical Applications” (Focus Group **F6**).

Based on the deep brain stimulation (DBS) research in **B5** in the first funding period, a transfer project **T1** in cooperation with the company Boston Scientific now plans on building a user-friendly imaging system to display the magnetically measured and reconstructed electrical currents within the individual magnetic resonance imaging (MRI) of the patient. This system will serve as a helpful tool for better programming of DBS patients. The work within the CRC will be supported by two service projects on MEMS sensor fabrication (**Z1**) and on

ME sensor characterization (**Z2**). An Integrated Research Training Group (**IRTG**) will foster the interdisciplinary collaboration within the CRC 1261 and provide the best possible research experience and training for our early career scientists. Furthermore, a Scientific Outreach Project (**SOP**) will be responsible not only for outreach to the public, school students and teachers but also for strengthening the interdisciplinary scientific communication within the CRC with a special focus on early career researchers.

The overall aim of the CRC 1261 is the establishment of a biomagnetic diagnostics system based on ME sensors for MEG, MCG, and other biomedical applications and to demonstrate its potential on selected medical diagnosis problems. The individual goals of the two remaining funding periods are grouped on the basis of the predicted limits of detection of the ME sensors at biomagnetically relevant frequencies ranging from 1 Hz to about 1 kHz. Based on the results of the first funding period with limits of detection in the range of $10 \text{ pT/Hz}^{1/2}$ at relevant frequencies, the selected application projects (**B7**, **B9**, **B10**, **T1**) are all feasible with the current sensor technology within the CRC but will of course profit from the expected improvement of the sensor performance during the second funding period.

Based on the planned projects and their expected results during the second funding period, the objective of the third funding period is achieving a closed-loop system of measurement and immediate actuation. For this, uncooled ME sensor arrays may then be implemented as a wearable device. A promising strategy is that measured data are processed in real time to develop a device for ME sensor-guided programming of patients with deep brain stimulators which can measure the stimulated area in patients outside of the magnetic chamber. Furthermore, uncooled ME-sensors to measure the MEG would open almost unlimited neuroscientific applications, e.g. brain-computer interface or closed-loop treatment of epilepsy based on the detection of the onset of epileptic spikes.

1.2.2 Detailed presentation of the research programme

1.2.2.1 Long-term prospects

The CRC 1261 has two long-term research objectives. **The first objective is the establishment of a closed-loop, uncooled, biomagnetic interface for diagnostics and immediate treatment in MEG and MCG.** Up to now, MEG and MCG have been predominantly realized in clinics using helium-cooled superconducting quantum interference devices (SQUID) as very sensitive magnetometers with a noise level in the low $\text{fT/Hz}^{1/2}$ range. Despite the proven advantages of MEG and MCG in many diagnostic problems compared to the widely used electroencephalography (EEG) and electrocardiography (ECG), MEG and MCG based on these SQUID sensors have found only very limited use in clinical applications. The reasons are mainly related to the complexity of the experimental setup and the high costs of investment and operation. Within the CRC 1261, we aim at a new biomagnetic interface approach based on ME composites as sensors for the detection of biomagnetic fields. These sensors avoid the disadvantages of SQUID sensors and enable new possibilities in MEG and MCG diagnostics as they will be operated at room temperature, will in general permit operation in unshielded environments, and will be much more cost-effective. Additionally, advantages of this technique in spatial resolution could enable physicians to rapidly answer complex clinical questions in cardiology and neurology at the bedside, such as a detection of the precise anatomical origin of arrhythmias or epileptic foci. Ultimately, invasive and costly procedures such as catheter-based electrophysiological studies may become obsolete, and ME sensor-based technology may even set the stage for novel methods of non-invasive treatment (e.g. ultrasound or radiation-based). Compared to electric measurements (ECG/EEG), advantages in the localization of the sources are envisaged due to the possibility of detecting vector fields in ME measurements. In comparison to existing concepts on the basis of EEG, removing the necessity to connect electrodes directly to the head would enable new, particularly long-term screening applications. These novel sensors could establish new visionary areas of applications such as mind control of prostheses, optimized learning, or novel body monitoring systems. Early promising applications that will be addressed within the CRC are movement detection and its analysis in neurological diseases as well as 3D measurements of magnetic particle distributions in biomaterial scaffolds (Fig. 1). For the latter, two approaches, magnetic particle mapping (MPM) and magnetic susceptibility particle mapping (MSPM), will be employed.



Figure 1: Application areas (brain, heart, cell imaging, and movement detection) and their prospects for the second and third funding period (from the center outwards).

The second long-term research objective is the investigation of different magnetic field sensor approaches based on ME composites with the aim of achieving a limit of detection in the sub-pT/Hz^{1/2} range for biomagnetically relevant frequencies (1 to 1 kHz). The different sensor approaches (direct measurements, ΔE -effect, piezotronic, electrically modulated and surface acoustic wave) and the aims for the second and third funding period (from the center outwards) are shown in Fig. 2.

ME materials are, in general, a subcategory of multiferroic materials, i.e. materials that show at least two ferroic properties (ferroelectric, ferro-/ferrimagnetic, or ferroelastic). Multiferroic materials are a relatively new but internationally very much noted class of materials due to their special properties such as multifunctionality, high energy conversion and good scalability for applications in micro- and nanotechnology. One can distinguish between natural and artificial multiferroics: the first consisting of one phase, the latter is a composite of two or more phases. In the case of ME materials, which have to be both ferroelectric and ferro-/ferrimagnetic, single phase magnetoelectrics are of very limited practical importance due to their limited effect sizes and low operation-temperatures, which are determined by the lower Curie temperature of the two ferroic transformations. Thus, within the CRC, research will be restricted to ME composites which rely on the combination of mechanically coupled piezoelectric and magnetostrictive phases. One should state that in a narrower sense composites which contain classical non-ferroelectric piezoelectric materials, based on ZnO, AlN, or quartz, are ME and thus within the scope of our research, but they are not multiferroic.

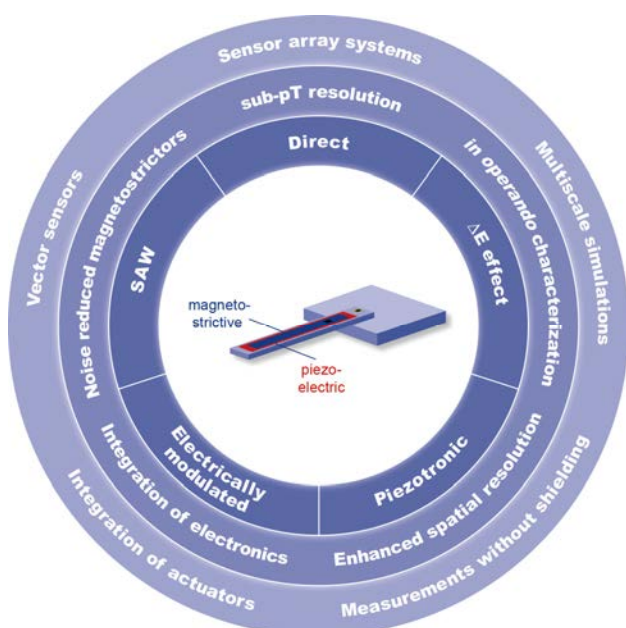


Figure 2: Different ME sensor approaches (direct measurements, ΔE -effect, piezotronic, electrically modulated and surface acoustic wave) and the aims for the second and third funding period (from the center outwards), which apply for all sensor approaches.

1.2.2.2 Magnetoelectric composites: different approaches for magnetic field sensors

The challenge of this CRC is the detection of natural as well as “artificial” biomagnetic fields arising from applications in cardiology, DBS, movement analysis (MA) and magnetic particle mapping (Fig. 3), which are all characterized by low field amplitudes and low frequencies. In summary, the required limits of detection (LOD) and frequency ranges are:

- In MCG 1 to 100 pT/Hz^{1/2} and 0.1 to 100 Hz,
- in MEG 10 fT/Hz^{1/2} to 1 pT/Hz^{1/2} and 1 to 1000 Hz,
- in DBS 1 pT/Hz^{1/2} and 130 – 170 Hz and at the higher harmonics up to 10 kHz,
- in the MSPM 10 pT/Hz^{1/2} to 1 nT/Hz^{1/2} and 1 and 10 Hz.

Furthermore, within the CRC there are two applications which rely on the detection of sinusoidal magnetic fields: MA and MPM. Here, the required LODs are in the pT/Hz^{1/2}-range at the excitation frequency which can be tuned to match the resonance frequency of the sensor employed.

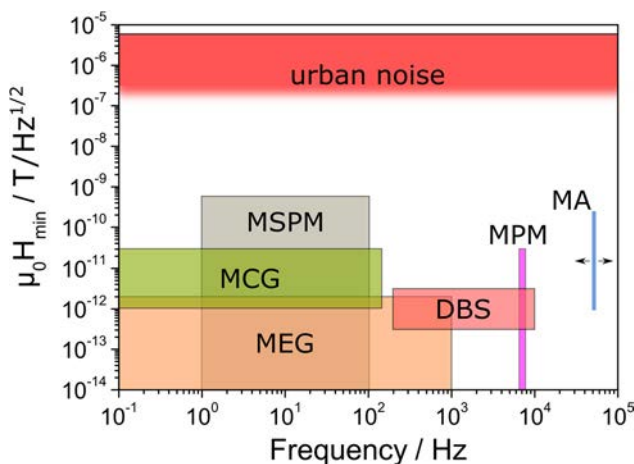


Figure 3: Required limits of detection (LOD) for the biomedical applications, which are the focus of the CRC 1261, as a function of frequency.

(DBS = deep brain stimulation
MA = movement analysis
MCG = magnetocardiography
MEG = magnetoencephalography
MPM = magnetic particle mapping
MSPM = magnetic particle susceptibility mapping)

As shown in Fig. 4a, the ME effect, which is the basis of the magnetic field sensors addressed in the CRC, connects the magnetic field with the electric polarization or the electric field with the magnetization (not shown). As explained in chapter 1.2.2.1, the direct (or natural) effect is small and restricted to low temperatures because the material has to be both ferroelectric and ferromagnetic. The CRC thus concentrates on artificial or composite magnetoelectrics which consist of a magnetostrictive and a piezoelectric phase.

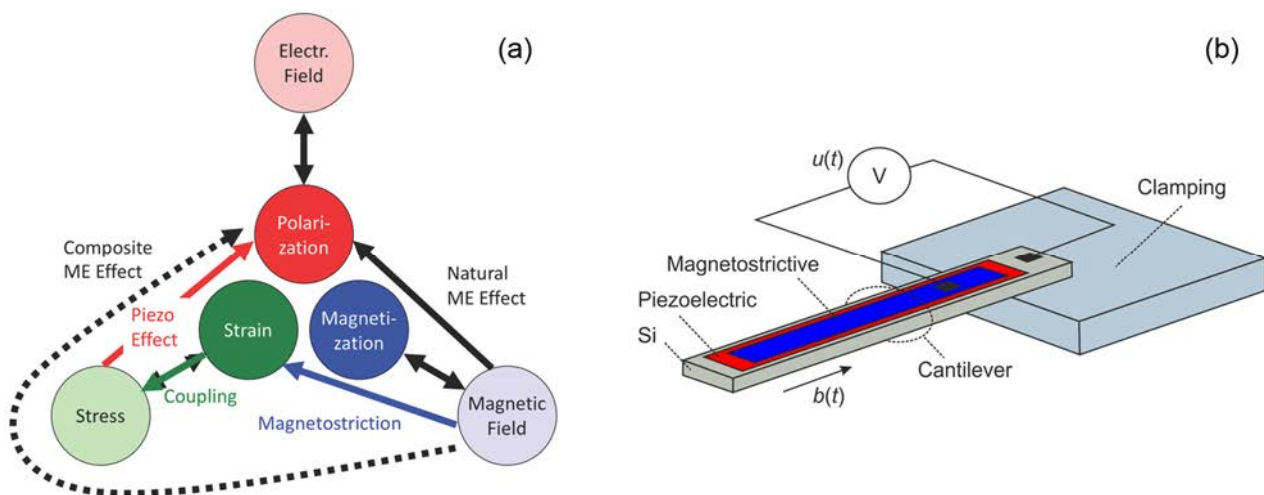


Figure 4: (a) Schematic representation of the direct ME effect and the composite ME effect, where the magnetostrictive strain is coupled to the piezoelectric phase. Only the direction usually used for magnetic field sensors, i.e. with magnetic field as the input, is shown. (b) Typical layout of a ME composite cantilever-type magnetic field sensor that was the starting point of the research in the CRC.

Their function – here for the application as magnetic field sensors – can be shown as a product property of the magnetostrictive strain, the mechanical coupling between the two phases and the piezoelectric effect [Su72, Fi05]¹. For applications as magnetic field sensors, the coefficient

$$\frac{\partial P}{\partial H} = \frac{\partial P}{\partial \sigma} \frac{\partial \sigma}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial H} = d_{ij} k_c d_{kl}^m \quad (1)$$

specifies the size of the ME effect. Here $\frac{\partial \varepsilon}{\partial H}$ describes the magnetostrictive strain ε induced by the magnetic field H , $\frac{\partial \sigma}{\partial \varepsilon}$ the transduction of the magnetostrictive strain to a stress σ in the piezoelectric material, and $\frac{\partial P}{\partial \sigma}$ the piezoelectric effect in the piezoelectric phase. Thus, these three partial derivatives are equal to the piezomagnetic coefficient d_{kl}^m , a coupling coefficient k_c , and the piezoelectric coefficient d_{ij} , respectively, which are in general dependent on the working point. The mechanical coupling depends on the volume fractions of the two phases, on their elastic properties, and, in the case of thin film composites, on the clamping to the substrate (Fig. 4b).

The limit of detection (LOD) can be determined by the ratio of the noise voltage density and the ME effect size all as a function of the frequency. For the cantilever-type sensors (Fig. 4b), calculations and measurements of the noise voltage density have revealed three major contributing noise sources from sensor and amplifier, namely Johnson-Nyquist noise of the sensor, as well as voltage and current (shot) noise of the amplifier. This results in three noise regimes for typical ME thin film sensors: $1/f$ dependency in the low frequency regime (approx. below 100 Hz) due to dominant current noise of the amplifier, $1/f^{1/2}$ dependence at medium frequencies (approx. between 100 Hz and 1 kHz) due to dominant Johnson-Nyquist noise of the piezoelectric phase, and a constant noise level for frequencies above 1 kHz due to dominant voltage noise of the amplifier (s. Fig. 5a) [Ja11a]. Assuming a frequency independent ME voltage coefficient outside the mechanical resonance and an amplification in resonance described by the quality factor Q (Fig. 5b), the LOD shows the same frequency dependence as the noise density level, however, the LOD is enhanced by the quality factor at the mechanical resonance (Fig. 5c, d). Additionally, it was found in the first funding period that the sensor-intrinsic thermal-mechanical noise limits the LOD but is only dominant in a very narrow range around the resonance frequency (f_{res}) [Du17].

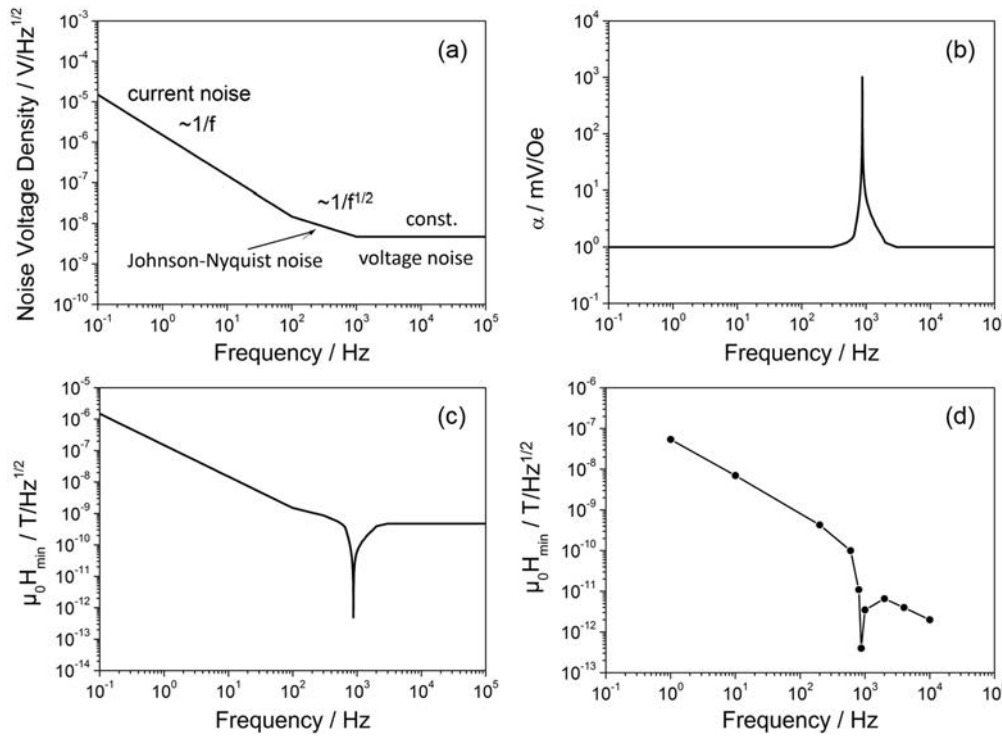


Figure 5: Schematic representation of: (a) the noise voltage density; (b) the ME voltage coefficient displaying the enhancement by the mechanical resonance and (c) the corresponding calculated limit of detection as a function of frequency. Typical data for thin film cantilever-type ME sensors as shown in Fig. 4b is presented. (d) Experimentally, this behavior was confirmed [Ya16].

By projecting the LOD of Fig. 5d into the biomagnetic fields versus frequency plot (Fig. 3), Fig. 6 is obtained. Considering that the mechanical resonance can be widely tuned, the result demonstrates that small-bandwidth applications at frequencies above 100 Hz (3D imaging of labelled cells and movement detection) are already

¹ [Su72] refers to references of the general information part given on page 27.

fully within reach of the present ME sensors when the mechanical resonance is close to the frequency of the application. The frequencies of the ME sensor, the MPM and the MA applications can be tuned in a wide range, thus matching is not a problem (Fig. 6)

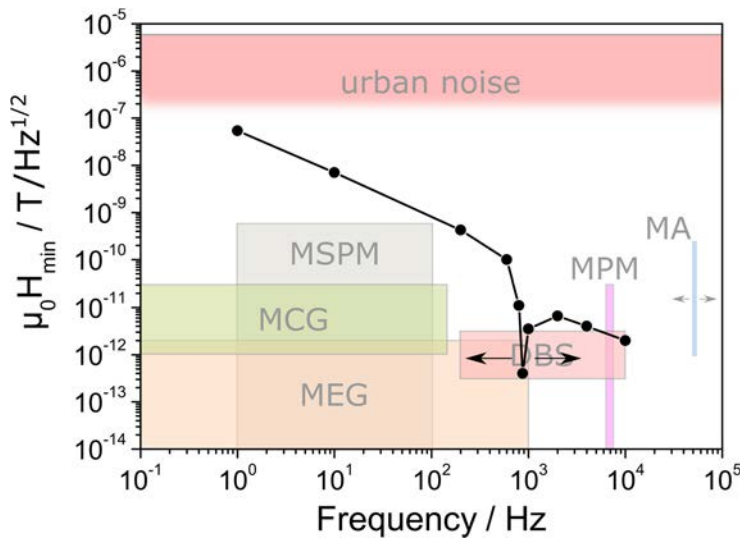


Figure 6: Typical LOD of a cantilever type ME magnetic field sensor (**Z1**) in comparison to the magnetic fields of applications, which are addressed within the CRC.

(DBS = deep brain stimulation
MA = movement analysis
MCG = magnetocardiography
MEG = magnetoencephalography
MPM = magnetic particle mapping
MSPM = magnetic particle susceptibility mapping)

This result leads to the following consequences:

1. For the applications using artificial sinusoidal magnetic fields (3D cell detection by MPM (**B7**) and MA (**B9**)), cantilever-type sensors as shown in Fig. 4b will be used in their mechanical resonance. Open questions are the use of exchanged biased magnetostrictive layers to avoid a DC magnetic bias field, the size of the sensor, its resonance frequency, and strategies to reduce cross-sensitivities. These questions will be central in **Z1** and **Z2**, respectively, and solutions will be based on the results mainly obtained by **A3** in the first funding period.
2. For the natural signals (MCG (**B10**), MEG), the DBS (**T1**) and the MSPM, a much higher bandwidth is required compared to cantilever-type sensors. Thus, modulation techniques will be employed: ΔE -effect sensors (**A4**), electrically modulated ME sensors (**A7**) and the surface acoustic wave sensors (**A9**). The generally very successful strategy of magnetic frequency conversion (MFC) will not be continued, as the required high frequency of the modulation field and possible crosstalk in sensor arrays are considered to be critical. Nevertheless, the related magnetostrictive multilayer development (**A1**, **A6**) for MFC will be transferred to or adopted by the other modulation approaches. The limits of detection obtained in the first funding period demonstrate the general feasibility of the application projects in project area B (Fig. 7).

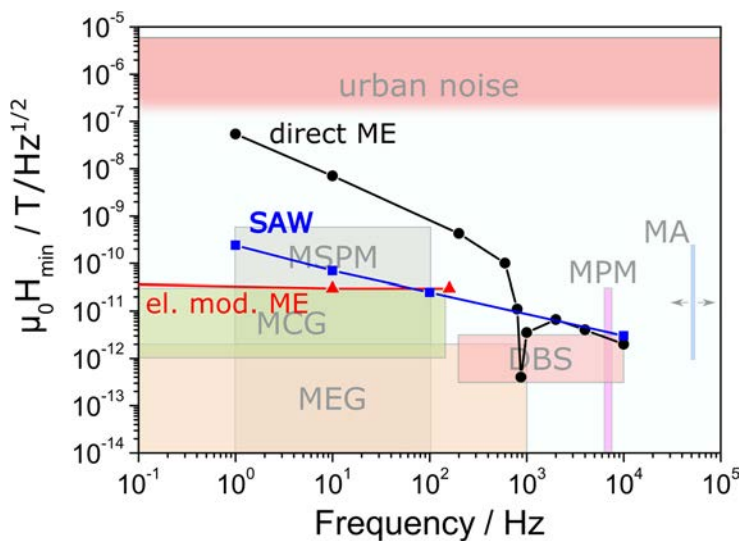


Figure 7: Comparison of detection limits achieved for the different sensor concepts (direct ME: cantilever type sensor (**Z1**), SAW: surface acoustic wave sensor (**A9**), and electrically modulated inverse ME sensor (**A7**)) within the first funding period.

(DBS = deep brain stimulation
MA = movement analysis
MCG = magnetocardiography
MEG = magnetoencephalography
MPM = magnetic particle mapping
MSPM = magnetic particle susceptibility mapping)

3. Different from modulation techniques, the ME sensors could be used in a passive, non-resonant mode. In this case, an enhancement of the ME-effect size of many orders of magnitude is required (Fig. 6). This should be achieved by novel, very soft ME composites, where clamping and other losses are

avoided. Here, particle / polymer composites as magnetostrictive phase and electrets as a pseudo-piezoelectric phase will be investigated (**A2**).

4. Additionally, we will continue with research on piezotronic readout (**A5, A6**), as this approach offers the possibility to enhance the effect size by amplification of the signal directly at the sensor and also the realization of extremely small ME sensors that could be suitable one day for invasive investigations, e.g. by using catheters.

More details on the different ME sensor concepts of the CRC are given in chapter 1.2.2.4.

1.2.2.3 Structure of the collaborative research centre

The work within the CRC is organized into two project areas and comprises 14 research projects and one transfer project. Project area **A**, "Sensor Technology", covers the range from materials research on novel ME composites and their constituents (**A1, A2**) to the research on new sensor concepts (**A4, A5, A7, A9**) including their *in situ* characterization (**A6, A10**) and materials and sensor modelling (**A8, A10**). Project area **B**, "Magnetolectric Sensor Systems for Medical Applications", uses sensor concepts of project area **A** and deals with analogue and digital signal processing (**B1, B2**) and three different life science applications (**B7, B9, B10**) that are considered to be in the range of the sensors' performance within the second funding period. The former project **B5** on deep brain stimulation will be continued as a transfer project **T1** with Boston Scientific as the industrial partner. The integration of medical projects at any stage is a specific characteristic of the CRC 1261. It will ensure the provision of specific sensor targets and specifications for medical applications as well as the evaluation of the sensors' performance using realistic and medically relevant problems and environments. Both are considered to be key factors for reaching the overall aims of the CRC. As a consequence, this approach requires a continuous, dedicated, interdisciplinary orientation of the CRC with the participation of internationally well-recognized groups from materials science, physics, electrical engineering, and medicine at Kiel University in collaboration with the Fraunhofer Institute of Silicon Technology (ISIT) and the Leibniz-Institute for Science and Mathematics Education (IPN) throughout all three funding periods. The two project areas will be complemented by two service projects (**Z1, Z2**), the Integrated Research Training Group (**IRTG**), the Scientific Outreach Project (**SOP**), and the Administrative Project (**Z3**). The structure and the main collaborations of the CRC 1261 are shown in Fig. 8. Further collaborations of the two project areas **A** and **B** and the two service projects are fostered by six focus groups, which are dedicated to organizing the work on the overarching topics "Magnetic layers" (**F1**), "Modelling" (**F2**), "Comparison of sensor concepts" (**F3**), "ME sensors" (**F4**), "Concepts based on ΔE -effect" (**F5**), and "Biomedical applications" (**F6**). More details on the focus groups are given in chapter 1.2.2.7. In the following sections, the project areas **A** and **B**, the Transfer Project, the Service Projects, and the collaborations within the CRC are discussed in more detail.

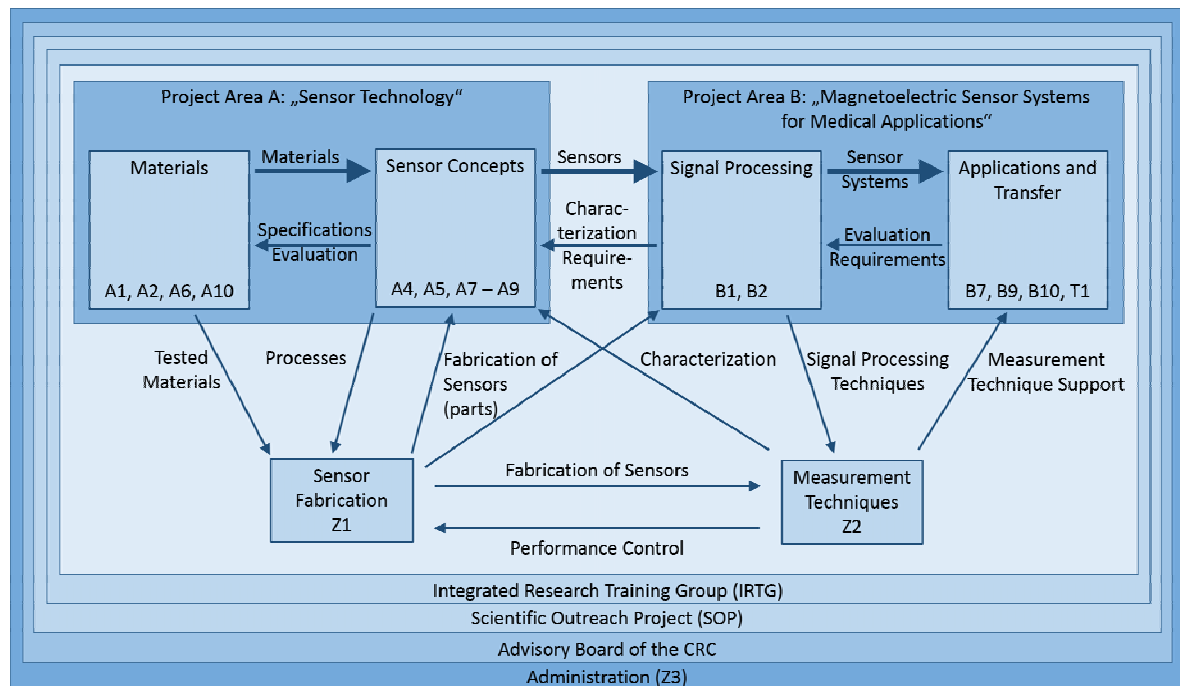


Figure 8: Structure of the CRC 1261 for the second funding period, also showing the main collaborations within the CRC. Besides the new projects, the installation of an Advisory Board is the main addition to the successful structure of the first funding period.

The projects **A3**, **B5**, and **B6** will not be continued in the second funding period. The reasons are as follows: (i) **A3** concentrated on resonant cantilever-type sensors. As the sensor performance at the mechanical resonance was found to be limited by thermal-mechanical noise, the expected gain with an increase in quality factor (Q) was reduced from proportional to Q to $Q^{1/2}$. Combined with the requirement of broadband sensors it was decided to transfer this work to the projects **A4** and **Z1**. Furthermore, the work on the new surface acoustic wave (SAW) sensors which was started in **A3** will be continued by **A9**. (ii) The work related to deep brain stimulation (**B5**) will be continued as a transfer project. (iii) In **B6** experiments have revealed that the magnetic field amplitudes are much smaller than initially expected. In combination with the very promising medical data obtained by alternative electrical measurements, it was decided to apply for a DFG project outside the CRC.

Three of the PIs of the first funding period – Bernhard Wagner (**A3**), Reinhard Knöchel (**B1**), and Ulrich Stephani (**B3**) – retired or will retire soon. Thus they will not continue as PIs in the CRC but agreed to be members of an **Advisory Board** which will be invited to the semi-annual retreats of the CRC. In this way, the CRC is expected to benefit from their broad knowledge and experience in MEMS, analogous electronics and epilepsy, respectively, in the second funding period.

1.2.2.4 Project area A

Project area **A** "Sensor Technology" focuses on research on sensor concepts based on ME composites and has evolved very dynamically during the first funding period. This is particularly reflected in the development of four novel sensor concepts: ME surface acoustic wave (SAW) sensors [Ki18a], electrically modulated ME sensors with pick-up coil [Vi18, Ha19], microwave sensors [Sa18a], and sensors with generator/transducer principle [Mi18]. The novelty of these approaches has also been demonstrated by the granted patents for three of these concepts [Ki16, Ha16, Sa18b]. Although main emphasis was put on investigation and understanding of these new concepts, very promising LOD values down to 30 pT/Hz^{1/2} at 10 Hz and 40 pT/Hz^{1/2} at DC were already achieved for the electrically modulated ME sensors, despite their quite early stage of development. It should be particularly pointed out that these sensor concepts promise the combination of a good LOD at biomagnetically relevant frequencies in combination with an appropriate bandwidth. Hence, much progress in the LOD and attractive applications in project area **B** are expected upon further investigations in the second funding period.

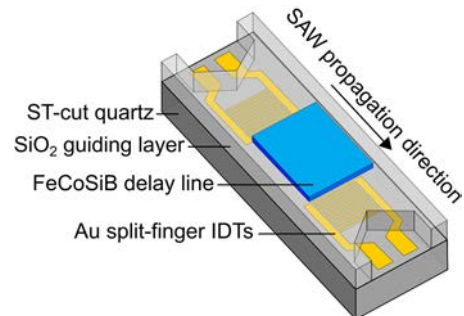


Figure 9: Sketch of a Love wave surface acoustic wave sensor based on a quartz substrate and a 4.5 μm thick SiO_2 guiding layer. The 200 nm thick magnetostrictive material FeCoSiB is deposited between the transducers on top of the delay line. The interdigital transducers have a periodicity p of 28 μm . Details are given in [Ki18a] as well as in **A9**.

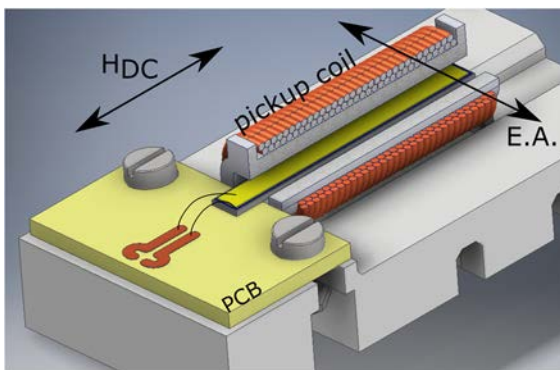


Figure 10: (a) Schematic of the novel electrically modulated ME sensor. The external magnetic field is applied along the long axis of the assembly (H_{DC}), orthogonally to the induced magnetic easy axis (E.A.). Details are given in [Ha18a] as well as in **A7**.

A sketch of a ME SAW sensor is shown in Fig. 9. This sensor was developed jointly in a cooperation of **A3**, **A4**, **A8**, **B1**, and **B2** and explores the ΔE effect, i.e. the change in the elastic modulus of a magnetostrictive layer in a magnetic field. In contrast to conventional ΔE -effect sensors, the change in shear modulus, which exhibits a higher magnetoelastic sensitivity, is used to change the wave velocity and thus the phase of a guided surface acoustic shear wave (so-called Love wave). The current version of the sensor already shows a LOD of 70 pT/Hz^{1/2} at 10 Hz and huge bandwidth (with the current readout electronics 50 kHz) and 120 dB dynamic range. The patented [Ki16] approach will be the focus of the new project **A9**.

The novel electrically modulated ME sensor with pick-up coil is shown in Fig. 10. It takes advantage of the dramatic enhancement of the converse ME effect for special high frequency mechanical resonances, so-called U modes that were discovered in **A7** [Ha19]. In the converse ME effect the piezoelectric layer is periodically strained, this

strain results in a stress in the magnetostrictive layer and thus in a change in the magnetization. Any external low frequency magnetic field – the field to be detected – then modulates this magnetization change. For readout, an inductor, matching the inductive self-resonance to the mechanical resonance, provides intrinsic amplification towards the converse ME effect, which thus forms an overall resonant circuit. So far, LODs as low as 30 pT/Hz^{1/2} at 10 Hz and 40 pT/Hz^{1/2} at DC were achieved.

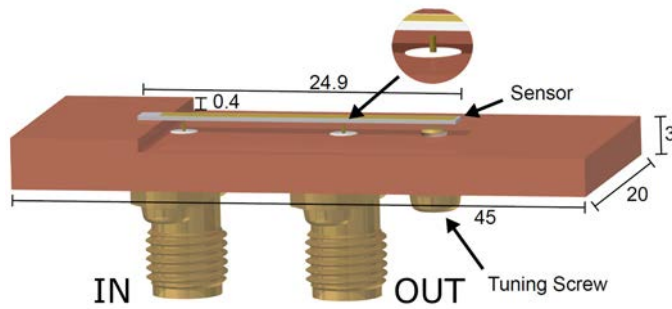


Figure 11: The cantilever acts as a transmission line microwave resonator with resonance frequency given by its geometric dimensions forming a quarter-wavelength resonator in longitudinal direction, accessed by input and output coupling with electric probes in the microwave stray field. Together with the ground plane the end tip of the cantilever forms a distributed capacitance which can be adjusted by a tuning screw. A magnetically induced bending of the cantilever changes this capacitance by ΔC , which thus results in a microwave resonator exhibiting a magnetic field dependent resonance frequency (see **B1** for further details).

In order to circumvent problems with the piezoelectric readout, a novel sensor concept has been investigated by **B1** and **A7** and patented [Sa18b]. Its basic structure is depicted in Fig. 11. In this structure, the cantilever is utilized as a magneto-mechanical transducer which behaves like a traditional ME cantilever, except for the missing piezoelectric layer. In this concept, the cantilever acts as a transmission line microwave resonator with a resonance frequency given by its geometric dimensions, typically in the gigahertz range. In one possible realization, the cantilever is unilaterally clamped close above a ground plane, forming a quarter-wavelength resonator. Together with the ground plane, the end tip of the cantilever can be regarded as a distributed capacitance $C_{\mu w}$, which can be adjusted by a tuning screw. A magnetically induced bending of the cantilever changes this capacitance by ΔC , which thus results in a microwave resonator with a magnetic field dependent resonance frequency. These frequency changes lead to both amplitude and phase modulation of the sensor's

electric output signal, which can be evaluated by classical readout systems. Initial measurements at the resonance frequency of the cantilever have shown limits of detection that are only restricted by thermal-mechanical noise [Du17] after noise from the microwave excitation and readout circuit had been suppressed by appropriate circuitry. For the low-frequency range, improved limits of detection in comparison to piezoelectric cantilevers are expected, because noise of the piezoelectric layer is eliminated. Moreover, the sensor can detect the magnetic field directly and thus, in principle, is capable of detecting static fields, in contrast to piezoelectric readout which is only sensitive for the time derivative of the magnetic field.

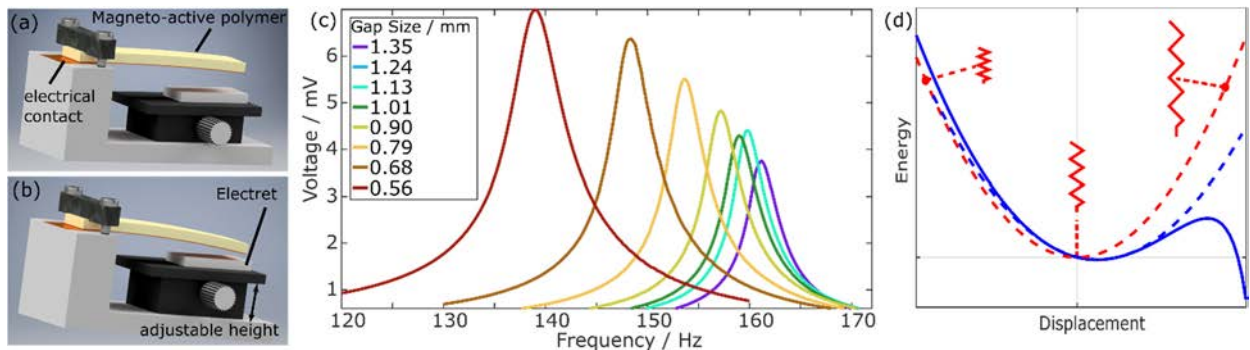


Figure 12: Electret mounted with a (a) large gap to the cantilever and (b) small gap. (c) Measured frequency response and sketch of the electret-based sensor for different gap sizes (in mm) between the cantilever and the electret (in blue). (d) Modeled potential energy over the displacement. The red dotted curve indicates the harmonic oscillator potential, the corresponding cantilever bar is then not further bent by the electret induced potential. If an electret layer is added, the cantilever is bent by the polarization and the equilibrium position is shifted. The blue dotted curve represents an approximation for small amplitude oscillations with the electret and illustrates the softening of the potential. The blue solid line shows the complete potential curve resulting from the oscillator potential in combination with the electret potential. It gets even softer the closer the beam gets to the electret (see [Mi18] and **A2** for further details).

Fig. 12 displays a scheme for a newly developed sensor which explores the electret generator/transducer principle. Here also the piezoelectric layer of the ME stack is eliminated and the readout occurs by means of an electret that contains permanent charges that induce polarization charges in the metallic electrode of the

bending beam. The resulting attractive force reduces the restoring force upon bending and leads to a strong effective softening of the vibrating beam. This effect is used in **A2** as an alternative approach to using intrinsically soft materials [Mi18]. The further development of such soft energy-efficient ME sensors operating in the direct mode will be continued in parallel with studies on sensors based on an electret generator/transducer principle. Encouraging new ideas to be investigated include substrate-free hybrid cantilevers with extremely low bending stiffness but very high stiffness in tension and compression, the use of highly porous electrets, and exploitation of the design freedom of 3D printing.

In addition to the abovementioned novel sensor concepts, the established concepts of ΔE -effect sensors [Za16] and of direct measurements with energy-efficient ME sensors [Ya16] will be continued in the second funding period. Based on comprehensive theoretical considerations and modelling as well as experimental investigation, the ΔE -effect sensor has now reached a level of understanding to explore its full integration together with the electronics for operation and readout (A4).

The investigations of the first funding period have clearly shown that the limit of detection of the different sensors is generally limited by the properties of the magnetostrictive layer and that further efforts on tailoring the magnetostrictive layer provide much space for increasing the LOD. Consequently, while continuing our successful studies on ME multilayers and domain tailoring in **A1**, we will increase our efforts on understanding the influence of imperfections on magnetic noise by the new **A10**, which encompasses both modelling and experiments. This project also involves advanced characterization methods combining local and global analysis. The characterization and modelling approaches will also be applied to the non-magnetic components of the sensors investigated in **A6** and **A8**, respectively.

The connection of the projects of project area **A** with the different sensor approaches is illustrated in Fig. 13.

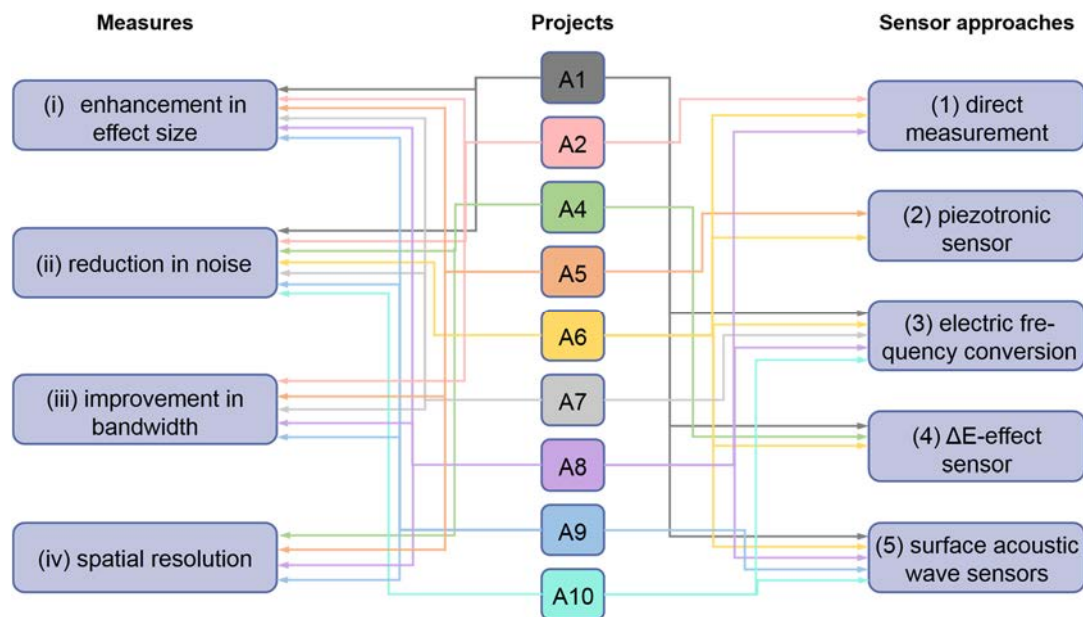


Figure 13: Main connections of Projects A1 to A10 with the sensor approaches pursued in the second funding period.

A1 studies magnetostrictive multilayers for ME sensors with emphasis on the magnetic domain processes. During the current funding period, this project turned out to be particularly important in view of the aforementioned results which have shown that magnetic noise contributions are generally the limiting factor for the achievable LOD. In close cooperation with **A10**, it will be investigated how magnetic domain induced noise contributions can be eliminated by the design of advanced magnetic multilayers. These will be prepared in a new sputter deposition cluster tool with nine sputter sources, which has already been put into operation. By magnetic field deposition, layering, and annealing procedures, magnetic anisotropies and exchange coupling will be adjusted in strength and orientation to achieve magnetic single domain behavior. Magnetic and magnetic domain investigations will be correlated to structural properties (**A6**). Thus, the foundations for ME composites with significantly improved sensing behavior for the different sensor concepts (**A4**, **A7**, **A9**) employed within the CRC will be established.

The aim of **A2** is the development of energy efficient magnetic field sensors that convert the magnetic field into an electric signal with minimum losses. The key for the realization of such a device is the reduction of passive materials and components like substrates and electrodes and the avoidance of energy transitions, particularly into the binding potential. In the second funding period, it is planned to extend the electret generator/transducer principle described above (Fig. 12). Inter alia, we intend to maximize the total chargeable electret surface by using highly porous materials as templates. Deposition by initiated chemical vapor deposition (iCVD) in conjunction with corona discharge already turned out to enable ultra-stable fluoropolymer electret thin films with tailored properties on complex porous substrates. The further development of the mechanically soft sensors operating in the direct mode will involve a number of new concepts, on substrate-free hybrid cantilevers with extremely low bending stiffness and very high stiffness in tension and compression. In addition, the design freedom of 3D printing of complex resonator geometries that are built up of mechanically soft composites, e.g. silicone filled with magnetic micro and nanoparticles, will be used.

The ΔE -effect magnetic field sensor in **A4** utilizes the frequency shift of a high frequency electromechanical resonator due to the change in the Young's modulus of a magnetostrictive component in a magnetic field. The sensor avoids the $1/f$ noise, allows broadband magnetic field measurements at low frequencies down to the DC range, and proves robust to vibrations. In particular, our current sensor concept does not require a magnetic AC modulation field and thus provides full device integrability. We now plan to develop fully integrated ΔE -effect sensors and sensor arrays including sensor electronics as a single unit. Initially, the development of the MEMS device and the electronics will occur on separate chips. The MEMS design can resort to entirely anisotropic magnetoelastic and electromechanical ΔE -effect models developed in the current funding period. The realization of the micromechanical design as a MEMS device using a piezoelectric AlN layer as well as the sensor electronics based on CMOS technologies is intended via Europractice, which provides prototyping and low volume production. The magnetic layer, which can also be a complex multilayer structure, will be deposited as a final step in Kiel. We also plan to explore sensor arrays with a large number of integrated sensors for increased resolution, noise reduction, and improved limit of detection. This will involve the development of proper grouping strategies as well as readout and excitation schemes.

A5 focuses on piezotronic readout for magnetoelectric sensors which provides a pre-amplification directly in the piezomaterial. ZnO and GaN needle-shaped sensors allow a very compact design, and therefore an envisioned biomedical application is a catheter-mounted sensor, for example, for intracardiac magnetic field detection as an alternative to the currently used tunnel magneto resistance (TMR) and giant magneto resistance (GMR) sensors. For comparison, more conventional miniaturized AlN piezotronic sensors will be explored as well. Consequently, in the second funding period it is proposed to examine and understand miniaturized piezotronic devices; in the third funding period, the biomaterial applications with the most successful piezotronic sensors are envisioned. The high resonance frequencies of the small needles require driving the sensors in ΔE mode. The intracardiac applications have different requirements compared to the external placement of magnetic field sensors: They have to be small and robust, the LOD is not as challenging due to the close proximity, but the signals have to be transferred a long distance via the catheter. Thus the piezotronic sensor concept seems to be very attractive, as the sensors have very small sizes, good sensor performance, and an intrinsic pre-amplification.

A6 focuses on the synergy of a combined methodical approach of transmission electron microscopy (TEM) and high resolution synchrotron-based X-ray scattering techniques on the sensors and their components. The applied methods and the synergetic strategy behind them yield complementary information on the local and global structure and structural defects, which are indispensable for further progress, especially in case of the complex multilayer magnetic materials (**A1**). A novel methodological combination for amorphous magnetostrictive (multi)layers linking synchrotron-based pair distribution analyses with complementary electron diffraction and X-ray spectroscopy techniques will be used to interrelate atomic and magnetic structure and composition. The results are particularly crucial for **A10**, which aims at a model-based structure-property description of the sensors. In addition, the effect of heat treatment on short-range ordering and magnetic properties will be addressed. The planned investigations also include crystalline piezomaterials (**A5**). Moreover, we intend to perform highly challenging *in situ* electron microscopy and *in operando* X-ray scattering measurements such as X-ray ptychography and advanced TEM imaging. These experiments require the development of novel devices for *in situ* straining and *in operando* measurements in a magnetic field (nano-XRD).

A7 will investigate electrically modulated ME sensors. In the second funding period, emphasis will be put on the novel electrically modulated ME sensor with pick-up coils, as discussed above (Fig. 10). This strategy exploits high frequency mechanical resonances. Here, the converse ME effect is further enhanced by matching the readout inductor self-resonance to the mechanical resonance. We expect to greatly improve by various

measures the currently achieved already very low LOD of $30 \text{ pT/Hz}^{1/2}$ at 10 Hz of the early prototype. These measures include: (1) a reduction of the magnetic noise by new magnetic materials developed in **A1** and **A10**, (2) a modified clamping and resonator design for achieving a spatially homogenous resonance mode, and (3) an increase of the resonance frequency of the employed U-mode resonance.

The aim of **A8** is a theoretical investigation of the behavior of ME sensors and sensor arrays based on piezoelectric and magnetostrictive composite materials in inhomogeneous biomagnetic fields. Emphasis will be laid on modelling of the SAW sensors of **A9** (Fig. 9) and of the electrically modulated cantilever sensors (**A7**). The simulation will be implemented by employing the finite element method (FEM). Noise modelling will be performed in cooperation with **B1**. A point of special interest will be the modelling of ME sensors and sensor arrays in inhomogeneous magnetic fields, which is a highly important aspect for biomagnetic applications. Moreover, the DBS system (**T1**) will be investigated with a multiscale approach including sensors in a sensor array and ME properties of the head.

In the new project **A9**, the aforementioned (Fig. 9) SAW sensors using the ΔE effect will be investigated for very sensitive, broadband magnetic field sensing. In these sensors, shear horizontal acoustic surface waves (Love waves) are guided by a fused silica layer with an amorphous magnetostrictive FeCoSiB thin film on top. A magnetic field changes the velocity of these waves due to magnetoelastic-induced changes of the shear modulus, which gives rise to a phase shift in the delay line (Fig. 9). Although the development of this sensor is still in an early stage, a remarkable LOD of $70 \text{ pT/Hz}^{1/2}$ at 10 Hz combined with a bandwidth of 50 kHz and a dynamic range of 120 dB has already been achieved. In the second funding period, we will investigate how the sensor performance is affected by the operational frequency, the use of ferroelectric crystals instead of quartz, the employment of exchanged biased magnetostrictive layers, the design of the interdigital transducers, and the use of polymeric guiding layers. Moreover, a polycrystalline AlScN thin film on a silicon substrate will be studied as a possible replacement for the piezoelectric bulk crystal because of its superior electro-acoustic coupling coefficients.

The aim of **A10** is to comprehend and quantify the exact influence of geometrical and physical imperfections on the magnetic noise of ME sensors, which is currently the limiting factor for the LOD. The project combines experimental and theoretical efforts in close cooperation with **A1**. Effects that are relevant for the magnetic properties include local geometrical errors, non-uniform magnetic material properties, local eigenstresses, and magnetic domains, and domain walls. Experimental techniques involve time-resolved *in situ* magneto-optical magnetic domain response analysis and local noise measurements. Highly resolved and adaptive micromagnetomechanical simulation and modelling techniques include adaptive discretization approaches and scale transition methods. With the starting point of noise investigations on well-defined model structures exhibiting artificial imperfections and tailored micromagnetic features, different sensor types will be addressed in cooperation with **A2**, **A4**, **A7** and **A9**. The results will permit fundamental understanding of the role of different scales in time and space, are expected to be crucial for the reduction of the magnetic noise and thus will lead to a major improvement in the LODs of the different sensors. The improvement will significantly extend the range of possible applications of the sensors being developed in project area **A**, which is a prerequisite for the success of the design of related sensor systems for biomedical applications in project area **B**.

1.2.2.5 Project area B

Project area **B** “Magnetoelectric Sensor Systems for Medical Applications” focused in the first funding period of the CRC on research on analogue and digital signal processing of the sensor concepts from project area **A** and on different biomedical applications that were considered to be in the range of the sensors’ performance. The research projects belonging to project area **B** were grouped (in the first CRC period) into three (sub-) areas:

- **B1** and **B2** performed research on converting the low-voltage or low-charge sensor output signals to enhanced digital signals. This included dedicated sensor, device, and circuit modelling (mainly for understanding the individual contributions to the noise statistics [Du17]) and sophisticated readout schemes (e.g. multi-carrier readout [Re16a]), as well as digital post processing, such as adaptive noise cancellation [Re16b].
- **B3** worked on inverse solutions for localization of biomagnetic activities for cardiologic and neurologic applications. Here, an entire processing chain that uses (patient-individual) *a priori* knowledge in terms of electric and magnetic parameter distributions obtained, e.g. from MRI, to compute so-called forward solutions was established. These forward solutions were combined with state-space-based brain and heart models to compute robust and precise inverse solutions that permit estimating current densities of brain [Ha17] and heart tissue [Ha18b].

- **B5**, **B6**, and **B7** investigated dedicated biomedical applications in the fields of neurologic applications (analyses of DBS (**B5**), nerve conduction (**B6**)), and cell analyses (imaging of magnetically labelled cells (**B7**)). In these biomedical application projects, the enhanced signals obtained from **B1** and **B2** as well as the models obtained from **B3** were utilized and several new research results could be obtained and published [e.g. Ya19, El19, Fr19].

Based on theoretical noise analyses that were confirmed by a multitude of measurements, low-noise amplification circuits were developed in **B1**. Dedicated printed circuit boards were designed for several sensor principles. The ones depicted in Fig. 14, for example, were used for the ME cantilever sensors of size 1 mm by 3 mm. Those sensors were used, on the one hand, in various experiments of the medical applications projects and to investigate the performance of multi-carrier readout in ΔE mode in **B2** [Re16a]. On the other hand, new applications such as movement (**B9**) or cardiologic analyses (**B10**) [Re18] used the boards for preliminary research that lead to corresponding proposals for the second funding period.

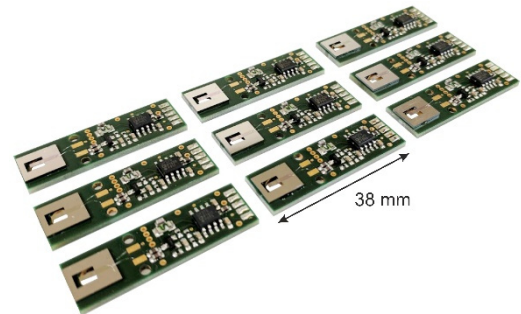


Figure 14: Cantilever-type ME sensors and corresponding low-noise amplifiers mounted on dedicated, printed circuit boards (PCBs) for biomedical experiments.

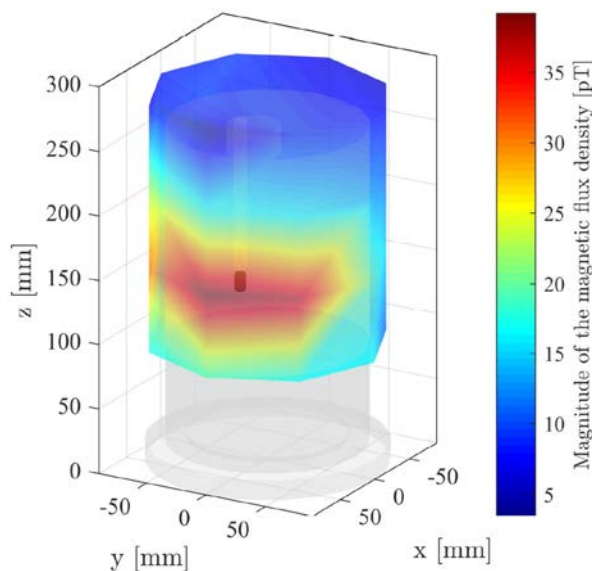


Figure 15: Measured magnetic field distribution for a bipolar electrode configuration (near-surface position) within a cylindrical phantom head. The phantom was filled with saline solution. The bipolar mode generates a more focused spatial distribution (compared to the monopolar mode) that can be used for electrode localization.

indicate a precision of the electrode localization scheme in the mm range [Ya19] (Fig. 15).

In the first

funding period **B3** success-fully investigated forward modelling and inverse solutions for MEG, MCG, as well as 2D cell analysis (**B7**). In the second funding period, this research work will be utilized and specifically extended in **B7** for 3D cell detection, in **B10** for the cardiologic applications and in **T1** for enhanced DBS electrode localization and estimation of the volume of tissue activated (VTA). Consequently, **B3** will not be continued in the second funding period.

The central objective of **B5** within the first funding period was to develop a method to measure with ME sensors the stimulated electrical field of a DBS electrode that is implanted into the brain of patients with Parkinson's disease. DBS involves implanting electrodes into certain, specific areas deep in the brain that are attached to an implantable pacemaker that is placed under the skin near the clavicle. This project represents an application which is of high clinical relevance and the magnetic fields generated by the DBS electrodes are stronger compared to the fields of human brain activity but still very challenging for achieving high spatial resolution. For the analysis in this biomedical application, different sensor types (single-sensor approaches) that are developed within the framework of the CRC were utilized. First results

Measurements in cooperation with the Physikalisch Technische Bundesanstalt (PTB) in Berlin showed that the magnetic nerve responses of the medianus nerve (electrically stimulated) have only amplitudes of about 20 fT. The response of the muscle that the nerve is connected to is about 1000 times larger (peak amplitudes of about 40 pT). Since the very small magnetic field amplitudes that originate directly from the nerve are currently not detectable with our ME sensors and the diagnostic advantages of the magnetic muscle measurements (in comparison to simpler electric ones) are not significant enough, we decided not to continue **B6** within this CRC. However, since the elaborated signal analyses (based on electric as well as magnetic signals) are very promising, we will continue the project outside the CRC, but only on the basis of electrical measurements.

In the first funding period, **B7** showed the feasibility of two approaches for the detection of magnetic nanoparticles using resonant ME sensors, which is called magnetic particle mapping (MPM), and ΔE -effect sensors, which is called magnetic susceptibility particle mapping (MSPM). The MPM system is shown in Fig. 16-a). MPM makes use of the nonlinear magnetization behavior of magnetic nanoparticles and measures the signal generated at the third harmonic. The MSPM system is shown in Fig. 16-b). MSPM measures the field generated by magnetic nanoparticles, aligned in an external magnetic field. Both methods use quasi 2D samples of magnetic nanoparticles and the resolution of the imaging techniques is in the range of the sensor to sample distance. Both approaches were used to detect magnetically labeled cells, which were also prepared within **B7**. The detection limit for MPM is about 300 ng at a sample to sensor distance of 1 mm and about 20 μ g at a distance of 8 mm for MSPM.

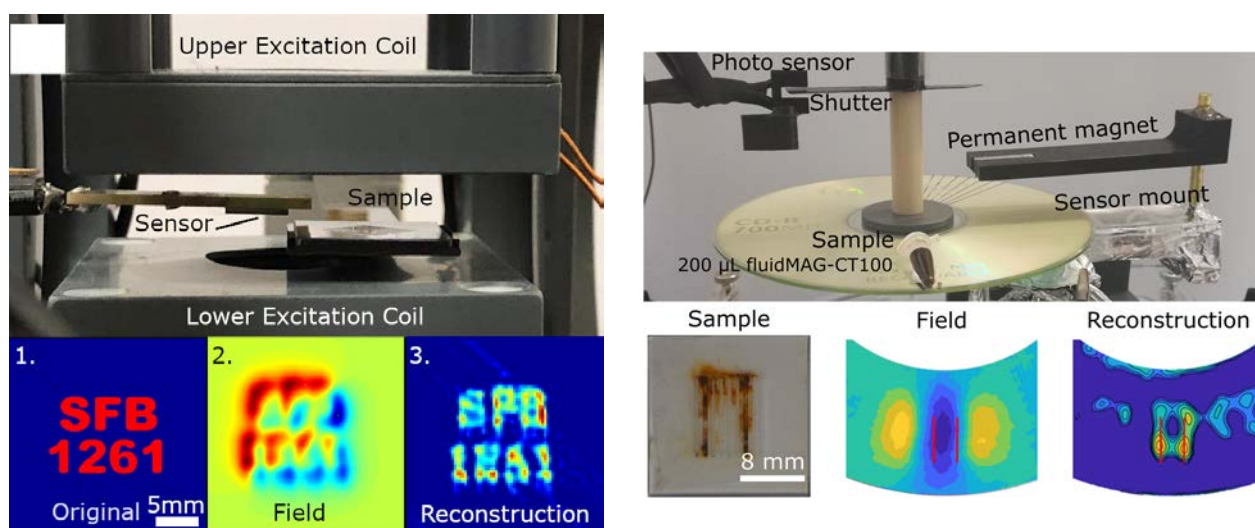


Figure 16: a) Magnetic particle mapping (MPM) setup for measuring the third harmonic generated by the nanoparticles due to their nonlinear magnetization behavior, subimages 1-3 show the initial distribution of magnetic nanoparticles, the measured magnetic field and the reconstructed distribution from the measured data, respectively. b) Magnetic susceptibility particle mapping (MSPM) setup for measuring the field generated by magnetic nanoparticles in a magnetic field. In the bottom line a sample for the determination of the spatial resolution, the field for the sample and the reconstructed particle distribution is shown.

In the second funding period, the projects in project area **B** as well as the transfer project **T1** will focus on two research aspects and corresponding objectives:

- research on system aspects and readout of entire ME multi-sensor systems (adaptive readout, cross-channel coupling reduction, combined analogue and digital signal enhancement), and
- research on applications of the ME multi-sensor systems for dedicated biomedical analyses.

These objectives are targeted by using several project connections within project area **B**, but also by considering various collaborations with the projects from project areas **A** and the service projects **Z**. The objective of creating entire multichannel sensor systems is addressed – as in the last funding period – mainly by **B1** and **B2**. The focus on multichannel systems should be strengthened in the second funding period, since all biomedical application projects will be able to enhance their analyses if a multitude of sensors are utilized in parallel. While **B1** focuses on the analogue part of the sensor system, **B2** addresses the digital part. Since best results can be obtained by combining analogue and digital approaches, both projects are strongly linked to each other. Multichannel ME sensor systems will be used in four different biomedical applications:

- the detection of magnetically labelled cells in **B7**,
- the analysis of human movement in **B9**,
- research on cardiologic applications (non-invasive mapping of arrhythmias) in **B10**, and
- the localization of electrodes of deep brain stimulation systems (position and orientation of the stimulation electrode) as well as the calculation of the volume of activated tissue, in **T1**.

B7 continues and extends its successful research, projects **B9** and **B10** are new projects, and the work of project **B5** is continued together with the company Boston Scientific as a transfer project **T1**.

As indicated in Figs. 17, projects in project area **B** are organized in two units (signal processing and biomedical applications), that have strong intra- as well as inter-unit connections. The sensor front-end system projects (**B1** and **B2**) create entire multichannel sensor systems with appropriate low-noise amplification hardware, readout principles that are specially tailored to the individual sensor concepts as well as multichannel signal enhancement by analogue, digital, and mixed analogue/digital means. To what extent analogue or digital approaches are used depends on the individual sensor concepts and on the frequency

range of operation. Whenever frequencies of 500 kHz and more are required, low-noise analogue mixing is applied. High-level modelling of the individual sensor principles is of great importance for **B1** and **B2**. In **B1** the noise models established in the first funding period will be extended and adapted to the new sensor concepts from project area **A**. In **B2** the system-theoretic models that were investigated in the first funding period will be extended to non-linear multichannel models, which will be the basis for research on multichannel signal enhancement schemes such as blind source separation and nonlinear equalization approaches. Besides pure data transmission via AD and DA converters, also additional information indicating, e.g., the state of control algorithms or the importance of individual sensors for the biomedical measurements is exchanged in real-time between the analogue and digital parts of the sensor frontend. This allows for optimal combination of analogue and digital approaches.

The biomedical applications addressed in **B7**, **B9**, **B10**, and **T1** have in common that they will compute first so-called forward solutions. Such solutions are obtained by solving quasi-static versions of the Maxwell equations. Each project computes appropriate inverse solutions that are based on the forward models.

B7 continues with detecting magnetic nanoparticles and cells by two setups: MPM and MSPM. In MPM, superparamagnetic nanoparticles are excited by a magnetic AC field and higher harmonics of the excitation frequency are generated due to their magnetic non-linearity that can be detected by ME sensors in resonance. MSPM employs, instead of AC fields, a motion-modulated DC field. This field is used to magnetize magnetic particles, but also to provide a bias field for a ΔE -effect sensor which records the resulting low frequency magnetic field. In the second funding period, **B7** will increase the sensitivity and resolution of both methods, e.g. by employing inhomogeneous magnetic fields and by using improved sensors from project area **A**.

B9 will use the direct readout in resonance of the ME sensors. To analyze movements of patients as well as of healthy controls a multitude of coils send out specially designed signals within the frequency range of maximum sensitivity of the ME sensors. These coils and ME sensors are positioned on clothes (jacket, trousers), which allows for a multitude of sender-receiver pairs (each ME sensor receives each coil signal). For each pair the distance as well as the corresponding orientation will be estimated, which thus permits for robust analyses of human movement. The magnetic analyses obtained will be compared and combined with conventional schemes based on IMU sensors (inertial measurement units, consisting of acceleration, and gyro sensors).

B10 will investigate combined ECG and MCG for non-invasive localization of malfunctioning heart tissue areas (scars) that are causing cardiac arrhythmias. Here, the forward models and the state-space-based inverse solutions that have been investigated in the first funding period within **B3** will be used and further extended. The main objective of **B10** is to answer the question whether invasive mapping of arrhythmic substrates (current standard) can be replaced by a completely non-invasive alternative, based on a ME sensor MCG. The transfer project **T1** is the continuation of **B5** and deals with individualized DBS for effective treatment of movement disorders including Parkinson's disease and essential tremor. A cooperation with the company

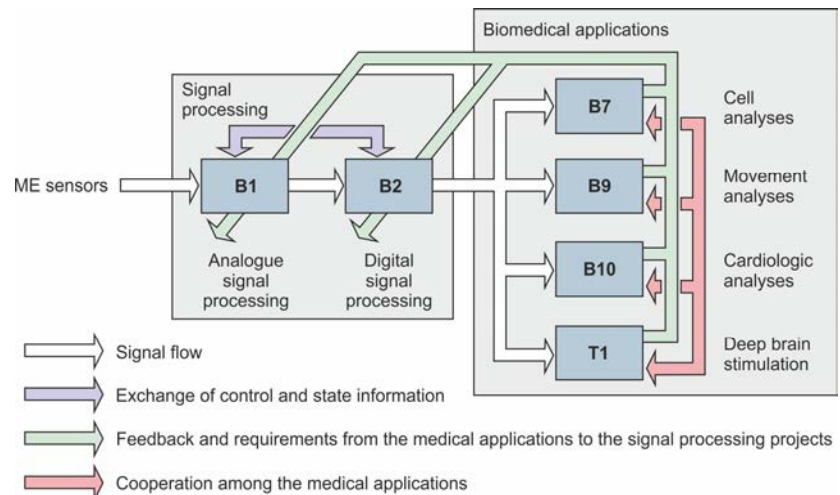


Figure 17: Project area **B** is grouped into two blocks: signal processing (for enhancing the magnetic signals by analog and digital means), biomedical applications (that use the enhanced signal for cell, movement, cardiologic, and DBS analyses).

Boston Scientific has been established, which is a producer of DBS equipment as well as surgical planning and programming software (GUIDE™ XT). The focus of the research will be in the localization of the position of the electrodes of DBS and the detection of the volume of activated tissue. For novel types of DBS electrodes, segmented contacts allow accurate treatment. Therefore, it is of highest interest to determine the proper orientation of the electrode in the brain with magnetic field measurements to avoid CT-measurements for patient safety reasons (radiation). In this transfer project the medical and industrial requirements will be considered and that the evaluation will be performed with state-of-the-art stimulators and industrial routines. Thus, the close collaboration and support by Boston Scientific will help to design a system for the calculation of the tissue activated by deep brain stimulation and to test its accuracy in various clinical studies where side effects can be clinically measured to validate this model.

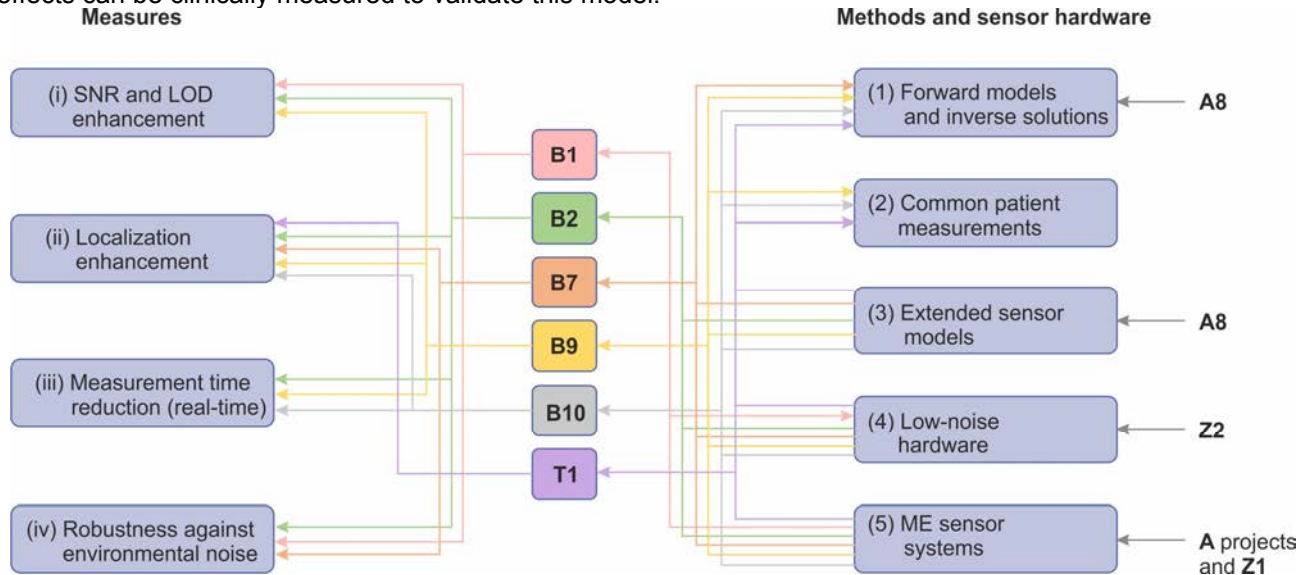


Figure 18: Cooperation within project area B (including T1) as well as with project area A and with the central projects.

All projects are strongly connected – both in terms of collaborations within this project area and by collaborations with project area A and the central projects. All sensors required for biomedical applications will be provided either directly from the project area A or from Z1. The same is true for low-noise analogue preprocessing which will be provided by B1 and Z2 (including measurement support). Furthermore, a close cooperation is planned for the research on forward models and inverse solutions (A8, B2, B7, B9, B10, T1). As soon as the extended sensor models in A8 are finished, they will be used in all projects that require forward models (B2, B7, B9, B10, T1). The real-time framework of B2 will be extended and used by B9 and B10. The sensor localization (based on fixed coils that are excited with specific signals) from B2 will be used in B10 and T1. Fig. 18 shows the most relevant collaborations of project area B. All others are described in the individual project descriptions.

1.2.2.6 Service projects

Scientific and technical support for the research projects will be provided by two service projects: Z1 “MEMS magnetoelectric sensor fabrication” and Z2 “Magnetoelectric sensor characterization”. These service projects enable the support in the MEMS fabrication of the ME sensors and the basic characterization of the ME sensors for the projects in project area A and the fabrication of sensor (array and vector-field measurement) systems for the projects in project area B. This also includes support for biomagnetic measurements in B. Furthermore, the connection to the research projects (Fig. 8) guarantees that up-to-date technology and knowledge is included in the portfolio of the service projects and is thus made available to all research projects. Additionally, the standardized fabrication and characterization techniques established in Z1 prevent redundancy in the research projects and permit a constant monitoring and comparison of the achieved LOD for the different sensor approaches.

The global objective of Z1 is to establish and maintain a common MEMS-based technology platform for the fabrication of a sufficiently large number of ME sensors based on the newest findings. This is achieved by combining the methods and techniques available at the Competence Center Nanosystem Technology (<http://www.kompetenzzentrum-nanosystemtechnik.uni-kiel.de/de/>) in Kiel and those at the Fraunhofer Institute for Silicon Technology (<https://www.isit.fraunhofer.de/>). Accordingly, this project assures a continuous delivery

of ME sensors from project area **A** on ME sensor research to project area **B** where ME sensors are evaluated for advanced biomedical applications. The service offered by **Z1** does not only include the fabrication of fully processed ME sensors but also the execution of separate process modules to relieve resources in project area **A** that are needed for pioneering new sensor concepts. New technologies investigated in project area **A** are gradually integrated into the technology platform **Z1**. This includes technological consultations and the operation of separate process modules that partly contribute to sensor fabrication. This finally results in a full fabrication flow executed and iteratively improved by **Z1**.

The first task of **Z2** in the second funding period is the functional characterization of ME sensors that are investigated in project area **A** and fabricated in **Z1**. It includes measurements on the spectral distribution of noise, the LOD, the bandwidth of operation, the robustness to acoustic noise and distortions produced by neighboring sensors as well as their directional characteristics. In order to evaluate the noise cancellation/suppression approaches of **B1** and **B2**, the characterization will be performed in magnetically shielded environments as well as in unshielded environments. As for the already established sensor types, the measurement procedures will be automated for new sensor concepts in project areas **A** and **B**. The researchers in these projects will be supported when using these measurement procedures and their results will be collected and the performance of different sensor concepts will be compared. In addition, sensor arrays will be investigated and their limits will be analyzed in order to arrive at viable systems for biomedical diagnosis. A further task is the fabrication of sensor (array) systems using the ME sensors fabricated in **Z1**. This includes the setup of the analogue and digital signal electronics for the readout of the sensors. **Z2** will also prepare measurement setups and support medical personnel during the measurements on healthy subjects and patients.

1.2.2.7 Collaborations within the CRC

Close collaboration between different projects and different disciplines is a key success factor in the CRC 1261. Collaboration and interaction are promoted by regular semi-annual retreats, focus group meetings, invited lectures in the CRC, and the IRTG activities for early career researchers (see section 1.4.1 and project **IRTG**). Two- to three-day retreats with all participating researchers were conducted twice per year either at the Akademie Sankelmark or at the Nordseeakademie in Leck to foster interaction and uninterrupted participation. At the beginning of the first funding period, we arranged the presentations by projects and included general discussion sessions. After the first year, the collaboration between projects was already so intense that we rearranged the presentations by topic starting with the retreat in April 2017. For example, on the new established topic “Surface-acoustic-wave sensors”, contributions were presented by **A1**, **A3**, **A4**, **A6**, **A8**, **B1**, **B2**, and **Z1**. This ordering by topic made for less repetition in the talks and a better understandability of the connections and the importance for researchers further away from a particular topic. On a daily basis, much of the interaction between projects was driven by the close collaboration of the young researchers. To give the collaboration between the semi-annual retreats a formal framework, we established focus groups. These focus groups are action groups spanning projects and foster exchange between projects on particular aspects. Each focus group has regular meetings for presentations, discussions, and comparisons of achieved results. The participating projects are committed to send at least one representative to the focus group meetings and to address overarching aspects. Joining forces in the focus groups minimizes redundancy among the projects and allows for common research on overlapping topics.

We started with three focus groups dedicated to “Modelling”, “Sensor Concepts”, and “Biomagnetic Signal Analysis”. As the focus group “Sensor Concepts” turned out to be very large (including about 70% of the CRC projects) resulting in long (and partly unfocused) meetings, we restructured the focus groups in 2018 with now six focus groups covering the topics “Magnetic Layers”, “Array Measurements”, “Modelling”, “Nerve and Heart Applications”, “Piezotronic”, “SAW, ΔE , and Hybrid Sensors”, and “Comparison of Sensor Concepts”. This dynamic approach in establishing demand-driven focus groups proved successful. In September 2019 we carried out a second round of adjustments resulting in the focus group constellation shown in Fig. 19. It also depicts the involvement of the different projects in the six focus groups.

Magnetic Layers

The performance of magnetic layers is a key cross-project topic. Here, material-related issues, such as deposition conditions and post deposition treatment, domain engineering for reduction of magnetic losses, stress control, alternative magnetostrictive materials as well as exchange coupling for self-biased magnetostrictive materials are discussed. The integration of advanced magnetostrictive multilayers into the sensor specific fabrication is a second focal point of the group. The focus group is coordinated by Dirk Meyners (**A1**, **Z1**).

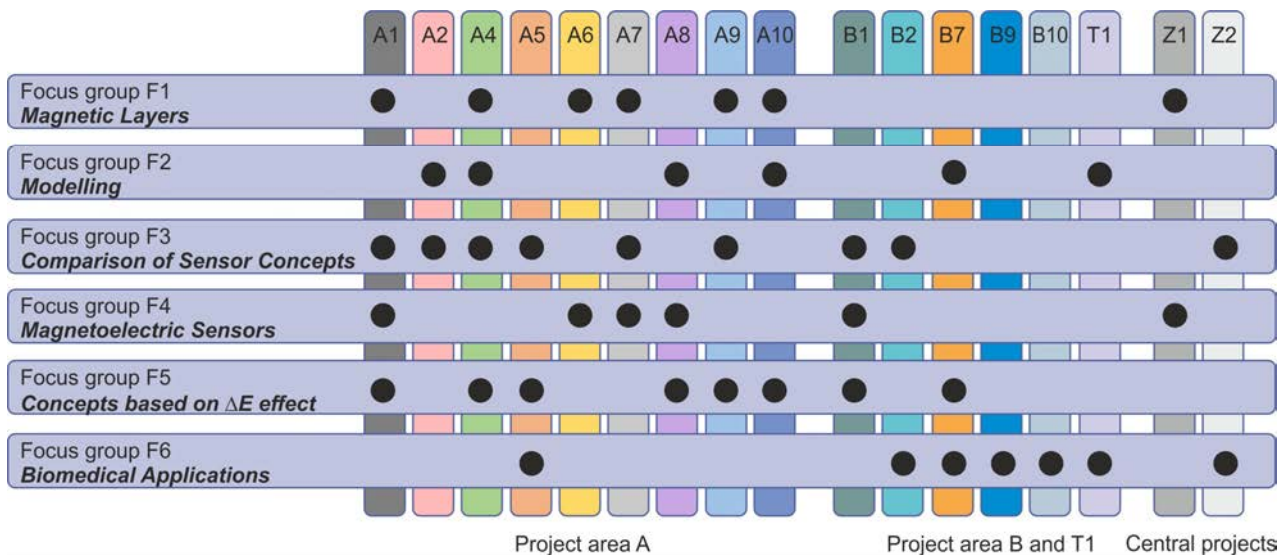


Figure 19: Participation of projects in focus groups.

Modelling

The focus group unites all activities on device and system modelling within the CRC 1261. All projects in the CRC include the modelling of particular aspects, e.g. material and domain modelling, modelling of non-linear effects, simulation of mechanical and electromagnetic characteristics, simulation of signal strengths and noise contributions as a function of frequency, and models for digital signal processing as well as for solving the inverse problem. A wide selection of simulation methods is employed within the CRC 1261, ranging from analytical equation-based and semi-analytical models to numerical techniques (in particular FEM) to iterative methods combining different software tools. Within the focus group, simulation approaches and algorithms will be compared, exchanged, and combined. The activities of this focus group are coordinated by Martina Gerken (A8).

Comparison of Sensor Concepts

This focus group is dedicated to establishing common definitions of sensor performance parameters such as sensitivity, frequency behavior, or LOD. Measurement procedures are defined to allow for comparability of performance results. The sensors developed in the CRC are compared to other types of magnetic field sensors. The focus group is coordinated by Michael Höft (B1, T1, Z2).

Magnetoelectric Sensors

This focus group bundles all activities on ME sensors based on piezoelectric and magnetostrictive composite materials. The investigation of all sensor concepts requires extensive characterization in terms of micro- and nanostructure, magnetic and piezoelectric properties and the resulting ME properties. The focus groups provide a platform for exchange on the different interlocking subjects relevant to the ME sensor research. This focus group is coordinated by Jeffrey McCord (A1, A10).

Concepts based on ΔE effect

In this focus group, all concepts based on a change of the elastic modulus by a magnetic field are considered. This includes ΔE -effect cantilever sensors as well as SAW sensors. This focus group is coordinated by Franz Faupel (A2, A4, B7).

Biomedical Applications

This group focuses on the use of magnetic field sensors in different applications. Joint topics include the mounting of sensors for measurements and multichannel measurements as well as signal processing and application related aspects. The activities of the focus group are coordinated by Gerhard Schmidt (B2, B9, B10, Z2).

A visible sign of the success of the collaboration between the projects is the high number of joint publications between different groups of the CRC. Within the first funding period 69 papers were published in the CRC 1261, thereof 50 were collaborations of several projects (29: two collaborating projects, 21: three or more collaborating projects)

1.2.3 Positioning of the Collaborative Research Centre within its general research area

1.2.3.1 Magnetic field sensors for biomagnetic applications

In the following, we provide a brief overview of existing magnetometer schemes for biomagnetic signal detection. We focus solely on the magnetometers that are currently the most relevant for biomagnetic applications. Therefore, magnetometers for which the required limits of detection (LODs) are out of range, which are too big in size, or cannot be easily assembled in sensor arrays are not considered here. Moreover, possible limitations for their application in MEG and MCG are discussed.

Since the beginning of the 1970s, biomagnetic recordings have mainly been performed with highly sensitive SQUID sensors [Ja65]. The first biomagnetic recordings of the heart and brain activity using SQUIDs were performed by D. Cohen [Co70]. The non-invasive recording, given spatial resolution, very good temporal resolution, and the lack of influence of all tissues beyond the heart or brain, led to the use of SQUID-based multichannel systems for MCG and MEG. The measurements are performed with simple magnetometers, axial or planar gradiometers, or a combination of magnetometers and gradiometers. The SQUID-based MCG and MEG have been used in the last three decades to study the healthy and pathological states of the heart [Lo04, Ko04, Fe05, Kw13] and brain [Lo04, Ha10a, Ha10b, Ha12, Da13].

Consequently, the benchmark for biomagnetic measurements is SQUID sensors. SQUID sensors provide a very low LOD in the range of a few fT/Hz^{1/2} for low frequency magnetic signals. SQUID sensors are routinely used for some of the biomagnetic applications mentioned above [Kö16]. Within Germany, systems with vectorially configured sensors have been installed at the Physikalische Technische Bundesanstalt (PTB) in Berlin and at the Biomagnetic Center Jena [Br09].

To maintain the superconducting elements of the device operating at liquid helium temperatures requires cryogenic cooling. Thus, the necessary apparatus makes the use of SQUID systems expensive and limits their applicability. Also, the cooling of the sensor in SQUID systems restricts the possibility of bringing the sensor close to the biomagnetic source. Due to this, the magnetic signal strength decreases strongly with increasing distance. Despite efforts to reduce the sensor-to-source separation, the advantage of a low LOD in relation to other sensor types is therefore partly reduced. Moreover, the increased source-to-sensor distance also aggravates the localization of the signal source. Related to that, the flexible adaption of SQUID sensor arrays to different patients is not an option; operation takes place in a fixed geometry. The use of high T_c superconductors for small-sized biomagnetometers eliminates some of the drawbacks of SQUID sensors [Fa17]. Some or all of these limitations have led to a limited operation of SQUID-based MCG or MEG devices, mostly in research settings in university hospitals.

A further drawback in relation to envisioned room temperature sensors is that *in vivo* inside-the-body measurements of biomagnetic signals are rather impossible. These points motivate the research into the development of other kinds of magnetic field sensors which could alleviate some of the limitations of SQUID devices and lead to a wider usage of MCG/MEG in clinics and research centers. In the following, several alternative concepts are discussed, starting with the ME composites that are the topic of the CRC.

As discussed in detail in the original proposal, ME composites consisting of magnetostrictive and piezoelectric materials are very attractive in comparison with single-phase ME materials because of their much higher ME coefficients and their much higher maximum operation temperatures. For earlier reviews, we refer to [Na08], [Ma11], [Wa14]. A recent review on ME composites as magnetic field sensors was given by Quandt, McCord and co-authors [Vi18]. Magnetic field sensors and other applications are covered in [Tu19], which also includes selected results of the CRC.

During the first funding period, published research on ME composites for magnetic field sensing focused on thin film devices. No significant progress was reported on bulk laminates, which can be considered as fully developed [Wa14]. For applications which require spatial resolution by sensor arrays and detection of low frequency signals (below 1 kHz) like MEG and MCG, bulk ME composites are not suitable due to their size, despite their fascinating properties. To realize magnetic field sensor arrays with the required resolution, the fabrication of small, identical, and low frequency resonant ME sensors can only be achieved by MEMS techniques. The different approaches for ME thin film composites focusing on applications as magnetic field sensors have been reviewed in the original proposal. Recent work includes antiparallel exchange biased multilayers [Ki19], frequency-tunable ME substrates [Rö18], and advanced characterization [Do18].

With regard to recently reported limits of detection, 100 pT/Hz^{1/2} were reported for multimode ΔE -effect sensors by Zabel et al. [Za16] in the range of 10 – 100 Hz. The group of Sun at Northeastern University investigated ΔE -effect sensors for DC magnetic field measurements and achieved a LOD of 800 pT/Hz^{1/2} [Li17]. Salzer et al. obtained 60 pT/Hz^{1/2} at 10 Hz by combining resonant ME sensors and magnetic frequency conversion [Sa18c]. Using the abovementioned Love wave surface acoustic wave concept, Kittmann et al. reported a LOD of about 100 pT/Hz^{1/2} at 10 Hz [Ki18a]. For the electrically modulated ME sensors, a concept using the converse effect and a so-called U-mode resonance at approximately 500 kHz, a LOD of 210 pT/Hz^{1/2} at DC and 70 pT/Hz^{1/2} at 10 Hz was reported [Ha19]. As discussed above in section 1.2.2.4 (see Fig. 5) much lower LODs as low as 30 pT/Hz^{1/2} at 10 Hz and 40 pT/Hz^{1/2} at DC were meanwhile achieved within **A7** (unpublished results) using antiparallel exchange bias multilayers from **A1** [Ki19].

The currently fast-growing field of research and development related to optically pumped magnetometers (OPMs) exemplifies the need of a non-cryogenic alternative to SQUID sensors. The operation of an OPM is based on the detection of the Larmor precession of alkali atoms in the vapor phase: for a brief review of the theory of OPMs, see e.g. [Ti19]. In this basic configuration, OPMs are scalar magnetometers in nature. However, detection limits competitive to that of SQUIDS have been demonstrated in advanced magnetically shielded environments [Da10]. The simplest OPM setup comprises a laser as light source, a commonly heated high-pressure vapor cell as magnetically responsive part, and a photodiode as detection unit. As a result and compared to thin film magnetic sensors, OPMs involve a rather complex sensor structure. Nonetheless, great effort have been undertaken to fabricate integrated sensor packages [Ki18b]. The first integrated sensors exhibited LODs in the range of 700 fT/Hz^{1/2} at 1 Hz [Sa12]. Further progress in the fabrication and operation of chip-scale OPMs lowered the achievable LOD to about 100 fT/Hz^{1/2} at 1 Hz [Al17]. As a drawback, such low detection limits of OPMs can only be reached when operated as zero magnetic field magnetometers [Du69]. In an unshielded environment, the required change of operational mode leads to a significant degradation of sensing performance by about one order of magnitude of the LOD [Al17].

In a shielded environment, commercially available optical magnetometers (QuSpin Inc., Louisville, Colorado) have been successfully applied to MEG [Bo18], MCG [Es17], [Ba18], and magnetic nanoparticle detection [Bo18b]. Interestingly, a comparison of fetal MCG measurements recorded by SQUIDS and microfabricated OPMs revealed a similar signal-to-noise level in the measurements, because the optical magnetometers could be brought much closer to the human body, i.e. to the sources of the magnetic field [Al15]. As a conclusion, all kinds of miniaturized sensors brought close to the biomagnetic field sources will benefit from the larger magnetic field strength.

Ongoing research addresses the application of OPMs in unshielded environments by more sophisticated optical pumping and gradiometric sensor arrangement [Be16], [Co16]. Concepts for optical vector magnetometers have also been demonstrated, e.g. optical modulation exploiting the Stark effect [Pa14], microwave fields as spatial references [Th18], and double resonances in modulated sensors [In18]. In general, these approaches come along with a higher complexity in sensor structure, optical pumping scheme, or readout, which makes sensor miniaturization and packaging more challenging. Also, the vapor cell of the OPMs need to be heated for operation. There are few attempts to simplify the OPM application such as the use of ⁴He instead of the often applied Rb or Cs vapors [Mo17]. ⁴He enables vapor cell operation at room temperature without heating. However, a HF discharge is necessary to excite the He atoms to metastable states as the ground state is insensitive to the Zeeman effect. Using centimeter-sized gas cells a detection limit of 210 fT/Hz^{1/2} at 10 Hz has been achieved.

Magnetoresistive (MR) sensors constitute another interesting class of magnetic field sensors (for a thorough review of the development of MR magnetic field sensors see [Zh19]). Despite the fact that state-of-the-art MR sensors do not reach detection limits low enough for the detection of biomagnetic signals from outside the human body without substantial averaging [Fu18], the possibility of MR-based MEG is predicted by an international consortium of renowned researchers working in that field [Zh19]. Tunneling magnetoresistive (TMR) magnetic field sensors suffer from 1/f noise of magnetic and non-magnetic origin limiting the achievable LOD to the lower nT/Hz^{1/2} regime at low frequencies [Eg09, Go06]. A substantial improvement has been demonstrated by using an array of numerous TMR junctions [Fr16]. Combining such an array of 640 TMR junctions with magnetic flux concentrators optimized by modelling, a detection limit LOD = 60 pT/Hz^{1/2} has been demonstrated at 1 Hz [De17]. This concept of sensor arrays combined with flux concentration will be transferred to miniaturized ME sensors in **A4**.

A path to circumvent the restrictions arising from the abovementioned LOD limitations is to bring the MR sensors as close as possible to the natural magnetic sources, i.e. into the body of the subject to be investigated.

This has been proven to be a feasible solution and demonstrated for giant magnetoresistive (GMR) sensors in the pioneering work of the group of Panntier-Lecoeur [Ba16]. With GMR microprobes the magnetic field from action potentials could be locally recorded *in vitro* on a mouse muscle. Furthermore, shaping the GMR microprobes into needles enabled intra-cortical magnetic recordings of neuronal activity in the visual cortex of a cat [Ca17]. Within the CRC, the ZnO-based ME sensors are the predestined candidates to adopt this approach to biomagnetic recording because of the miniature size, needle-like shape, and integrated piezoelectric readout (A5).

An alternative approach with a LOD in the $\text{pT/Hz}^{1/2}$ range at room temperature are giant magnetoimpedance (GMI)-based magnetometers. In the most promising configuration, an amorphous ferromagnetic and glass-coated wire is used as the core inside an inductive coil. The GMI effect is based on a large change in the complex impedance of a soft ferromagnetic conductor excited by an alternating or pulsed current when subjected to an external magnetic field [Mo15]. Magnetic sensors based on the pulse magnetoimpedance effect have been used for the measurement of biomagnetic signals. The equivalent magnetic noise level of GMI magnetometer presents a $1/f$ behavior at low frequencies. In recent developments, with an optimized GMI sensor system employing a time-differential measurement scheme, a noise level as low as $2 \text{ pT/Hz}^{1/2}$ at low frequencies was achieved [Ma19]. Measurements of heart and brain signals were demonstrated by using a gradiometric sensor configuration [Wa17, Uc17], by which magnetic background noise is eliminated. GMI sensors are operated at room temperature and can be brought very close to the human body by which the magnetic field detected at a GMI sensor is about 20 times higher than for a SQUID sensor setup [Wa15]. Despite the recent progress, averaging of data is needed for the extraction of the weak biomagnetic signals.

Another alternative approach is based on the use of fluxgate magnetometers. The fluxgate magnetometer allows for the extraction of the direction and magnitude of the magnetic field. The principle of a fluxgate is based on a soft magnetic core that is periodically driven into saturation. A detection coil around the magnetic core measures the induction voltage and detects the signal at double the frequency. Similar to GMI sensors, the magnetic active element consists of a high susceptibility amorphous ribbon. The measurement of magnetocardiograms using orthogonal fluxgate arrays was demonstrated [Ka15], [Ha15]. A LOD of below $5 \text{ pT/Hz}^{1/2}$ has been achieved for low frequency [Sa18d] measurement fields. Pros and cons in relation to SQUID sensors are very similar to GMI sensors.

GMI and fluxgate sensors are the most analogous devices to ME sensors. They incorporate many of the advantages that will be realized in a similar way for ME sensors. Despite recent developments, they still outperform ME sensors with respect to biomagnetic applications. Yet, in all cases the main sensor feature is a special amorphous wire or ribbon. In fact, for GMI and fluxgate demonstrations of measuring biomagnetic signals, the ferromagnetic core materials came from single individual laboratories for each of the sensor types. This demonstrates that reproducibility for achieving the best LOD with the quenched magnetic material is a critical issue. As neither of the sensor types is based on thin film technology, integration of the structures and miniaturization is another critical issue. Thin film-based GMI and fluxgate sensors are so far inferior to their ribbon- and wire-based counterparts and do not achieve the performance of thin film ME sensors.

1.2.3.2 Biomagnetism in medical diagnostics

Biomagnetism can provide novel medical diagnostic strategies but to the best of our knowledge there is worldwide no funded research activity which focuses on the whole process: from the development of new magnetic field sensors to dedicated applications in biomagnetic medical diagnostics. Closest to our CRC is perhaps the Nanosystems Engineering Research Center for Translational Applications of Nanoscale Multiferroic Systems (TANMS) funded by the National Science Foundation, USA, (EEC-1160504) since 2012. TANMS is a center at the University of California, Los Angeles, with the partner institutions California State University, Northridge, Cornell University, Northeastern University, University of California, Berkeley, and University of Texas at Dallas and works to engineer a revolution in miniature electromagnetic electronics through development of a new class of nanoscale multiferroic materials (<http://www.tanms-erc.org/home/about>). It has only limited activities in ultra-sensitive magnetic field sensors.

As the research on magnetic field sensors suited for biomedical applications is already described in 1.2.3.1., this chapter concentrates on projects for the utilization of natural biomagnetism in medical diagnostics. For the artificial fields (deep brain stimulation, magnetic particle detection, and movement analysis) the relation to the state-of-the-art is discussed in the individual projects.

The pioneering experiment in MEG was conducted in 1969 by D. Cohen and F. Zimmermann at Harvard Medical School using SQUID sensors [Co70]. Today, this research is continued at the Athinoula A. Martinos Center for Biomedical Imaging at Massachusetts General Hospital, which is one of the world's premier

research centers devoted to development and application of advanced biomedical imaging technologies (<https://www.martinos.org/>), including work on biomagnetism. Here, the researchers use MEG - often in conjunction with EEG, MRI, fMRI, and optical imaging - to obtain maps of brain activity in cognitive neuroscience studies of the normal and damaged brain.

To our knowledge, more than 150 laboratories in the world are dedicated to MEG research (<http://megcommunity.org/groups-jobs/groups>). In Germany, 13 institutes are using SQUID-technology including the PTB Berlin and the Universities in Düsseldorf, Erlangen, Frankfurt, Heidelberg, Konstanz, Magdeburg, Münster, Hamburg, Leipzig, Jena, Jülich und Tübingen. The CRC 1261 is currently collaborating with the PTB Berlin (Prof. Koch, TP B6), Düsseldorf (Prof. Schnitzler, TP B5) and Münster (Prof. Wolters, TP B3). Their core interests are questions related mostly to system neuroscience, and as far as we know, none of these institutes except for the PTB Berlin are developing magnetic field sensors. Their projects are not related to the clinical application projects of the current proposal. The value of the SQUID-MEG is documented by almost 10 000 publications in Pubmed, and without this technology modern neuroscience is unthinkable. Many key findings of systems neuroscience have been developed with the MEG, like the functions of sensory systems or the motor system. In addition, cognitive neuroscience exploits extensively the independence of the magnetic wave from the transporting medium. In contrast, the clinical use of MEG is much more limited and mostly attached as clinical studies to existing research centers because of the high costs for the use of SQUID technology.

In SQUID-based MCG, there is much less activity worldwide. Major developments are related to the Biomagnetik Park GmbH, Hamburg (<https://biomagnetik.com/en/homepage>), which in close collaboration with the Korean Research Institute of Standard and Science (KRISS) works on the MCG technology to provide a diagnostic system that is able to detect cardiac diseases without any chemical agents, radiation, or strong magnetic fields. The developed technology was used with more than 6 000 patients examined in Hong Kong and at several sites in Germany and has proven its general feasibility [Kw13].

In general, it has to be stated that in both MEG and MCG clinical use is very limited due to the restrictions of using liquid He-cooled SQUID sensor systems in a magnetic shielded environment. The huge potential of sensors at room temperature being capable of operating in a non-shielded environment is also documented by the increased research activities with OPMs [Ho18, lw19, Os18]. Because the ultra-sensitive OPMs saturate in magnetic fields in the 10 nT range, they still need shielding, which motivates even more the search for magnetic field sensors with an appropriate LOD and a high dynamic range as addressed in our proposal.

Literature

- [Al15] O. Alem, T. H. Sander, R. Mhaskar, J. LeBlanc, H. Eswaran, U. Steinhoff, Y. Okada, J. Kitching, L. Trahms, S. Knappe, Fetal magnetocardiography measurements with an array of microfabricated optically pumped magnetometers. *Physics in medicine and biology*. **60**, 4797–4811 (2015).
- [Al17] O. Alem, R. Mhaskar, R. Jiménez-Martínez, D. Sheng, J. LeBlanc, L. Trahms, T. Sander, J. Kitching, S. Knappe, Magnetic field imaging with microfabricated optically-pumped magnetometers. *Optics express*. **25**, 7849–7858 (2017).
- [Ba16] F. Barbieri, V. Trauchessec, L. Caruso, J. Trejo-Rosillo, B. Telenczuk, E. Paul, T. Bal, A. Destexhe, C. Fermon, M. Pannetier-Lecoeur, G. Ouanounou, Local recording of biological magnetic fields using Giant Magneto Resistance-based micro-probes. *Sci. rep.* **6**, 39330 (2016).
- [Ba18] M. Batie, S. Bitant, J. F. Strasburger, V. Shah, O. Alem, R. T. Wakai, Detection of Fetal Arrhythmia Using Optically-Pumped Magnetometers. *JACC. Clinical electrophysiology*. **4**, 284–287 (2018).
- [Be16] G. Bevilacqua, V. Biancalana, P. Chessa, Y. Dancheva, Multichannel optical atomic magnetometer operating in unshielded environment. *Appl. Phys. B*. **122**, 92003 (2016).
- [Bo18] E. Boto, N. Holmes, J. Leggett, G. Roberts, V. Shah, S. S. Meyer, L. D. Muñoz, K. J. Mullinger, T. M. Tierney, S. Bestmann, G. R. Barnes, R. Bowtell, M. J. Brookes, Moving magnetoencephalography towards real-world applications with a wearable system. *Nature*. **555**, 657–661 (2018).
- [Bo18b] L. Bougas, L. D. Langenegger, C. A. Mora, M. Zeltner, W. J. Stark, A. Wickenbrock, J. W. Blanchard, D. Budker, Nondestructive in-line sub-picomolar detection of magnetic nanoparticles in flowing complex fluids. *Sci. rep.*, **8**, 3491 (2018).
- [Ca17] L. Caruso, T. Wunderle, C. M. Lewis, J. Valadeiro, V. Trauchessec, J. Trejo Rosillo, J. P. Amaral, J. Ni, P. Jendritza, C. Fermon, S. Cardoso, P. P. Freitas, P. Fries, M. Pannetier-Lecoeur, In Vivo Magnetic Recording of Neuronal Activity. *Neuron*. **95**, 1283-1291.e4 (2017).
- [Co16] R. J. Cooper, D. W. Prescott, P. Matz, K. L. Sauer, N. Dural, M. V. Romalis, E. L. Foley, T. W. Kornack, M. Monti, J. Okamitsu, Atomic Magnetometer Multisensor Array for RF Interference

- Mitigation and Unshielded Detection of Nuclear Quadrupole Resonance. *Phys. Rev. Applied*. **6** (2016).
- [Co70] D. Cohen, E. A. Edelsack, J. E. Zimmerman, Magnetocardiograms taken inside a shielded room with superconducting point-contact magnetometer. *Appl Phys Lett*, **16**, 278-280 (1970).
- [Da10] H. B. Dang, A. C. Maloof, M. V. Romalis, Ultrahigh sensitivity magnetic field and magnetization measurements with an atomic magnetometer. *Appl. Phys. Lett.* **97**, 151110 (2010).
- [Da13] F. L. da Silva, EEG and MEG: relevance to neuroscience. *Neuron*, **80**, 1112-1128 (2013).
- [De17] J. G. Deak, Z. Zhou, W. Shen, Tunneling magnetoresistance sensor with pT level 1/f magnetic noise. *AIP Advances*. **7**, 56676 (2017).
- [Do18] C. Dong, M. Li, X. Liang, H. Chen, H. Zhou, X. Wang, Y. Gao, E. Mcconney, J. G. Jones, G. J. Brown, B. M. Howe, N. X. Sun, C. Dong, M. Li, X. Liang, H. Chen, H. Zhou, B. M. Howe, N. X. Sun, Characterization of magnetomechanical properties in FeGaB thin films, *Appl. Phys. Lett*, **113**, 262401 (2018).
- [Du17] P. Durdaut, S. Salzer, J. Reermann, P. Hayes, D. Meyners, E. Quandt, G. Schmidt, R. Knöchel, M. Höft, Thermal-Mechanical Noise in Resonant Thin-Film Magnetoelectric Sensors. *IEEE Sens. J.* **17**, 2338–2348 (2017).
- [Du69] J. Dupont-Roc, S. Haroche, C. Cohen-Tannoudji, Detection of very weak magnetic fields (10–9 Gauss) by ⁸⁷Rb zero-field level crossing resonances. *Physics Letters A*. **28**, 638–639 (1969).
- [Eg09] W. F. Egelhoff, P. Pong, J. Unguris, R. D. McMichael, E. R. Nowak, A. S. Edelstein, J. E. Burnette, G. A. Fischer, Critical challenges for picoTesla magnetic-tunnel-junction sensors. *Sensors and Actuators A: Physical*. **155**, 217–225 (2009).
- [El19] E. Elzenheimer, H. Laufs, W. Schulte-Mattler, G. Schmidt, Signal Modelling and Simulation of Temporal Dispersion and Conduction Block in Motor Nerves, *IEEE Transactions on Biomedical Engineering*, early access (2019). <https://doi.org/10.1109/TBME.2019.2954592>.
- [Es17] H. Eswaran, D. Escalona-Vargas, E. H. Bolin, J. D. Wilson, C. L. Lowery, Fetal magnetocardiography using optically pumped magnetometers: a more adaptable and less expensive alternative? *Prenatal diagnosis*. **37**, 193–196 (2017).
- [Fa17] M. I. Faley, J. Dammers, Y. V. Maslennikov, J. F. Schneiderman, D. Winkler, V. P. Koshelets, N. J. Shah, R. E. Dunin-Borkowski, High- Tc SQUID biomagnetometers. *Supercond. Sci. Technol.* **30**, 83001 (2017).
- [Fe05] R. Fenici, D. Brisinda, A. M. Meloni, Clinical application of magnetocardiography, *Expert Rev. Mol. Diagn.* **5**, 291-313 (2005).
- [Fr16] P. P. Freitas, R. Ferreira, S. Cardoso, Spintronic Sensors. *Proc. IEEE*. **104**, 1894–1918 (2016).
- [Fr19] R. M. Friedrich, S. Zabel, A. Galka, N. Lukat, J.-M. Wagner, C. Kirchhof, E. Quandt, J. McCord, C. Selhuber-Unkel, M. Siniatchkin, F. Faupel, Magnetic particle mapping using magnetoelectric sensors as an imaging modality, *Sci. Rep.*, **9**, 2086 (2019).
- [Fu18] K. Fujiwara, M. Oogane, A. Kanno, M. Imada, J. Jono, T. Terauchi, T. Okuno, Y. Aritomi, M. Morikawa, M. Tsuchida, N. Nakasato, Y. Ando, Magnetocardiography and magnetoencephalography measurements at room temperature using tunnel magneto-resistance sensors. *Appl. Phys. Express*. **11**, 23001 (2018).
- [Go06] A. Gokce, E. R. Nowak, S. H. Yang, S. S. P. Parkin, 1/f noise in magnetic tunnel junctions with MgO tunnel barriers. *Journal of Applied Physics*. **99**, 08A906 (2006).
- [Ha10a] R. Hari, L. Parkkonen, C. Nangini, The brain in time: Insights from neuromagnetic recordings, *Annals of the New York Academy of Sciences*, **1191**, 89-109 (2010).
- [Ha10b] P. Hansen, M. Kringelbach, R. Salmelin, (Eds.): MEG: an introduction to methods. *Oxford University Press* (2010).
- [Ha12] R. Hari, R. Salmelin, Magnetoencephalography: from SQUIDs to neuroscience: Neuroimage 20th anniversary special edition, *Neuroimage*, **61**, 386-396 (2012).
- [Ha15] S. Harada, I. Sasada, F. Hang, Development of a One-Dimensional Fluxgate Array and Its Application to Magnetocardiogram Measurements. *Electron Comm Jpn.* **98**, 20–26 (2015).
- [Ha16] P. Hayes, R. Knöchel, A. Piorra, E. Quandt, Magnetoelktrische Magnetfeldmessung mit Frequenzumsetzung, EP 15 170 985.
- [Ha17] L. Hamid, A. Al Farawn, I. Merlet, N. Japaridze, U. Heute, U. Stephani, A. Galka, F. Wendling, M. Siniatchkin, Source reconstruction via the spatiotemporal Kalman Filter and LORETA from EEG time series with 32 or fewer electrodes. 39th Int. Conf. IEEE EMBS, Jeju Island, 2218-2222 (2017).
- [Ha18a] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yarar, A. Piorra, R. Knöchel, Y.K. Fetisov, E. Quandt, Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing. *Journal of Physics D: Applied Physics*, **51**, 354002 (2018).
- [Ha18b] N. Habboush, L. Hamid, M. Siniatchkin, U. Stephani, A. Galka, Pipeline for Forward Modelling and Source Imaging of Magnetocardiographic Recordings via Spatiotemporal Kalman Filtering. 40th Int. Conf. IEEE EMBS, Honolulu, 199-202 (2018).

- [Ha19] P. Hayes, M. Jovičević Klug, S. Toxværd, P. Durdaut, V. Schell, A. Teplyuk, D. Burdin, A. Winkler, R. Weser, Y. Fetisov, M. Höft, R. Knöchel, J. McCord, E. Quandt, Converse Magnetoelectric Composite Resonator for Sensing Small Magnetic Fields. *Sci. rep.*, **9**, 16355 (2019).
- [Ho18] N. Holmes, J. Leggett, E. Boto, G. Roberts, R. M. Hill, T. M. Tierney, V. Shah, G. R. Barnes, M. J. Brookes, R. Bowtell, A bi-planar coil system for nulling background magnetic fields in scalp mounted magnetoencephalography, *NeuroImage*, **181**, 760–774, (2018).
- [In18] S. J. Ingleby, C. O'Dwyer, P. F. Griffin, A. S. Arnold, E. Riis, Vector Magnetometry Exploiting Phase-Geometry Effects in a Double-Resonance Alignment Magnetometer. *Phys. Rev. Applied*, **10** (2018).
- [Iw19] G. Z. Iwata, Y. Hu, T. Sander, M. Muthuraman, V. C. Chirumamilla, S. Groppa, D. Budker, A. Wickenbrock, Biomagnetic signals recorded during transcranial magnetic stimulation (TMS)-evoked peripheral muscular activity, preprint: <http://arxiv.org/pdf/1909.11451v1>, (2019).
- [Ja65] R. C. Jaklevic, J. Lambe, J. E. Mercereau, A. H. Silver, Macroscopic quantum interference in superconductors, *Physics Review*, **140**, A1628 (1965).
- [Ka15] H. Karo, I. Sasada, Magnetocardiogram measured by fundamental mode orthogonal fluxgate array. *Journal of Applied Physics*, **117**, 17B322 (2015).
- [Ki16] A. Kittmann, S. Zabel, E. Yarar, F. Faupel, R. Knöchel, M. Höft, P. Durdaut, E. Quandt, Sensorelement für Magnetfelder mit hoher Frequenzbandbreite, DE 10 2016 123 274 B4
- [Ki18a] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, F. Faupel, E. Quandt, Wide Band Low Noise Love Wave Magnetic Field Sensor System, *Sci. Rep.*, **8**, 278 (2018).
- [Ki18b] J. Kitching, Chip-scale atomic devices. *Applied Physics Reviews*, **5**, 31302 (2018).
- [KI19] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. Salzer, M. Höft, E. Quandt D. Meyners, J. McCord, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors, *Applied Physics Letters*, **114**, 192410 (2019).
- [Ko04] H. Koch, Recent advances in magnetocardiography, *Journal of electrocardiology*, **37**, 117-122 (2004).
- [Kö16] R. Körber, J.-H. Storm, H. Seton, J. P. Mäkelä, R. Paetau, L. Parkkonen, C. Pfeiffer, B. Riaz, J. F. Schneiderman, H. Dong, S. M. Hwang, L. You, B. Inglis, J. Clarke, M. A. Espy, R. J. Ilmoniemi, P. E. Magnelind, A. N. Matlashov, J. O. Nieminen, P. L. Volegov, K. C. J. Zevenhoven, N. Höfner, M. Burghoff, K. Enpuku, S. Y. Yang, J.-J. Chieh, J. Knuutila, P. Laine, J. Nenonen, SQUIDS in biomagnetism. *Supercond. Sci. Technol.*, **29**, 113001 (2016).
- [Kw13] J. S. Kwong, B. Leithäuser, J. W. Park, C. M. Yu, Diagnostic value of magnetocardiography in coronary artery disease and cardiac arrhythmias: A review of clinical data, *International journal of cardiology*, **167**, 1835-1842 (2013).
- [Li17] M. Li, A. Matyushov, C. Dong, H. Chen, H. Lin, T. Nan, Z. Qian, M. Rinaldi, Y. Lin, N. X. Sun, Ultra-sensitive NEMS magnetoelectric sensor for picotesla DC magnetic field detection, *Appl. Phys. Lett.*, **110**, 143510 (2017).
- [Lo04] O. V. Lounasmaa, H. Seppä, SQUIDS in neuro-and cardiomagnetism, *Journal of Low Temperature Physics*, **135**, 295-335 (2004).
- [Ma11] J. Ma, J. Hu, Z. Li, C.W. Nan, Recent Progress in Multiferroic Magnetoelectric Composites: from Bulk to Thin Films, *Adv. Mater.*, **23**, 1062-1087 (2011).
- [Ma19] J. Ma, T. Uchiyama, Alpha Rhythm and Visual Event-Related Fields Measurements at Room Temperature Using Magneto-Impedance Sensor System. *IEEE Trans. Magn.*, **55**, 1–6 (2019).
- [Mi18] M. Mintken, M. Schweichel, S. Schröder, S. Kaps, J. Carstensen, Y. K. Mishra, T. Strunskus, F. Faupel, R. Adelung, Nanogenerator and piezotronic inspired concepts for energy efficient magnetic field sensors. *Nano Energy*, **56**, 420–425 (2019).
- [Mo15] K. Mohri, T. Uchiyama, L. V. Panina, M. Yamamoto, K. Bushida, Recent Advances of Amorphous Wire CMOS IC Magneto-Impedance Sensors. *Journal of Sensors*, **2015**, 1–8 (2015).
- [Mo17] S. Morales, M. C. Corsi, W. Fourcault, F. Bertrand, G. Cauffet, C. Gobbo, F. Alcouffe, F. Lenouvel, M. Le Prado, F. Berger, G. Vanzetto, E. Labyt, Magnetocardiography measurements with 4He vector optically pumped magnetometers at room temperature. *Physics in medicine and biology*, **62**, 7267–7279 (2017).
- [Na08] C.W. Nan, M. Bichurin, S. Dong, D. Viehland, G. Srinivasan, Multiferroic magnetoelectric composites: Historical perspective, status and future directions, *Journal of Applied Physics*, **103**, 031101 (2008)
- [Os18] J. Osborne, J. Orton, O. Alem, and V. Shah, Fully integrated standalone zero field optically pumped magnetometer for biomagnetism, Proc. SPIE 10548, Steep Dispersion Engineering and Opto-Atomic Precision Metrology XI, 105481G, (2018)
- [Pa14] B. Patton, E. Zhivun, D. C. Hovde, D. Budker, All-optical vector atomic magnetometer. *Physical review letters*, **113**, 13001 (2014).

- [Re16a] J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, F. Faupel, G. Schmidt, Adaptive Readout Schemes for Thin-Film Magnetoelectric Sensors Based on the delta-E Effect, *IEEE Sensors Journal*, **16**, 4891-4900 (2016).
- [Re16b] J. Reermann, C. Bald, S. Salzer, P. Durdaut, A. Piorra, D. Meyners, E. Quandt, M. Höft, G. Schmidt, Comparison of Reference Sensors for Noise Cancellation of Magnetoelectric Sensors, *IEEE Sensors*, 1-3 (2016).
- [Re18] J. Reermann, P. Durdaut, S. Salzer, T. Demming, A. Piorra, E. Quandt, N. Frey, M. Höft, G. Schmidt, Evaluation of Magnetoelectric Sensor Systems for Cardiological Applications, *Measurement (Elsevier)*, 230-238 (2018).
- [Rö18] V. Röbisch, A. Piorra, R. Lima de Miranda, E. Quandt, D. Meyners, Frequency-tunable nickel-titanium substrates for magnetoelectric sensors, *AIP Advances*, **8**, 125320 (2018).
- [Sa12] T. H. Sander, J. Preusser, R. Mhaskar, J. Kitching, L. Trahms, S. Knappe, Magnetoencephalography with a chip-scale atomic magnetometer. *Biomedical optics express*. **3**, 981–990 (2012).
- [Sa18a] S. D. Salzer, C. Kirchhof, E. Quandt, M. Höft, R. Knöchel, Magnetoelectric Microwave Magnetic Field Sensor at 3 GHz, *Asia-Pacific Microwave Conference (APMC)*, 10.23919/APMC.2018.8617346 (2018).
- [Sa18b] S. Salzer, R. Knöchel, E. Quandt, L. Thormählen, Mikrowellenresonator-Magnetfeldmessvorrichtung sowie Magnetfeldmessverfahren, DE102018110511.
- [Sa18c] S. Salzer, V. Röbisch, M. Jovičević Klug, P. Durdaut, J. McCord, D. Meyners, J. Reermann, M. Höft, R. Knöchel, Noise Limits in Thin-Film Magnetoelectric Sensors With Magnetic Frequency Conversion, *IEEE Sensors Journal*, **18**, 596-604 (2018).
- [Sa18d] I. Sasada, Low noise fundamental mode orthogonal fluxgate (FM-OFG) magnetometer built with an amorphous ribbon core, *IEEE Trans. Magn.*, **54**, 1-5 (2018).
- [Th18] T. Thiele, Y. Lin, M. O. Brown, C. A. Regal, Self-Calibrating Vector Atomic Magnetometry through Microwave Polarization Reconstruction, *Physical review letters*. **121**, 153202 (2018).
- [Ti19] T. M. Tierney, N. Holmes, S. Mellor, J. D. López, G. Roberts, R. M. Hill, E. Boto, J. Leggett, V. Shah, M. J. Brookes, R. Bowtell, G. R. Barnes, Optically pumped magnetometers: From quantum origins to multi-channel magnetoencephalography, *NeuroImage*. **199**, 598–608 (2019).
- [Tu19] C. Tu, Z.Q. Chu, B. Spetzler, P. Hayes, C.Z. Dong, X.F. Liang, H.H. Chen, Y.F. He, Y.Y. Wei, I. Lisenkov, H. Lin, Y.H. Lin, J. McCord, F. Faupel, E. Quandt, N.X. Sun, Mechanical-Resonance-Enhanced Thin-Film Magnetoelectric Heterostructures for Magnetometers, Mechanical Antennas, Tunable RF Inductors, and Filters, *Materials* **12**, 2259 (2019).
- [Uc17] T. Uchiyama, T. Takiya, Development of precise off-diagonal magnetoimpedance gradiometer for magnetocardiography. *AIP Advances*. **7**, 56644 (2017).
- [Vi18] D. Viehland, M. Wuttig, J. McCord, E. Quandt, Magnetoelectric magnetic field sensors, *MRS Bull.* **43**, 834–840 (2018).
- [Wa14] Y. Wang, J. Li, D. Viehland, Magnetoelectrics for magnetic sensor applications: status, challenges and perspectives, *Materials Today* **17**, 269-275 (2014).
- [Wa15] K. Wang, S. Tajima, D. Song, N. Hamada, C. Cai, T. Uchiyama, Auditory evoked field measurement using magneto-impedance sensors, *J. Appl. Phys.*, **117**, 17B306 (2015).
- [Wa17] K. Wang, C. Cai, M. Yamamoto, T. Uchiyama, Real-time brain activity measurement and signal processing system using highly sensitive MI sensor. *AIP Advances*. **7**, 56635 (2017).
- [Ya16] E. Yarar, S. Salzer, V. Hrkac, A. Piorra, M. Höft, R. Knöchel, L. Kienle, E. Quandt, Inverse bilayer magnetoelectric thin film sensor, *Appl. Phys. Lett.*, **109**, 022901 (2016).
- [Ya19] M. Yalaz, A. Teplyuk, M. Muthuraman, G. Deuschl, M. Höft: The Magnetic Properties of Electrical Pulses delivered by Deep Brain Stimulation Systems, *IEEE Trans on Instrumentation and Measurement*, paper accepted (2019).
- [Za16] S. Zabel, J. Reermann, S. Fichtner, C. Kirchhof, E. Quandt, B. Wagner, G. Schmidt, F. Faupel, Multimode delta-E effect magnetic field sensors with adapted electrodes, *Appl. Phys. Lett.*, **108**, 222401 (2016).
- [Zh19] C. Zheng, K. Zhu, S. Cardoso de Freitas, J.-Y. Chang, J. E. Davies, P. Eames, P. P. Freitas, O. Kazakova, C. Kim, C.-W. Leung, S.-H. Liou, A. Ognev, S. N. Piramanayagam, P. Ripka, A. Samardak, K.-H. Shin, S.-Y. Tong, M.-J. Tung, S. X. Wang, S. Xue, X. Yin, P. W. T. Pong, Magnetoresistive Sensor Development Roadmap (Non-Recording Applications). *IEEE Trans. Magn.* **55**, 1–30 (2019).

1.2.4 National and international cooperation and networking

The CRC 1261 closely cooperates with other national and international working groups that also aim to investigate highly sensitive magnetic field sensors for biomedical applications. This is, for example, reflected

by the number of conferences or symposia at conferences that were organized by principal investigators of the CRC (Table 1).

Table 1: Conferences and Symposia at conferences co-organized by principal investigators of the CRC 1261

Conference	Symposium, topic, involved principal investigators (bold)
14.-19.08.2016, Cancun, Mexico	International Materials Research Congress (IMRC), Symposium C.3 Interfacing Nanometer and Micrometer-Scale Structures to the Bio-World (E. Quiroga González, M. Sailor, C. Selhuber-Unkel)
21.-26.08.2016, Glasgow, Scotland	7th Joint European Magnetic Symposia 2016 (JEMS), Symposium on Magnetic thin films, surface, interfaces and patterned thin films. (J. McCord , Dan Alwood, Francesca Casoli)
26.01.2017, DESY, Hamburg, Germany	Workshop: High resolution diffraction at solid and liquid interfaces, (B. Murphy , F. Bertram)
24.04.-28.04.2017, Dublin, Ireland	IEEE International Magnetism Conference Intermag 2017, program co-chair (J. McCord)
07.-09.06.2017, Kiel, Germany	3 rd Euro Intelligent Materials, Conference chairs (C. Selhuber-Unkel , E. Quandt)
14.-16.06.2017, Kaunas, Lithuania	Nanotechnology and Innovation in the Baltic Sea Region 2017 (NIBS), conference chair (F. Faupel)
26.11.-01.12.2017, Boston, USA	MRS Fall Meeting 2017, Symposium EM02 — Multiferroics and Magnetoelectrics (F. Faupel)
08.-11.5.2018 Seoul, South Korea	4th International Conference on Nanogenerators and Piezotronics (NGPT 2018), chairman of the piezotronic session (R. Adelung)
30.05.-01.06.2018, Sønderborg, Denmark	Nanotechnology and Innovation in the Baltic Sea Region 2018 (NIBS), Conference chair (F. Faupel)
03.-07.09.2018, Mainz, Germany	9th Joint European Magnetic Symposia 2018 (JEMS), Symposium 13. Complex oxides, multiferroics and composite multiferroics (E. Quandt , S. van Dijken)
09.-12.09.2018, Kiel, Germany	Conference of the German Association of Chemistry and Physics Education (GDCEP), Symposium on interfaces between Science Communication and Science Education, together with other SOPs (L. Kampschulte, C. Enzinger , I. Parchmann)
17.-19.9.2018 Garching, Germany	German Conference for Research with Synchrotron Radiation, Neutron and Ion Beams at Large Facilities (SNI 2018) (B. Murphy , A. Schneidewind, G. Dollinger)
26.-28.09.2018, Darmstadt, Germany	Materials Science and Engineering (MSE) 2018, Symposium Cell-instructive hydrogels (C. Lee-Thedieck, C. Selhuber-Unkel , P. van Rijn)
03.-04.05.2019, Kiel, Germany	DBS-workshop, New Studies for DBS (A.-K. Helmers , G. Deuschl , D. Berg, M. Synowitz, S. Paschen)
05.-08.06.2019, Poznan, Poland	Nanotechnology and Innovation in the Baltic Sea Region 2019 (NIBS) (F. Faupel)
15.-17.06.2019, Beijing, China	4th International Conference on Nanoenergy and Nanosystems, chairman of the piezotronic session (R. Adelung)
17.-19.06.2019, Kiel, Germany	4th Euro Intelligent Materials, conference chairs (C. Selhuber-Unkel , E. Quandt)
29.06.-02.07.2019, Oslo, Norway	5th congress of the European Academy of Neurology, President of EAN (G. Deuschl)
18.-23.08.2019, Vienna, Austria	23rd European Crystallographic meeting, Symposium: In situ and in operando analysis of functional materials (B. Murphy , A. Neels)
02.-05.09.2019 Berlin, Germany	Microscopy Conference 2019, Session Material sciences 6, Nanostructured materials (L. Kienle , M. Ritter)
01.-06.12.2019, Boston, USA	MRS Fall Meeting 2019, Symposium EL03: Multiferroics and Magnetoelectrics (N. Sun, J. Chang, S. Priya, E. Quandt)
01.-06.12.2019, Boston, USA	MRS Fall Meeting 2019, Symposium SB06: Bringing mechanobiology to materials: From molecular understanding to biological design (J.E. Curtis, M. Paszek, K. Poole, C. Selhuber-Unkel)
11.-13.03.2020, Kiel, Germany	Workshop on Biosignals, Workshop Processing of bio-electric and bio-magnetic signals (A. Bahr , E. Elzenheimer , G. Schmidt)

22.-25.09.2020, Darmstadt, Germany	Materials Science and Engineering (MSE) 2020, Topic organizer „Biomaterials“ (A. Boccaccini, H.-W. Kim, C. Selhuber-Unkel) and Symposium Biostructive Polymers (C. Lee-Thedieck, C. Selhuber-Unkel , P. van Rijn)

A close scientific network on ME sensor technology, e.g., with Prof. Sun (Northeastern University, USA), with Prof. Viehland (Virginia Tech, USA) and with Prof. Priya (Penn State, USA) exists and will be sustained. Especially, Prof. Priya is the PI of the Penn State – American Ceramic Society – University of Kiel (PACK) International Research Experience Fellowship. PACK is a National Science Foundation (NSF) funded international research fellowship opportunity for US graduate students to conduct research at Kiel University. Within 3 years 18 students in total will participate in this program. Furthermore, Prof. Nian Sun just recently received the Humboldt Award and will spend approximately 6 weeks in Kiel for intense collaboration with several PIs of the CRC. Additionally, existing contacts of the first funding period as, e.g., with Prof. Wang (Beijing, China), and Prof. Schilling (TU Braunschweig) will be continued and strengthened in the second funding period.

There are further intense scientific collaborations in the scientific field of the CRC between groups at Kiel University and national and international working groups at other universities (in alphabetical order), which are of importance for the planned research work:

The **Adelung group (A2, A5)** closely cooperates with the group of Prof. Tiginyanu from the Academy of Science in Moldova about the production of piezoelectric ZnO and GaN crystals. A long-lasting cooperation about the synthesis and the electronic and optical characterization of the ZnO crystals exists with Prof. Ronning (Universität Jena). With Prof. Ya Yang from the Chinese academy of sciences in Beijing, a collaboration has been started in the first funding period for the magneto-electric composite hybrid sensors.

The **Deuschl group (T1)** has cooperations with Prof. Agid (Paris) in the area of deep brain stimulation. In the research area of tremor, there are cooperations with Prof. Bhatia (London), Prof. Eble (Springfield, USA), and Prof. Hallett (Bethesda, USA). Furthermore, the group cooperates with Prof. Schnitzler (Düsseldorf) and Prof. Muthuraman (Mainz/Frankfurt) in the area of recording of SQUID-MEG and data analysis.

The **Faupel group (A2, A4, B7)** cooperates in the field of initiated chemical vapor deposition of polymers with Prof. Karen Gleason (MIT, Boston) and Prof. Anna Coclite (University of Graz). In the field of ΔE -effect sensors there is a cooperation with Prof. Nian Sun (Northeastern University, Boston). Furthermore, in the field of Magnetic Particle detection and Magnetic Particle Imaging there are cooperations with Prof. Meinhard Schilling and Prof. Frank Ludwig (TU Braunschweig) as well as Prof. Thorsten Buzug (Lübeck University).

The **Frey group (B9)**, as a founding member of the DZHK (Deutsches Zentrum für Herz- Kreislau fforschung), cooperates with several German university cardiology departments in multicenter clinical trials (phase II-IV) which include electrophysiological trials (eg SMART-MI, TU Munich).

The **Gerken group (A8)** cooperates with Dr. Hadi Heidari (Glasgow University) on the modelling and simulation of magnetic-field sensors and with Prof. Carsten Wolters (Münster University) on finite-element-method head models.

Ann-Kristin Helmers (T1) cooperates with the group of Prof. Schlaier (Regensburg) and Dr. Jakobs (Heidelberg) on diffusion tensor imaging (DTI) and neuromodulation for deep brain stimulation and for the use of rechargeable impulse generators.

The **Höft group (B1, T1, Z2)** cooperates with Prof. Rubiola and Prof. Friedt (FEMTO-ST Institute, France) in the field of noise analysis of SAW sensor systems, with Prof. Pohl (Ruhr Universität Bochum) for radio frequency integrated circuits and with Prof. Jacoby (Technische Universität Darmstadt) in the field of tunable microwave devices.

The **Kienle group (A6)** cooperates with Dr. Kübel (KIT-KNMF, Karlsruhe), Dr. Lotnyk (IOM Leipzig), and Prof. Johnson (University of Oregon) in the field of high resolution microscopy and electron crystallography. Moreover, collaboration with Prof. Tiginyanu from the Academy of Science in Moldova on GaN-based piezotronic material systems and Prof. Johnson (University of Oregon) on transition metal dichalcogenides will be strengthened.

Fabian Lofink (A9) cooperates closely with Prof. Ambacher (Albert-Ludwigs-Universität Freiburg) in the field of surface acoustic wave devices.

The **Maetzler group (B9)** collaborates with Prof. Jeff Hausdorff (Tel Aviv University, Israel) and Kamiar Aminian (EPFL, Switzerland) to better assess gait and balance changes associated with aging and disease by using digital devices such as inertial measurement units. The group is also involved in several European consortia such as the IMI2 projects Mobilise-D (connecting digital mobility assessment to clinical outcomes for regulatory and clinical endorsement) and IDEA-FAST (identifying digital endpoints to assess fatigue, sleep and activities of daily living in neurodegenerative disorders and immune-mediated inflammatory diseases, see 1.5 for funding details).

The **McCord group (A1, A10)** cooperates with Prof. Nian X. Sun (Northeastern University, Boston) on issues of magnetic domain effects in ME and similar sensor structures based on magnetic thin films.

Dirk Meyners (A1, Z1) cooperates with Prof. Nian X. Sun (Northeastern University College of Engineering, Boston) in the field of amorphous magnetic materials and with Prof. Holger Kersten (Kiel University) in the field of plasma-based sputter deposition of thin films.

The **Murphy group (A6)** cooperates with Dr. Krywka (HZG, Geesthacht) and Prof. Burghammer (ESRF, F) in the field of nano X-ray diffraction methods and with Prof. Collins (Diamond, UK), Dr. Bouchenoire (ESRF, F) and with Dr. Bertram (X-ray diffraction) and Dr. Sprung (coherent X-ray diffraction CXDI) (DESY, Hamburg). For the X-ray CXDI, they collaborate with Prof. Shpyrko and Dr. Hrkac (UCSD, USA) along with Dr. Ross Harder (APS, USA).

Florian Niekiet (Z1) cooperates with the group of Prof. Butz (University Siegen) in the field of structural characterization of functional materials.

The **Parchmann group (project SOP)** closely cooperates with the Deutsches Museum, where the former PI Lorenz Kampschulte now leads the education programs. Furthermore, the IPN has a continuous exchange and cooperation with Prof. Ron Blonder (Weizmann Institute of Science, Israel) in the field of outreach in nano science. Through the Kiel Science Outreach Campus KiSOC, additional cooperations are provided, e.g., with Prof. Ayelet Baram-Tsabari (Technion, Israel) or the National Institute for Science Communication (NaWiK). The exchange with other SOPs has led to joint conference symposia and will be continued to establish a formal network.

The **Quandt group (A7, A9)** cooperates with Prof. Wuttig (University of Maryland, USA), Prof. Sun (Northeastern University, USA), Prof. Viehland (Virginia Tech, USA), and Prof. Priya (Penn State University, USA) in the field of ME composites and magnetic field sensors.

The **Rieger group (A4)** cooperates with Prof. John T. Taylor (University of Bath, UK) in the field of monolithic integrated circuit design for multichannel biomedical signal recording.

The **Schmidt group (B2, B9, B10, Z2)** cooperates with Prof. Hansen (University of Dallas, Texas, USA) in the field of pattern recognition and machine learning as well as with Dr. Sander-Thömmes (PTB, Berlin, Germany) in the field of biomagnetic measurements.

The **Selhuber-Unkel group (project B7)** collaborates with Jan Lammerding (Cornell University), Carsten Grashoff (University of Münster), and Anne Staubit (Universität Bremen) in the fields of biomedicine and responsive materials, respectively.

The **Wulfinghoff group (project A10)** cooperates with Prof. Manfred Kohl (Karlsruhe Institute of Technology, Germany) in the field of sensors and actuators with piezoelectric components.

1.3 Research profile of the applicant university

1.3.1 Strategy and planning

As described in detail in the original proposal, the Collaborative Research Centre 1261 is integrated into the research focus “Kiel Nano, Surface and Interface Science” (KiNSIS) of Kiel University, which was created as a consequence of the long-lasting successful research in the area of nanoscience and nanotechnology. According to the strong interdisciplinary character of nanotechnology, KiNSIS has members from various fields including physics, chemistry, materials science, electrical engineering, medicine, and biology. Together with

the Collaborative Research Centre 677 “Function by Switching”, the Transregional Collaborative Research Centre 24 „Fundamentals of Complex Plasmas“ (in collaboration with University of Greifswald), and the Research Unit 2093 “Memristive Devices for Neural Systems”, the CRC 1261 formed the initial backbone of the research focus. The TCRC 24 and the CRC 677 ended in 2018 and 2019, respectively. In 2016, the Research Training School 2154 “Materials for Brain” was established, and in 2019, an interdisciplinary team of KiNSIS scientists submitted a draft for the new CRC 1461 “Neurotronics”. The draft was positively evaluated and the DFG recommended the submission of a full proposal for this CRC.

The concept of the CRC 1261 fully reflects the strong, interdisciplinary approach of KiNSIS in particular and of the Kiel University in general. Colleagues from the Faculty of Engineering, the Faculty of Mathematics and Natural Sciences, and the Faculty of Medicine of Kiel University as well as colleagues of the Fraunhofer Institute for Silicon Technology (Fraunhofer ISIT, Itzehoe) and of the Leibniz Institute for Science and Mathematics Education (IPN) collaborate within the CRC 1261. Their research areas range from materials science, physics, electrical and information engineering to neurology, and cardiology. During the last years, the CRC 1261 has been stimulating research into sensors and sensor systems at Kiel University in an even broader community. As a result, the University submitted a proposal for an “Innovation Center for Interconnected Sensor Systems” for funding by the European Union and the state of Schleswig-Holstein within the EFRE program. The proposal achieved first-stage approval and was recently submitted for final approval. The Innovation Center shall provide the necessary R&D infrastructure for achieving research results in the area of networked sensors and for transferring these results to marketable products together with companies. It provides approximately 3000 m² of new laboratory and office space.

In recent years, the European Union, the state of Schleswig-Holstein, and Kiel University have strongly supported the priority research area KiNSIS by investing in the corresponding research infrastructure of the participating faculties. Special emphasis was put on the Kiel’s Nanolab, which was built in 2008 and was continually developed further. Without Kiel’s Nanolab, many of the research activities within the CRC 1261 would not be possible. Within the EFRE program Kiel’s Nanolab is funded as a Competence Center for Nanosystems Technology since 2013. With this funding, various new devices (sputter deposition devices, laser scanning microscope) have been installed in Kiel’s Nanolab. Examples of recent funding within the DFG Scientific Instrumentation and Information Technology program are a new photoelectron spectroscopy instrument (683 k€) and a new state-of-the-art transmission electron microscope (2600 k€). The microscope will be equipped with several detectors for recording atomically resolved images of light and heavy atoms. Moreover, atomically resolved EDX analysis is possible as well as EELS with sub 1 eV energy resolution. The CRC 1261 will directly benefit from both instruments.

Fraunhofer ISIT is part of the Forschungsfabrik Mikroelektronik Deutschland (FMD) started in 2017, a grant by the BMBF to 13 non-university institutes to strengthen the research and development capabilities in the field of microelectronics totaling 350 Mio €. As part of the FMD, ISIT received 19.3 Mio € to invest in its research infrastructure. The CRC 1261 will directly benefit from this investment, e.g. from the new deposition and characterization tools for piezoelectric thin films and high resolution lithography equipment.

The close collaboration between the faculties involved in the CRC 1261, particularly the Faculty of Engineering and the Faculty of Medicine, also has important effects on teaching, particularly at the graduate level. This is specifically reflected in the integrated research training group (IRTG) but also by a close collaboration with the Research Training Group 2154 “Materials for Brain”, which involves many PIs from medicine and materials science. Meanwhile, a close cooperation between the RTG 2154 and the CRC 1261 has been established.

1.3.2 Staff situation

The CRC 1261 involves 22 principal investigators, from which eight hold full professorships, six hold associate professorships and seven are in a wider sense junior group leaders. Prof. Deuschl has retired but holds the first senior professor position at Kiel University and has a permission contract with UKSH / Kiel University to undertake the work described within this proposal. Prof. Faupel successfully applied for a shift of his retirement to ensure his participation over the full second funding period. Prof. Bahr and Prof. Rieger were appointed as additional junior and associate professors in electrical engineering, respectively, to strengthen the activities of the CRC. As a consequence, the CRC consists of a team comprising of well-renowned senior scientists in combination with highly qualified younger scientists and thus guarantees a well-balanced expertise for the suggested work program. Eight of the contributing principal investigators belong to the Institute for Materials Science, five are within the Institute of Electrical and Information Technology, four are with the University Hospital Schleswig-Holstein, Campus Kiel, one is with the Institute of Experimental and Applied Physics, two are with the Leibniz-Institute for Science and Mathematics Education in Kiel, and two are with the Fraunhofer

Institute of Silicon Technology in Itzehoe. Thus, the team represents the broad interdisciplinary competence that is a key signature of this CRC.

Many of the professors within the CRC were appointed at Kiel University within the last ten years: Adelung (2010), Höft (2013), Kienle (2010), McCord (2011), Parchmann (2009), Rieger (2018), Schmidt (2010), Selhuber-Unkel (2010), Wagner (2009) and Wulfinghoff (2018). Three of them (Adelung, Kienle, McCord) were initially appointed as Heisenberg professors and were tenured later. For any future calls to Kiel University a possible involvement in the CRC will be a key criterion for the selection of the candidates. External calls were successfully repelled (Adelung, Gerken (three times), Kienle, Selhuber-Unkel, Bahr). Recently, Prof. Selhuber-Unkel received an external call for a full professorship from the University of Heidelberg, which is still pending. Two of the principal investigators (Gerken, Selhuber-Unkel) have been awarded with an ERC Starting Grant. Prof. Quandt received a Reinhard Koselleck Grant from the DFG.

1.3.3 Research infrastructure

The research infrastructure at all participating institutions is very good for carrying out the work planned for the second funding period of the CRC. A modern cleanroom facility is available at the Faculty of Engineering. The cleanroom is part of the **Kieler Nanolabor**, which was founded in July 2008 as a central facility for the nanosciences and their applications at Kiel University. The Nanolabor is open to all scientists at the Kiel University. As a part of the Kieler Nanolabor, the cleanroom belongs to the Faculty of Engineering, with the Chair for Inorganic Functional Materials (Prof. Quandt) responsible for its operations. The cleanroom is listed as a core facility within the RIsources portal for Research Infrastructure operated by the German Research Foundation, http://risources.dfg.de/detail/RI_00368_de.html. The available 300 m² in this facility comprises work areas of the classes ISO-5 and ISO-6, whereas its equipment corresponds to those of a lab oriented to research on micro- and nanotechnology. This way, many devices for thin film deposition, patterning, and characterization have been installed and are available to the users. This equipment includes sputter deposition and CVD devices, spin coaters and mask aligners, wet benches, dry etch and ion milling tools, etc. Further details on the cleanroom equipment, rules (articles), registration, and those in charge can be found at <http://www.tf.uni-kiel.de/matwis/afm/en/nanolab>. In 2013, the Kieler Nanolabor was extended by the state of Schleswig-Holstein, in collaboration with the EU, to the **Competence Center Nanosystem Technology**. This center promotes cooperation projects between academia and industry, which includes not only established technology companies but also local and regional SMEs and spin-offs from the University.

The **Transmission Electron Microscopy (TEM) center** of the Faculty of Engineering of Kiel University is also listed as a core facility within the RIsources portal operated by the German Research Foundation (cf. http://risources.dfg.de/detail/RI_00354_de.html). The statutes of the TEM center (<http://srs.matwis.tf.uni-kiel.de/temzentrum/satzung>) provide detailed information about personnel, hardware, and costs. Instrumentation includes a field emission TEM (Tecnai F30 STWIN G2) which is equipped with advanced analytical capabilities, particularly the GIF Tridiem energy filter, tomography, heating and cooling stages, and the DigiStar device for precession electron diffraction. The facilities of the two TEM preparation labs for dimpling, ion beam milling (low energy PIPS), chemical etching (jet polishing), and a Dual Beam FIB milling (FEI Helios established in the Nanolabor) enable the production of electron transparent samples with the aid of the best available technology. A second TEM (Jeol 2100) optimized for tomography was installed in 2013. Moreover, a probe-corrected scanning electron microscope (STEM with atomic resolution) will be installed in 2020 at the Faculty of Engineering. The relevant funds of 2.6 M€ were granted on 09.07.2019 by the DFG (INST 257/620 FUGG). The instrument will be equipped with dedicated sample holders, e.g., for in situ heating and electrical biasing, a cold field emitter for high resolution EELS, an atomically resolving wide-angle EDX detector, and diverse image detectors providing not just Z-contrast but also enhanced contrast for light-element imaging. Access to scanning electron microscopes (e.g. Zeiss Gemini plus) for preliminary examination is guaranteed.

For the **simulation** of ME sensors and sensor arrays in **A8** as well as the micromagnetomechanical simulations in **A10**, sufficient capacity is available on simulation computers including, in particular, the server with 256 GB RAM and 1 TB HDD purchased in the first funding period for SAW simulations. Additionally, particularly large simulations may be carried out in the Kiel University Computing Centre. For finite-element method (FEM) simulations, the software package COMSOL Multiphysics and FEAP (Finite Element Analysis Program, Berkeley, USA) are available. Matlab, Mathcad, and Mathematica are available for analytic calculations.

An **X-ray photoelectron spectroscopy system** (currently Omicron Full Lab, to be replaced by a Prevac Multichamber XPS system in December 2019) as well as several sputter deposition chambers constructed in-

house are operated by the Faupel group in their laboratories at the Institute for Materials Science. The laboratories also afford three small chambers for initiated chemical vapor phase deposition.

At the Institute of Materials Science, there is a fully equipped **cell culture laboratory** (GMO class: S2) available, including sterile benches, incubators, an autoclave, a spinning disc confocal microscope, and further phase contrast and fluorescence microscopes. In the biomaterials laboratory, chemistry hoods, a 3D bioprinter (CellInk+), as well as a microindentation machine and two atomic force microscopes are available for characterization.

At the Institute of Electrical Engineering and Information Technology, an integrated circuit design environment with high performance computing server, industry design software (Cadence IC design) and state-of-the-art IC design process design kits and fabrication possibilities (Europractice, MPW) are available. Computer servers, software structure and licensing agreements are in place to support the design and test of integrated electronic circuits (ASIC) and MEMS.

A further improvement is expected at the Faculty of Engineering as a remodelling of the campus is planned to take place between 2020 and 2023. This includes the construction of the “Innovation Center for Interconnected Sensor Systems”. Some PIs of the CRC (Bahr, Gerken, Höft, Rieger, Schmidt) will move into the new building with their groups. During construction, all existing laboratories remain operational such that the conduction of the CRC is not affected. The new Innovation Center will provide laboratory and office space for additional junior groups and spin-off companies. It has in total 1600 m² lab space.

The **Fraunhofer Institute for Silicon Technology** in Itzehoe offers access to its **MEMS cleanroom facility** (1000 m²) which started operation in 2015. The cleanroom is equipped with specific 200 mm wafer MEMS technology processing tools such as LPCVD, PECVD, epitaxy, ALD, sputtering of AlN, AlScN and PZT, spray coating, fluorine and chlorine RIE of Si, Si-compounds, and piezoelectric materials, CMP, XeF₂ and Si enriched TMAH release etch, wafer bonding, electroplating of Au, Cu, Sn, and In.

Within the Neurocenter of the UKSH Kiel, close collaborations exist between the Department of Neurology (deputy head: Prof. Walter Maetzler), the Department of Neurosurgery and the Department of Radiology and Neuroradiology Campus Kiel (head: Prof. Olav Jansen). The Department of Neurology has access to >10 500 outpatients and >3800 inpatients per year as well as a mobility lab including an optical movement tracking system and a split-belt (relevant to **T1** and **B9**). The large portfolio of cutting edge mobile health technology systems with unlimited access to raw data include Noraxon®, GaitUp®, Movisens®, McRoberts and Mobility-Lab®, enabling the in-house development and validation of mobility and non-motor algorithms (**B9**). **T1** runs an EGI-256 channel Electroencephalogram for movement related brain activation with sufficient computational power to analyze movement related potentials and source analysis. Modern Brain-lab software is available through the Department of Neurosurgery. The Department of Radiology and Neuroradiology provides special imaging facilities and expertise (scanning protocols relatively insensitive to artifacts) in imaging with magnetic resonance (MR) peripheral nerves and both pre- and postoperatively of patients subject to deep brain stimulation (given MR compatibility of the implanted device as per the manufacturer).

The Department of Neurology with its imaging and data analysis labs provides sufficient computational power to solve problems described in projects **B9** and **T1**. During the first funding period, this department was equipped with a number of modern **high-power computers** (10 – 20 high-speed Intel processors with 60 – 120 GB RAM and multiple GPU processors for parallel processing in each, as well as modern servers for data storage). The computers are linked within a network so that it is possible to use shared computational capacities. Moreover, if additional computational capacities are needed, the infrastructure of the Computational Center (Rechenzentrum) of Kiel University can be used.

The Department of Cardiology, Angiology and Intensive Care Medicine (**B10**) sees more than 10 000 outpatients and >600 inpatients per year and has developed a clinical trial infrastructure with dedicated clinical trial physicians and several study nurses (currently 6). The department has 4 modern cardiac catheterization laboratories, including an electrophysiology lab that is equipped with state of the art mapping technology (CARTO). Besides a year-long established cooperation with the Faculty of Engineering, in particular the group of Prof. Schmidt, close cooperations exist with the department of radiology and radiation therapy.

In project **T1**, simultaneous recordings of MEG (with new ME sensors) and EEG are planned. For that purpose, both the Department of Neurology is running **modern EEG systems**. During the first funding period an EEG system Electrical Geodesics EGI Co. with 128 and 256 EEG channels was successfully used. This and other systems (2 systems of Brain Products amplifiers BrainVision MR+ for 128 channel recordings) may be applied

for MEG-EEG recordings in the current CRC. Moreover, the Department of Neurology can provide a number of commercial and non-commercial software packages which are necessary for data processing within the projects **B9** and **T1** as well as **B7** (CURRY, BESA, BrainVision analyser, Brain Voyager, FieldTrip, FSL, Cartool, EEG Lab, Simbio, SPM).

1.4 Support structures

1.4.1 Early career support

Education and support of doctoral and postdoctoral researchers is an essential part of the CRC 1261. The Integrated Research Training Group (IRTG) was successfully established in the first funding period and a total of 30 early stage researchers have participated. It promotes scientific independence and interdisciplinary training of all early stage researchers within the CRC 1261. The IRTG includes four action areas: supervision, competence development, interdisciplinary exchange, and international experience. All doctoral researchers and their advisors sign a supervision agreement at the beginning, which lays out the individual rights and responsibilities of both parties. Furthermore, the planned research as well as the planned qualification measures are discussed with two thesis advisors and recorded in the research and qualification plan every six months. The IRTG contains a strong peer-teaching and peer-coaching component with a student-organized booster phase for all new IRTG members as well as mandatory biweekly student-only seminars. Furthermore, doctoral researchers organize annual summer school sessions corresponding to their needs and they also invite external speakers. All CRC members, including all early-stage members, have a retreat every six months for the interdisciplinary exchange. Additionally, an extensive training and qualification program with respect to technical as well as cross-curricular skills is offered. This includes lectures, competence workshops as well as contributions by invited external guests. The Graduate Center and other existing institutions at Kiel University already provide a large variety of courses and also offer extra courses tailored to the requests of the CRC. The fourth action area of the IRTG is the achievement of international excellence. A mandatory research stay abroad of up to three months as well as international conference participation is funded for all IRTG members. Particularly, the external research stays proved to be a very effective measure for advancing the knowledge and global networking of early career researchers. All activities within the IRTG are discussed in detail in the project **IRTG**. Bachelor and master students are involved in the CRC as student assistants as well as for performing their thesis research. Advanced students participate in IRTG and CRC events.

Another important aim of the CRC is to support designated young researchers by giving them the opportunity to participate in the CRC as a principal investigator. E.g., Andreas Bahr was integrated successfully into the CRC as junior professor. He finished his doctorate in 2017, joined the Institute of Electrical and Information Engineering the same year, and heads the research group of sensor system electronics. For the second funding period, Stephan Wulfinhoff is a new principal investigator. He got his doctoral degree in 2014 and was recently appointed as W2 professor of Computational Material Sciences. Fabian Lofink also finished his doctorate in 2014 and was already PI in the first funding period and continues as a PI in the second funding period. He is with the Fraunhofer ISIT. Florian Niekel is another young researcher from ISIT who joins the CRC as a new PI. Ann-Kristin Helmers is integrated into the CRC as PI of project T1. Carolin Enzingmüller is a new PI in project SOP. Overall, six of the 22 PIs are young researchers (less than 8 years after doctoral degree). We plan to recruit additional junior groups on the topic of ME sensors during the second funding period. These groups will benefit from the excellent research environment and will be included in the activities of the CRC.

Table 3 Contracts of researchers within the CRC 1261.

Project	Surname, first name	Type of funding	Topic	Duration
B2	Bald, Christin	Doctoral researcher	Multichannel Analysis for Magnetoelectric Sensor Systems	11/17-06/20
A2	Baytekin-Gerngroß, Melike	Doctoral researcher	Nanoscale Sculpturing of Metals for adhesion improvement of electrets.	11/16-12/16
B1	Durdaut, Phillip	Doctoral researcher	Analog Signal Processing and Frontends with Maximum Signal-to-Noise Ratio for Magnetoelectric Sensors in Biomedical Applications	07/16-06/20
B6	Elzenheimer, Eric	Doctoral researcher	Multimodal Mapping of Nerve Pathology with Magnetoelectric Sensors	07/16-06/20

SOP	Enzingmüller, Carolin	Postdoc	Design and evaluation of science outreach	09/16-06/20
B7	Friedrich, Ron-Marco	Doctoral researcher	Imaging of magnetically labelled cells	01/17-06/20
B3	Galka, Andreas	Senior researcher	Inverse solutions for localization of biomagnetic activity in heart and brain	08/16-12/18
A1	Golubeva, Elizaveta	Doctoral researcher	Investigation and methodological reduction of magnetically induced noise in magnetostrictive multilayers	08/19-06/20
B3	Habboush, Nawar	Doctoral researcher	Inverse Solutions for Localization of Biomagnetic Activity in Heart	08/16-06/18
B3	Habboush, Nawar	Doctoral researcher	Inverse Solutions for Localization of Biomagnetic Activity in Heart	07/18-08/18
B3	Habboush, Nawar	Doctoral researcher	Inverse Solutions for Localization of Biomagnetic Activity in Heart	01/19-06/20
B3	Hamid, Laith	Doctoral researcher	M/EEG source imaging via the spatiotemporal Kalman filter and its applications in epileptology	08/16-12/18
B3	Hamid, Laith	Postdoc	M/EEG source imaging via the spatiotemporal Kalman filter and its applications in epileptology	01/19-06/20
A7	Hayes, Patrick	Doctoral researcher	Electrically modulated magnetoelectric sensors	07/16-06/18
A7	Hayes, Patrick	Doctoral researcher	Electrically modulated magnetoelectric sensors	07/18-09/18
A7	Hayes, Patrick	Doctoral researcher	Electrically modulated magnetoelectric sensors	09/18-12/18*
A7	Hayes, Patrick	Doctoral researcher	Electrically modulated magnetoelectric sensors	10/19-12/19
A7	Hayes, Patrick	Doctoral researcher	Electrically modulated magnetoelectric sensors	12/19-06/20
A1	Holländer, Rasmus	Doctoral researcher	Dynamics of functional magnetic microstructures	06/18-12/18
A6	Hrkac, Stjepan	Doctoral researcher	Nanofokus-Röntgenstreuung an komplex magnetoelektrischen Mikrokompositen	08/16-09/16
A6	Hrkac, Stjepan	Doctoral researcher	Nanofokus-Röntgenstreuung an komplex magnetoelektrischen Mikrokompositen	10/16-10/16
A6	Hrkac, Stjepan	Doctoral researcher	Nanofokus-Röntgenstreuung an komplex magnetoelektrischen Mikrokompositen	11/16-12/16
A6	Jordt, Philipp	Doctoral researcher	In-situ study of microstructure in magnetoelectric and piezotronic materials	07/16-10/18
A6	Jordt, Philipp	Doctoral researcher	In-situ study of microstructure in magnetoelectric and piezotronic materials	10/18-06/20
A1	Jovicevic Klug, Matic	Doctoral researcher	Investigations of Magnetostrictive Multilayers for Magnetoelectric Sensors	07/16-06/19
A5	Kalu, Chima Obobi	Doctoral researcher	Impedance spectroscopy on piezotronic sensors	08/19-09/19*
A5	Kalu, Chima Obobi	Doctoral researcher	Impedance spectroscopy on piezotronic sensors	09/19-12/19*
A2	Kaps, Sören	Postdoc	Basics of polymer-metal-magnetic composites	09/16-06/17
A6	Kamp, Marius	Doctoral researcher	Test measurements for evaluation of a novel approach of X-ray spectroscopy with sub-nm resolution	07/19-06/20
Z1	Kirchhof, Christine	Postdoc	Resonante magnetoelektrische Sensoren zur Detektion niederfrequenter Magnetfelder	07/16-06/20
A3	Kittmann, Anne	Doctoral researcher	Resonant Magnetoelectric Sensors	07/16-06/20
A8	Krantz, Matthias	Senior researcher	Modelling of Magnetoelectric Sensors	07/16-06/20
B7	Lukat, Nils	Doctoral researcher	3D-imaging of magnetically labelled Cells	07/16-06/19

B7	Lukat, Nils	Doctoral researcher	3D-imaging of magnetically labelled Cells	07/19-06/20
A1	Müller, Cai	Doctoral researcher	Magnetic domains in functional magnetic films	01/18-12/18
A1	Müller, Cai	Doctoral researcher	Magnetic domains in functional magnetic films	08/19-11/19
Z1	Niekiel, Florian	Postdoc	Resonant Magnetoelectric Sensors	03/17-06/20
B2	Reermann, Jens	Doctoral researcher	Signal Processing for Magnetoelectric Sensor Systems	07/16-09/17
A1	Röbisch, Volker	Doctoral researcher	Magnetoelectric Sensors with Exchange Bias	07/16-06/17
A1	Röbisch, Volker	Doctoral researcher	Magnetoelectric Sensors with Exchange Bias	07/17-09/17
A3	Schell, Viktor	Doctoral researcher	Surface Acoustic Wave Magnetic Field Sensors	08/18-12/18
A3	Schell, Viktor	Doctoral researcher	Surface Acoustic Wave Magnetic Field Sensors	10/19-06/20
A8	Schmalz, Julius	Doctoral researcher	Analyse und Optimierung von Elektrodenstrukturen für Magnetfeldsensoren zur Erhöhung der Sensitivität	07/16-01/18
A8	Schmalz, Julius	Doctoral researcher	Analyse und Optimierung von Elektrodenstrukturen für Magnetfeldsensoren zur Erhöhung der Sensitivität	02/18-01/19
A8	Schmalz, Julius	Doctoral researcher	Analyse und Optimierung von Elektrodenstrukturen für Magnetfeldsensoren zur Erhöhung der Sensitivität	02/19-06/20
A2	Schröder, Stefan	Doctoral researcher	Initiated chemical vapor deposition of polytetrafluoroethylene for magnetic field sensors	07/16-06/18
A2	Schröder, Stefan	Doctoral researcher	Initiated chemical vapor deposition of polytetrafluoroethylene for magnetic field sensors	07/18-06/19
A2	Schröder, Stefan	Doctoral researcher	Initiated chemical vapor deposition of polytetrafluoroethylene for magnetic field sensors	07/19-06/20
A5	Schütt, Fabian	Doctoral researcher	Highly porous 3D interconnected Networks from low-D materials	07/16-06/17
A5	Schütt, Fabian	Doctoral researcher	Highly porous 3D interconnected Networks from low-D materials	07/17-09/17
A2	Schweichel, Marleen	Doctoral researcher	Development and characterization of mechanically soft magnetostrictive composite materials for hybrid magnetoelectric sensors	07/17-12/17
A2	Schweichel, Marleen	Doctoral researcher	Development and characterization of mechanically soft magnetostrictive composite materials for hybrid magnetoelectric sensors	01/18-06/20
A4	Spetzler, Benjamin	Doctoral researcher	ΔE -effect Sensors	07/19-06/20
A5	Stölting, Mona	Doctoral researcher	Development and Characterization of piezotronic magnetoelectric composites	07/17-06/20
A6	Strobel, Julian	Doctoral researcher	Transmission Electron Microscopy on amorphous thin films	07/18-10/18
A4	Strunskus, Thomas	Senior researcher	ΔE -effect sensors	07/16-06/20
A3	Su, Jingxiang	Doctoral researcher	Resonant Magnetoelectric Sensors	04/18-06/20
Z2	Teplyuk, Oleksandr	Senior researcher	Magnetoelectric Sensor Characterization	07/16-06/20
A1	Thormählen, Lars	Doctoral researcher	Fabrication and development of magnetostrictiv multilayers for magnet field sensors	10/17-06/20
B1	Toxvaerd, Sebastian	Doctoral researcher	Noise Analysis and Analogue Signal Processing for Magnetoelectric Sensors in Biomedical Applications	07/16-01/19
B1	Toxvaerd, Sebastian	Doctoral researcher	Noise Analysis and Analogue Signal Processing for Magnetoelectric Sensors in Biomedical Applications	01/19-01/20
B7	Wagner, Jan-Martin	Senior researcher	Solution of inverse problem	08/16-12/16

A4	Wiegand, Patrick	Doctoral researcher	Integrated Circuits for Biomedical Signal Acquisition and Processing	11/18-06/20
A6	Wolff, Niklas	Doctoral researcher	Defect structures and deformation characteristics of magnetoelectric and piezotronic sensor components for biomagnetic field sensing application	07/16-06/18
A6	Wolff, Niklas	Doctoral researcher	Defect structures and deformation characteristics of magnetoelectric and piezotronic sensor components for biomagnetic field sensing application	07/18-06/19
A6	Wolff, Niklas	Doctoral researcher	Defect structures and deformation characteristics of magnetoelectric and piezotronic sensor components for biomagnetic field sensing application	07/19-06/20
B1	Wolfram, Henrik	Doctoral researcher	Noise Analysis and Analogue Signal Processing for Magnetoelectric Sensors in Biomedical Applications	06/19-01/20
B1	Wolfram, Henrik	Doctoral researcher	Noise Analysis and Analogue Signal Processing for Magnetoelectric Sensors in Biomedical Applications	01/20-06/20
B5	Yalaz, Mevlüt	Doctoral researcher	Individualized Deep Brain Stimulation	12/16-06/20
Z1	Yarar, Erdem	Postdoc	Inverse-Bilayer AlN/(Fe ₉₀ Co ₁₀) ₇₈ Si ₁₂ B ₁₀ Magnetoelectric Composites	06/18-07/18*
Z1	Yarar, Erdem	Postdoc	Inverse-Bilayer AlN/(Fe ₉₀ Co ₁₀) ₇₈ Si ₁₂ B ₁₀ Magnetoelectric Composites	07/18-03/19*

* pregnancy representation

Table 4: Durations of contracts in the CRC 1261

Duration of contract	Number of contracts for doctoral researchers		Number of contracts for postdoctoral researchers		Number of researchers in total
	male	female	male	female	
up to 12 months	30	3	4	0	24
up to 24 months	8	0	0	0	7
up to 36 months	5	3	0	0	8
up to 48 months	5	2	3	0	10

Most of the very short contracts were related to pregnancy representation.

1.4.2 Gender equality and family-friendly measures

Gender equality

Equal opportunity of women and men is a strategic goal at Kiel University and its promotion forms part of the University's mission. Kiel University is an equal opportunity employer with very strong and committed interest in affirmative actions to promote female scientists. Kiel University has a comprehensive gender equality program and, although not yet at its goal of parity in appointments at all levels in the University, has made considerable headway in recent years. One Vice President of the University Board is responsible for diversity including gender equality. Detailed gender equality goals have been negotiated between Kiel University and the State Government (2013), and subsequently, gender equality indicators have been included in the allocation of funds for (since 2014) and within (from 2015 onwards) the University. A major aim in the concept of equal opportunities of the University is a significant increase of female professorships and women in leading scientific positions. In order to achieve this important goal, the University allocates funds and carries out a variety of measures at different career levels. In addition, Kiel University Clusters of Excellence funded within the excellence initiative since 2006 have been particularly efficient at attracting highly qualified female scientists to Kiel. Kiel University was successful in all rounds of the Program for Women Professors I (2008), II (2013) and III (2018) with the approved maximum funding of three professorships for women in round I and II. Funding for two professorships in the third round of the program has been approved in 2019. Several of our measures have been included into the toolbox for the DFG's Research-Oriented Standards on Gender Equality. The initial statement (2009), the interim report (2011) and the final report (2013) of Kiel University on the Research-Oriented Standards on Gender Equality were all ranked with the second best mark of stage 3 attesting that the University has a convincing overall concept that is for the most part already implemented. A new *GenderConsulting service* in particular for collaborative research projects started in June 2019.

Kiel University actively promotes a research environment free of gender bias. The support of female scientists is viewed as a central task and as an integral part of the University profile. Measures included in the gender equality concept of the Graduate Center support female doctoral researchers. Since 2010, *via.mento*, a mentoring program for female postdoctoral researchers from all faculties and disciplines has been established at Kiel University. Up to 18 female postdoctoral researchers can take part in each round of the program which became a permanent measure from 2017 onwards. For female junior professors, Kiel University has launched a special, tailor-made support program in 2014. On the University level, seed-money is offered for female post-docs and junior professors to support their research, an interdisciplinary science network enables exchange and cooperation between postdoctoral female scientists, and gender-fair regulations are applied during the appointment procedure of professors at Kiel University. Guidelines will also be developed for open, gender-fair, transparent, and merit-based recruitment for all research personnel at Kiel University. Furthermore, gender training is offered to members of recruitment commissions, the use of gender sensitive language is promoted in all documents, and several workshops on the integration of gender aspects into teaching are offered.

Family-friendly university and campus

Family friendliness for students and staff is a central issue in University politics. Kiel University was certified with the “*audit familiengerechte Hochschule*” by the *berufundfamilie GmbH* as nationwide first comprehensive university in 2002. The process to receive the certificate for the sixth time started in October 2019. At Kiel University, family orientation has reached a high level, is implemented throughout the University structures, and is well used by students and staff. Kiel University is the ambassador of Schleswig-Holstein for the company network “*Standortfaktor Familienfreundlichkeit*”. Kiel University has established crib-places and day care centers directly on campus in the past years and holds places in co-operating facilities near the campus. Currently, 135 spaces for children aged 0 to 3 (five places exclusively for children of staff of the Faculty of Engineering at day care close to the faculty’s campus) are provided and 177 spaces for children aged 3 to 6. Additionally, flexible childcare is organized by the office for family services also during congresses, seminars, or meetings held in or near Kiel. During most school holidays, schoolchildren of employees can take part in a holiday-program (30 places). The family-friendly campus at Kiel University includes parent-child workrooms, mobile toy boxes, baby changing-rooms, a playground, and facilities for children in the canteens.

The office for family services at Kiel University, existing since 2007, supports and advises scientists and students in the compatibility of family and career/studies. This includes specific matters such as childcare, parental leave, work-contract situations and financial aspects. It coordinates and implements new family-friendly measures in cooperation with the governing board, the commissioners for family affairs at each faculty (Prof. Christine Selhuber-Unkel has held this position at the Faculty of Engineering since May 2015), the Equal Opportunities Commissioner and student representatives.

First funding period: Implemented CRC-specific measures to promote gender equality

In addition to the above listed strategies of Kiel University, the CRC has organized and implemented its own measures and activities adapted to its needs. Since April 2017, Tina Kerby (RTG 2154 “Materials for Brain” manager) is jointly coordinating the gender equality activities of the CRC 1261 and RTG 2154, supported by Julia Jedtberg (IRTG 1261 manager). Due to the thematic overlap of the CRC and RTG, similar demands exist for the involved scientists regarding gender equality. Therefore, the activities have been merged and were offered to the members of both DFG-projects. This not only increased the group size and the dynamic and mutual exchange within and between the groups, but also improved the synergetic effect of the measures offered.

The demands and needs for gender equality measures are changing between school and university level as well as in the various stages of career and life. With consideration of these different levels and stages, the gender equality measures and activities of the CRC can be divided into three categories:

- (1) Individual support (e.g. soft-skills workshops, coaching, child care)
- (2) General activities and measures at group level up to events for all CRC members (e.g. gender equality meetings, networking events, talks, mini-workshops)
- (3) Events and measures aiming to sustainably increase the number of women in science and in the CRC by approaching and motivating female pupils, bachelor and master students (e.g. Girl’s Day, aid in career planning of students, introduction to scientific work).

However, for the organized measures, a clear distinction between the three categories is not always possible. The overall objective is to support families and to increase the proportion of women in science on a long-term and sustainable basis, which in the end is reflected in a synergetic effect of all three categories.

Individual support mainly referred to measures promoting the personal development of female CRC members as well as the support of pregnant members and child care recipients:

- Student assistants: support for a post-doc and doctoral researcher during pregnancy.
- Child care: provision of child care to enable the participation of parents at meetings, retreats, and summer schools.
- Motive analysis tool *Profile Dynamics*[®]: analysis revealing individual patterns, motives, needs, and talents.
- Workshop “*Career strategies accompanying the doctorate: building potential – tapping professional pathways*”: support for female doctoral researchers in strategically planning their future career.
- Workshop “*Sicheres Auftreten*”: improvement of self-perception, voice, speech, and strengthening of confidence.
- Leadership coaching: specific coaching for a female professor regarding negotiations on executive leadership level.

Various events were addressed to all CRC members and/or involved smaller groups. On a regular quarterly basis, CRC members met for gender equality meetings to receive feedback and discuss ideas for future activities. Further, the CRC invited internal and external guests to give talks, seminars, and mini-workshops:

- Workshop “*Gleichstellungsmaßnahmen - was hilft wirklich?*”: ideas and discussions for new gender equality measures.
- Seminar “*Möglichkeiten und Unterstützung bei Schwangerschaft während der Doktorarbeit und in der Elternzeit*”: support possibilities of Kiel University in case of pregnancy and parental leave.
- Seminar “*Experiences, challenges, and strategies on my career path*”: introduction and discussion of female CRC project leaders personal career path experiences.
- CRC & RTG organized workshop “*Women in Science and Engineering Breakfast*” taking place at the 4th Euro Intelligent Materials 2019, Kiel: outstanding female scientists shared their experiences on various family and career topics.
- Talk and workshop “*Bedürfnisse, Wünsche, Kompetenzen – (M)Ein Weg nach der Promotion!*”: needs, wishes, and getting to know one’s own competences on the way to a doctorate and beyond.
- Seminar “*Unconscious bias*”: identifying unconscious thinking patterns and stereotypes and sensitizing for this issue.

The CRC implemented various activities and measures to support the long-term aim of a sustainable increase in the number of women in science. The CRC offered the following activities to pupils as well as students to get young women interested in its research areas, to inform them about their options and opportunities in these fields, and to motivate and support them in their career decision:

- *Girls’ Days* projects “*Materialwissenschaften - wie aus Sand ein Handy wird*” and “*Mikroskopie: die faszinierende Mikrowelt im großen Maßstab*”: female pupils had the opportunity to perform scientific experiments and gained insight into laboratories.
- *Physik Projekt Tage*: the four-day-workshop in collaboration with the Department of Physics (Kiel University) was selected as a model case in the DFG Toolbox (now Center of Excellence Women and Science - CEWS). Female pupils worked on elaborate projects such as “*Magnetfeldsensoren in der Medizin*”.
- Seminar “*Promotion – ja oder nein?*”: support and motivation for bachelor and master students in their decision-making process regarding their future career.
- Student assistant positions: outstanding female master students were specifically introduced to research and science. The concept includes (1) career counselling and mentoring by CRC project leaders, (2) accompanying tandem formation (student + female doctoral researcher as a mentor).
- Conference participation: female master student assistants were given the opportunity to attend a conference to promote their personal and professional development. Each student was accompanied by a mentor who acted as a support and contact person and introduced the student to his/her network.

Second funding period: Planned CRC-specific measures to promote gender equality

To further support gender equality in the second funding period, the CRC will continue with the successful measures of the first funding period, and will further extend the concept of promotion at different levels and stages with various measures. In the first funding period, on the project leader level, a female share of 19% was achieved which will increase to 26% in the second funding period (Table 1). On the doctoral researcher’s level, the CRC aimed for a female share of 25% in the first funding period, which was met by 26%. On the post-doc level, 1 of 6 positions (17%) were filled by a female post-doc (Table 2). Following the “cascade” model, the CRC aims at a target proportion of women at each career level at least equal to the proportion of women at the next lower level. Given the large number of positions in the engineering disciplines of the CRC, and the comparatively low proportion of female students in these disciplines (14% to 25%), the CRC ambitiously targets for the second funding period a female share of 25% for both doctoral students and post-doc researchers.

In the second funding period, the coordination of gender equality measures will remain with Tina Kerby (RTG 2154 manager), supported by Julia Jedtberg (IRTG 1261 manager). To further improve the organizational and structural standard and to better meet the members' needs, a gender equality consortium will be established to involve the different groups (males and females, doctoral researchers up to professor, CRC and RTG) more closely. The consortium will consist of one CRC and one RTG member each from the areas management, project leaders, and doctoral researchers. Of the six members, at least one must be male. The consortium will meet quarterly to discuss, plan, and organize activities.

Individual support will be continued as described above and will also be extended by measures such as voice training, application training, and individual coaching. The needs will be queried via surveys, and measures will be organized accordingly. Besides the existing support (student assistants, Kiel University child care) for parents and new mothers, the CRC will extend the support to facilitate their return to research. This concerns, e.g., a stronger support for working in a home office or attending conferences. In the latter case, family members who take over child care during the conference, receive funding for their travel expenses. To further support female researchers in their scientific career, the CRC and RTG have established a "*Mentoring for Women*" program for their female doctoral researchers. The program aims to support the doctoral researchers' career planning, promotion of personal competences, building and integrating a network, and the exchange of experience and knowledge in the individual mentoring relationship. The doctoral researchers receive financial travel support to visit their mentors. In the future, project leaders will proactively promote this program. This also applies to the Kiel University mentoring program *via:mento* for CRC post-docs.

To reach more members regarding gender equality topics, the CRC will integrate talks, mini-workshops, or seminars in future retreats. In this way, the talks and seminars of invited experts will reach most of the members. Furthermore, throughout the year experts dealing with gender topics specifically will be invited for talks and seminars (e.g. glass ceiling, gender bias-free recruiting) to increase general awareness for gender equality. As female scientists also serve as a role model for an academic career, the CRC will prioritize the invitation of female colloquia speakers. In addition, the speakers will give a seminar dealing with career or family related topics.

There is great potential for increasing the proportion of women in the natural sciences among pupils and students. The CRC will continue its participation in the Girls' Days with at least one project offered per year. This also applies to the collaboration with the Physics Department and prospective *Physik-Projekt-Tage*. The support of outstanding and highly motivated female master students will be carried on and installed as a structured *Career Mentoring Program*. The program includes a student assistant job accompanied with individual mentoring. Candidates will be selected upon their letter of motivation, degree certificate, and reference from a professor. The *Career Mentoring Program* consists of:

- Individual coaching: via individual analysis and coaching the student gets to know about her behavioral patterns, needs, talents, and how to best develop her potential.
- Career mentoring and counselling by a female CRC project leader: support via individual sessions, advice regarding studies, career, and personal support options.
- Participation at CRC retreats: getting insight into the CRC-projects and opportunity to network with doctoral researchers and project leaders.
- Participation at a conference: the student accompanies a project leader to a conference, someone who will act as a mentor and will support the student in establishing contacts and networks.

By integrating female students into a structured framework at such an early stage and supporting them in their personal and professional development, the chances that they will remain in science increase. Furthermore, since the student assistant job involves a bonding to the CRC, chances increase that these students will remain in this research field and apply for a doctoral position at the CRC.

Table 5: Female share of project leaders during the first funding period and for the second funding period.

Position	1 st Funding Period				2 nd Funding Period	
	Proportion of women [%] According to proposal for 1 st funding period	Current number of men / women Reference date: proposal for 2 nd funding period		Current proportion of women [%] Status Quo Reference date: proposal for 2 nd funding period	Number of men / women	
		m	w		m	w

Postdoctoral researchers	0	2	0	0	1	1	50
Research group leaders, junior research group leaders, junior professors	33	2	1	33	3	2	40
Professors C3/W2	25	3	1	25	5	1	17
Professors C4/W3	17	9	2	18	8	2	20
Total	19	16	4	20	17	6	26

Table 6: Female share of doctoral and postdoctoral researchers during the first funding period and targeted portion of women for the second funding period.

	1 st Funding Period				2 nd Funding Period
	Targeted proportion of women [%] According to proposal for 1 st funding period	Current number of men / women Reference date: proposal for 2 nd funding period		Current proportion of women [%] Status Quo Reference date: proposal for 2 nd funding period	Targeted proportion of women [%]
		m	w		
Doctoral researchers	25	17	6	26	25
Postdoctoral researchers	25	5	1	17	25

1.4.3 Management of research data and knowledge

This data management plan acts as a CRC guideline for all principle investigators (PIs). Exceptions may be made due to legal, ethical, copyright, or other reasons.

1.4.3.1 Data collection and documentation

Data definition

This project will generate and work with the following data types:

- 1) experimental data (e.g., measurement, quantification, or pseudonymised medical data)
- 2) fabrication data (sensor and sample fabrication)
- 3) simulation data (code, results)
- 4) personal medical data

The data will be stored in digital form, either in the format in which it was originally generated or in a compressed form. If originally recorded on paper, the data will be converted into a digital form via scanning (file format: tiff or jpeg). Measurements and quantification of the images will be recorded in spreadsheet files. The data is expected to reach 45TB over the course of the CRC.

A special role is taken by sensitive and personal medical data (as explained below) which is expected to reach 10TB over the course of the project.

Data collection and generation

After generation, experimental, fabrication and simulation data (data types 1, 2, and 3) will first be stored on laptops and/or desktop PCs of the individual project members and on collaborative storage devices of the contributing working groups/institutes. All files will be collected in data type-dependent folder structures. For data types 1, 2, and 3, each directory will contain an info.txt file documenting the data generation process (e.g.

the experimental protocol used in a certain experiment). Experimental data will be collected along with a written procedure recorded in an electronic laboratory notebook. Any deviations from the protocol and other useful contextual information will also be recorded. This should allow the data to be understood by other CRC-members and add contextual value to the dataset, should it be reused in the future. Each dataset will be accompanied by a readme.txt file which will describe the directory hierarchy. A common naming convention based on the following norms will be adopted for the structure of folders and file names used to organize the data:

- ISO 8601 format for date and time information: YYYYMMDDThhmmss±hhmm or YYYYMMDD
- semantic versioning scheme (Major.Minor.Patch), e.g., 2.0.0
- unified file names: Project_Experiment_Scientist_20180523T134241+0100_1.0.0.csv

In the case of nanoanalytical data a unique file name and documentation system is well established, where unique sample and specimen IDs are used for data identification including further information of the instrumentation, technique and possible specimen modifications (e.g. ID1000_01h_Instrument_Method_count). The compatibility with the ISO 8601 standard is possible by this nomenclature. For type 3 data (simulation code), the Git code revision management system will be employed. Sensitive personal and experimental medical data (data type 4) will be recorded using pen and paper versions of questionnaires and clinical tests as well as using detection systems as described in detail in the individual project descriptions (**T1**, **B9**, **B10**). This data will be stored pseudonymously in the REDCap database of the Department of Neurology. Experimental medical data will be collected in analogy to data types 1, 2, and 3 but stored pseudonymously on REDCap. Within T1, only limited data will be collected and stored on hard discs.

For **B10** (cardiology), a certified clinical trial unit is in place, which follows several standard operating procedures regarding patient data storage and protection. Moreover, the department of Cardiology and its use case “heart failure” is part of the BMBF-funded HighMed consortium, which aims at standardizing clinical data (pseudonymized) in order to make them available for scientific exploitation.

Documentation and Metadata

Experimental, simulation-based and fabrication data (data types 1, 2, and 3) will be accompanied by contextual documentation according to DFG best practice principles. In particular, these include spreadsheets documenting preparation conditions and text files which detail the experimental, simulation, and sample characterization procedures. Files and folders will be named as given in the previous section, which includes for each dataset identifications to the researcher, the date, the study, and the type of data as metadata. The final dataset, as deposited in the chosen data repository, will also be accompanied by a readme.txt file listing all files and folders comprising a certain data set, outlining the file-naming convention used and explaining how the files relate to each other, what format they are in, or whether particular files are intended to replace other files.

Two types of metadata will be considered within the frame of the CRC, corresponding to the project publications and to the published research data. Metadata will form a subset of data documentation that will explain the subject, creator, origin and description of a data collection. Furthermore, the metadata will contain information on the resource type (e.g. image, audio), data formats, time reference, access conditions, and terms of use.

1.4.3.2 Ethics, legal and security issues

Ethical issues – addressing and handling

For experimental, simulation-based and fabrication data (data types 1, 2, and 3), no ethical issues are expected. Sensitive experimental medical data (data type 4) will be pseudonymized. The correspondence table for sensitive / personal and experimental data will be encrypted, stored at the respective study centers of the University hospital and access will be restricted to the PIs and key personnel for the specific project (e.g. doctoral researcher working on the project).

B9, **B10** and **T1** will include research on human participants. The dataset will consist of approximately 80 patients over the course of the CRC for **B6** and up to 30 patients for **T1**. The necessary ethical authorization for this project has already been obtained or are submitted from the ethics committee of the medical faculty at Kiel University (number D438/18). For **B10**, approx. 60 patients will be included and an ethics permission will be sought as well. Only data from participants that have given written informed consent prior to participation in the study will be recorded. Participants are informed that they can refuse participation or drop out of the study at any time without any consequences for the participant.

Data access and security

All research data and otherwise relevant data of the CRC will remain private within the CRC until published with agreement of the relevant PIs. All published papers, presentation slides, and posters containing data types 1, 2, and 3 are shared through the SAMBA file share at the Kiel University Computing Centre. Additionally pseudonymization of data type 4 will be performed using an encrypted, locally-stored correspondence table. Access to this table is restricted to the PIs and key personnel (e.g. doctoral researcher working on the project). This data will be stored in the REDCap database of the Department of Neurology. The data is only seen and processed by REDCap users from the Department of Neurology that are specifically authorized to access this project (i.e. PIs, study nurses, and students working on this project).

Copyright and intellectual property rights

The PIs for each project as the “owner” of the data shall decide what happens with the data in accordance with the DFG code of good scientific practice and the guideline on research data management of Kiel University. Experimental, fabrication, and other derived data will be published with an Open Data Common Attribute digital identifier (ODC-BY 1.0). Simulation data will be shared under the GPL v3 GNU General Public license. The written software will be owned by the PIs and the individuals creating it. In general, experimental, fabrication, medical, and other data is owned by the individuals creating the data.

1.4.3.3 Data storage & preservation**Storage & Backup during research**

Storage and backup of data types 1, 2, and 3 will be done on laptops and/or desktop PCs of the individual project members and on backup shares located at the CAU Computation Centre (except for data related to ethics issues, see previous section). The PIs of the projects will be responsible for the storage and backup of data. Backups shall be done on a daily basis via rsync-based backup scripts (e.g. duplicity on UNIX-systems and DeltaCopy on Microsoft Windows Systems) that are set up to run on every weekday. The files shall be synced to personal SAMBA shares located at the University Computing Centre of Kiel University using an encrypted connection. As mentioned above, sensitive and personal medical data will be stored in a pseudonymized fashion at the Department of Neurology and entered into REDCap (established and EU GDPR compliant database for clinical research).

Data preservation plan

As a general guideline, quality assured data which is the foundation of research findings in this CRC, will be stored for at least 10 years. Extensions and exceptions from this guideline can be made by the PIs of the individual projects. Reasons for these might be, but are not limited to:

- Reusability of the data: quality of metadata, integrity and accessibility of data, license allowing reuse, readability of data (chosen file formats)
- Value of the data: indispensable data, completeness of the data or data set, uniqueness, possibility to reproduce the data in the same conditions and at what cost, interest of the data, potential of reuse
- Ethical and sensibility considerations

The data selection is related mainly to the long-term value of the data and its potential value for re-use. Data preservation does not necessarily mean publication (e.g. personal sensitive data may be preserved but never published), but publication means generally preservation.

1.4.3.4 Data sharing and reuse**Sharing**

Evaluated research data are published in renowned research journals with supplementary material to make the results available for the public long-term. In general, the CRC's data sharing policy aims to publish data being relevant for the research community on general open repositories (e.g. Zenodo, Dryad, Figshare) respecting the FAIR principles (findable, accessible, interoperable, re-usable) based on the following guidelines. Quality assured experimental, fabrication and simulation data (data types 1, 2, and 3 as well as other derived data), which is the foundation of the research findings made in this CRC, should be published under the Open Data Commons Attribution License after a moratorium of 6 months, preferably on Zenodo. Original simulation codes will be published on GitHub. Experimental medical data of B9 will follow the rules as described above for experimental data (data type 1). Sensitive and personal medical data will not be shared with any collaboration partner, neither within nor without the CRC.

In general, repositories maintained by non-profit organizations are preferred. Possible exceptions include the intent to ensure the visibility of research results if comparable data is usually published on a well-established

but commercial digital repository. This includes data related to experimental and simulation results. On the experimental side, it is planned to publish extensive documentations including, e.g., specimen composition and dimensions, process conditions including possible heat treatments as well as the experimental conditions and relevant raw measurement data. On the simulation side, the researchers shall not only publish the relevant simulation results but also the related source code and input files necessary to reproduce the data. Data sharing on open repositories is planned to be usually initiated at the time of publication of the respective scientific output. Exceptions might be made due to legal, ethical, copyright, confidentiality, or other clauses.

Limitations to protect sensitive data

Experimental, simulation, fabrication, and related derived data must not be published if sensitive data is to be protected. Sensitive and personal medical data will never be shared. The same applies to the pseudonymised experimental data where appropriate.

1.4.4 Knowledge transfer and public relations

Kiel University provides several well-established structures for public outreach into different fields of societal impact, which includes education. Public Outreach is a common rationale of all leading research areas at Kiel University. The Clusters of Excellence as well as the Collaborative Research Centres have developed and implemented different structures and forms of outreach programs and activities, such as print and digital media products, exhibitions, lab activities, school programs, the Kiel Children University, meetings and conferences, and regular press releases. One of Kiel University's Vice President's responsibilities focuses explicitly on public outreach connected to teacher education and higher education. This leading focus aims to strengthen and to sustainably establish the rationale of public outreach as an integrated component of research and education at Kiel University.

The University Office for Press, Communication and Marketing Services supports researchers through different means and advice. Press releases are regularly written and submitted in cooperation between the researchers and the press office. Recipients are the local press for regional information and political support, as well as national and international channels. Additionally, the press office regularly issues a University newspaper (4 times per year, number of copies: 110,000) that is published along with the local newspaper *Kieler Nachrichten*. It features research projects, international guest scientists, conferences, public lectures, and much more. Furthermore, project websites are supported by the press office. As social media channels (Facebook, Twitter, Flickr, blogs) continue to grow in importance when it comes to directly communicating with stakeholders (the public, students, sponsors, partners) and to enhancing news and stories (research results, people, events, etc.) with photos, videos, charts and graphics, the press office continually works on broadening its online presence. Based on a well-grounded concept, Kiel University's online activities so far have resulted in ever-growing public outreach. In addition, there are several public events such as the „Night of the Profs“ and „kieler uni live“ (presentation during Kiel Week, the world's biggest sailing event with three million visitors each year) each attracting up to 10,000 visitors every time with lectures, exhibitions, science slams, and more public activities. These offer platforms for researchers who want to put across their scientific interests to the public. The office also supports conferences and other public and/or scientific events both during the organizing and marketing process and with press releases before and after the event. Current examples are the exhibitions for the 350th anniversary of the University, showing outstanding researchers and outcomes from past and present programs such as medicine and nano science and technology (<http://www.cau350.uni-kiel.de/en/exhibitions/>). In the press office, two science communicators work who are in charge of research foci of Kiel University. One is solely responsible for increasing public visibility of Kiel Nano, Surface and Interface Science (KiNSIS). The CRC 1261 will have access and can make use of the public outreach instruments that were especially designed for this institution. Networks with industry, such as the job fair „contacts“, provide another foundation for exchange between the University, its students, and researchers and societal infrastructures.

With regard to education, Kiel University has set up a lab environment for students of all age groups named „Kieler Forschungswerkstatt KiFo“ (Kiel Research Workshop). The Kieler Forschungswerkstatt offers programs for different research areas such as ocean science, nano science and technology, or energy. School students visit the labs as whole classes (focus on stimulating interest for STEM (Science-Technology-Engineering-Mathematics) fields) or in special voluntary programs (focus on fostering interests and talents). Teacher education programs, both pre- and in-service are additionally implemented. Both areas are accompanied by research provided by the close link and cooperation between Kiel University and the IPN, the Leibniz Institute for Science and Mathematics Education, which has led to the establishment of the *Kiel Science Outreach Campus KiSOC* in 2016. The KiSOC and the KiFo now form an environment that forms systemic links between scientists and science educators and communicators that leads to co-designed and an empirically tested outreach environment. KiSOC and KiFo also provide several regional, national, and

international networks for the distribution of Kiel University's research programs and activities. The network of student research centers in Schleswig-Holstein offers talented students environments to explore and get in touch with outstanding scientific projects at Kiel University. The EU-Interreg funded project PANaMa (prospects on the labor market with science and mathematics) develops teaching units and enrichment environments at interfaces between science, industry, and society and involves different areas of the CRC sciences.

1.5 Other sources of third-party funding for project leaders

All projects, which are in operation at least until July 2020 or which are proposed, are listed.

Project leaders	Project	Project title	Funding period	Funding agency
Adelung	A2, A5	PorSSi - Entwicklung und Charakterisierung von großflächigen, porösen Si-Film-Anoden für Lithium-Schwefel-Silizium-Energiespeicher	09/17 – 08/20	BMBF 03XP0126B
Adelung Faupel	A2, A4, A5, B7	Forscherguppe: Memristive Bauelemente für neuronale Systeme (FOR 2093), TP A2 "Memristive und memsensorische Bauteile für Filament-freie niedrig verknüpfte CNT Netzwerke"	01/18 – 12/20	DFG AD 183/12-2 FA 234/24-2
Adelung	A2, A5	Prevon – CleaNet „Entwicklung und Charakterisierung eines Fouling-Release-Beschichtungsmaterials für Aquakulturnetze	04/19 – 03/21	BMWi VDI VDE IT 16KN078723
Adelung	A2, A5	Funktionale intrinsische Hybridverbunde mit aktiven Elementen und strukturierten Metalloberflächen	08/18 – 07/21	DFG AD 183/23-1
Adelung	A2, A5	Hochporöse 3-dimensionale Kohlenstoff-Aeromaterialien für energieeffiziente, ultraschnelle und selektive Gassensoren	08/19 – 07/21	DFG AD 183/27-1
Adelung	A2, A5	Smart Mat & Surf - Print4Sense "Additive 3D-Fertigungsverfahren für die chemische Sensorik"	03/19 – 08/21	BMWi VDI VDE IT 16KN062028
Adelung	A2, A5	NanoKomp - Gedruckte Schraubenkompressoren aus nanostrukturierten Mikropartikeln im Komposit; Prozessentwicklung und -optimierung zur Strukturierung von Al-Legierungs-Mikropartikeln sowie Konzeption, Konstruktion und Anlagenbau zur Strukturierung von Al/Al-Legierungs-Mikropartikeln	05/19 – 11/21	BMWi AiF Projekt GmbH ZF4463403WO9
Adelung	A2, A5	Promotionsstipendium Theseen Riaz	10/18 – 10/20	DAAD 91686407
Adelung	A2, A5	EU Graphene Core 2 Aerographene in WP13	04/18 – 03/20	EU 785219
Deuschl	T1	Earlystim follow-up study	2013-2020	Medtronic (Earlier BMBF, clinical study program)
Faupel,	A2, A4, B7	In-situ investigations of condensation, nucleation and growth of metal films and nanostructures on organic surfaces during sputter deposition	12/16 - 12/20	DFG FA 234/23-2
Faupel	A2, A4, B7	In-situ-Analyse plasmainduzierter Materialmodifikationen an Nanopartikeln für funktionelle Anwendungen	05/19 - 05/22	DFG PO 2299/1-1
Faupel,	A2, A4,B7	Ultradünne breitbandige solare Absorber für den UV- und UV-NIR-Bereich basierend auf einem skalierbaren plasmonischen Metamaterial	06/19 - 06/22	DFG FA 234/32-1

Faupel, Adelung	A2, A4, A5, B7	Materials for Brain (M4B): Dünnschichtbasierte Funktionsmaterialien für die minimal-invasive Therapie von Erkrankungen des Gehirns TP P4: Kontrolle der Wirkstofffreisetzung durch Barrierschichten TP P5: Sensor-Aktor-System zur signalgesteuerten Freisetzung von Medikamenten im Gehirn	04/17 - 09/21	DFG GRK 2154 - TP P4 and TP P5
Frey	B10	Targeting mechanotransduction in cardiac hypertrophy and failure	01/19-12/20	BMBF DZHK-TP2.4
Frey	B10	Role of microRNA-582 in cardiac signal transduction, hypertrophy and heart failure	11/18-11/21	DFG FR1289/13-1
Gerken	A8	Ein Innovationsprojektzentrum für Rolle-zu-Rolle prozessierte flexible Devices	04/16 – 09/20	Interreg 5A
Gerken	A8	Entwicklung einer mikrofluidischen Sauerstoffsonde	05/18 – 10/20	ZIM
Gerken	A8	Optoelektronisch-mikrofluidisches System zur Detektion von fluoreszenzmarkierten Nukleinsäuren	04/19 – 03/22	EFRE + State
Gerken	A8	Entwicklung einer mikrofluidischen Funktionseinheit mit nanostrukturierter Oberfläche als Signalwandler zur parallelen optischen Detektion von verschiedenen Biomolekülararten	10/19 – 03/22	ZIM
Gerken	A8	Beam-forming OLED with nanostructured fluorescence layer (Proof of Concept)	proposed	ERC
Gerken	A8	Zentrum für vernetzte Sensorsysteme	proposed	EFRE + State
Gerken	A8	Modelling of metal growth on nanostructured optical substrates	proposed	Humboldt Foundation
Höft	B1, T1, Z2	Novel Filter Topologies and Synthesis Techniques for Addressing the Challenges of Future Communication Systems	05/19-04/21	DFG HO 5539/6-2
Höft	B1, T1, Z2	MWDSV - Mikrowellengerät nach dem Durchstrahlverfahren (ZF4558804PR8)	09/17-03/21	BMW/i AiF/ZIM
Höft	B1, T1, Z2	Advanced Technologies for future European Satellite Applications (TESLA), EU H2020-MSCA-ITN-2018 Project 811232	01/19-12/22	EU
Höft	B1, T1, Z2	Konzepte und Synthese Flüssigkristallbasierter Filter mit kontinuierlich steuerbarer Mittenfrequenz und Bandbreite im Ka-Band	granted 07/19, duration 3 years	DFG HO 5539/9-1 JA 921/72-1
Kienle	A6	Chromchalkogenid-basierte Thermoelektrika	08/17 – 08/20	DFG KI 1263/16-1
Kienle	A6	Lasergenerierte magneto-plasmonische Fe-Au-Nanopartikel: Bildungsmechanismus, Realstruktur und Eigenschaften	11/16 – 10/20	DFG KI 1263/15-1
Kienle	A6	FOR 2093 Forschergruppe „Memristive Bauelemente für neuronale Systeme“ Teilprojekt B2 „Strukturelle und chemische Nanoanalyse an memristiven Bauelementen“	10/18 – 09/21	DFG KI 1263/12-2
Kienle	A6	Neue Instrumente für in-operando-TEM: Plasmamodifikation live	06/19 – 05/22	DFG KI 1263/17-1
Kienle	A6	Exzellenzcluster ROOTS, Subcluster 6, Conflicts in Conciliation	08/19 – 01/23	DFG EXC 2150
Kienle, Lofink	A6, A9	SALSA “Erforschung disruptiver Mikroelektronikbauelemente auf Basis eines neuartigen ferroelektrischen Materials“	2019 - 2023	BMBF
Maetzler	B8	Keep Control: Industrial Academic Initial Training Network towards specific diagnosis and treatment of age-related gait and balance deficits	03/17-02/21	EU Horizon 2020 ITN

Maetzler	B8	BraViva: Quantitative assessment of motor fluctuations and bradykinesia in Parkinson's disease using wearables	10/18-09/20	Lundbeck
Maetzler	B8	GUIDE-IBD: Molecular-medicine based therapy guidance in inflammatory bowel disease	10/19-09/22	BMBF
Maetzler	B8	Mobilise-D: Connecting digital mobility assessment to clinical outcomes for regulatory and clinical endorsement	04/19-03/24	EU Horizon 2020 IMI2
Maetzler	B8	IDEA-FAST: Identifying digital endpoints to assess fatigue, sleep and activities of daily living in neurodegenerative disorders and immune-mediated inflammatory diseases	11/19-01/25	EU Horizon 2020 IMI2
McCord	A1	Multifunktionalemagnetooptische Sensoren zur Messung von Magnetfeldern, elektrischen Messgrößen und Temperatur.	01/18-12/21	DFG MC 9/20-1
McCord	A1	Magnetische Oberflächen zur kontrollierten Manipulation superparamagnetischer Mikroperlen.	01/18-01/21	DFG MC 9/13-2
McCord	A1	Dom-MagDzMo_Domänenwanddynamik und Verhalten magnetischer Strukturen in magnetischen Schichten mit Dzyaloshinskii-Moriya Wechselwirkung.	03/18-02/21	DFG MC 9/19-1
McCord	A1	Skymionics: Topologische Spin-Phänomene im Realraum für Anwendungen.	11/18-11/21	DFG MC 9/21-1
Murphy	A6	Pump-Probe Platform for fast and ultrafast Dynamics of liquid interfaces	07/19-06/22	BMBF F05K19FK2
Parchmann	SOP	Network School student research in Schleswig-Holstein	2017 - 2027	Joachim Herz Foundation and State Schleswig-Holstein
Parchmann	SOP	OER@IPN - Transfer and Promotion of Research-based STEM education	2018-2021	Leibniz Association
Parchmann	SOP	Zukunft des MINT-Lernens (The Future of STEM Learning)	2019-2021	Deutsche Telekom Stiftung
Parchmann	SOP	KiSOC – Kiel Science Outreach Campus (Leibniz Science Campus)	2016-2020	Leibniz Association
Parchmann	SOP	Perle - Qualitätspakt Lehre (Quality pact for teaching)	2017 - 2020	BMBF
Parchmann	SOP	LeaP@CAU II – Lehramt mit Perspektive an der CAU zu Kiel (teaching profession with perspective at CAU Kiel)	2019-2024	BMBF
Parchmann	SOP	PANaMa – Perspektiven am Arbeitsmarkt mit Naturwissenschaft und Mathematik (Perspectives on the labor market with science and mathematics)	2019-2020	EU- Interreg 5a
Quandt	A7, A9	Reinhart Koselleck Projekt: Kristallographisch kompatible keramische Formgedächtniswerkstoffe	07/16 – 06/21	DFG QU 146/23-1
Quandt	A7, A9	Die Rolle der Superkompatibilität auf die Ermüdung von Formgedächtnislegierungen	06/19 – 05/22	DFG QU 146/24-1
Quandt	A7, A9	Kooperative Aktorsysteme für Nanomechanik und Nanophotonik (SPP 2206: KOMMMA)	09/19 – 09/22	DFG QU 146/25-1
Quandt	A7, A9	GRK 2154 Materials for Brain: Thin film implants based on magnesium alloys	04/17 – 09/21	DFG P1a, GRK 2154
Quandt	A7, A9	GRK 2154 Materials for Brain: Thin film flow-diverter stents based on superelastic shape memory alloys	04/17 – 09/21	DFG P2a, GRK 2154
Rieger	A4	Wearable Electronics for Long-term Camptocormia Monitoring	proposed	DFG
Schmidt	B2, B9, B10, Z2	Untersuchungen zur Mehrkanalsignalverarbeitung für Dünnschichtsensoren	01/19 – 12/21	WTD WAS900/I0668

Schmidt	B2, B9, B10, Z2	Messtechnik und Analyseverfahren für die Bewertung und Entwicklung von Algorithmen für die Verbesserung von Innenraumkommunikationssystemen im Fahrzeug; Neue Modelle zur systemnahen Analyse und zur Verbesserung von Algorithmen für Innenraumkommunikationssysteme	09/19 – 04/21	AiF ZF4558807SS9
Schmidt	B2, B9, B10, Z2	DAAD Forschungsstipendium - Promotion in Deutschland	10/17 – 09/21	DAAD 91646138
Schmidt Quandt	A7, A9	Untersuchungen zu Mehrkanalsignalverarbeitung für Dünnschichtsensoren	02/19 – 12/21	WTD 71 E/E71Z/I0668/9F 246
Selhuber-Unkel	B7	KOMMMA-SPP 2206, "Schaltbare, bistabile Mikroaktuatorssysteme aus stimuli-responsiven Polymeren"	11/19 – 10/22	DFG SE 1801/4-1
Selhuber-Unkel	B7	"Surviving under pressure: Adaptation to mechanical forces as a key step in the evolution of multicellular life"	02/20-01/25	Volkswagen-stiftung 96733
Selhuber-Unkel	B7	GRK 2154 Materials for Brain: Embedding implant materials into structured hydrogels.	04/17-09/21	DFG P6, GRK 2154
Selhuber-Unkel	B7	ERC Proof of Concept "Strainstiff: Strain-stiffening polymer structures for orthotics"	04/19-09/20	EU Grant-No. 812943
Selhuber-Unkel	B7	"Molecularly controlled, stimuli-sensitive hydrogels for dynamically adjustable biohybrid actuators"	01/18-01/21	Volkswagen-stiftung 93415
Wulfinghoff	A10	SFB/TRR-136, M05 Numerisch effiziente, mehrskalige Materialmodelle für Prozesse mit thermischer und chemischer Hauptwirkung	01/18 – 12/21	DFG SFB/TRR-136
Wulfinghoff	A10	SFB/TRR-87, A6 Mehrskalige Modellierung des Schädigungs- und Bruchverhaltens nanostrukturierter Schichten	07/18 – 06/21	DFG SFB/TRR-87
Wulfinghoff	A10	GRK „Materials for Brain“, P12 Chemomechanische Kontinuumsmodellierung von biokompatiblen Abbauprozessen in Dünnschichtimplantaten	proposed	DFG
Wulfinghoff	A10	SPP 2206 Cooperative Actuator Systems for Nanomechanics and Nanophotonics	09/19 – 08/22	DFG WU 847/3-1

2 Existing funds and requested funds

2.1 Existing funds

2.1.1 Overview of existing funds for direct costs

(All figures in k€)

Funding period	Core support provided by applicant university/universities	Core support provided by other participating institutions	Other funds	Total
2016/2	59.70	9.00	0	68.70
2017	119.30	18.00	0	137.30
2018	119.30	18.00	0	137.30
2019	119.30	18.00	0	137.30
2020/1	59.70	9.00	0	68.70
Ending funding period	477.30		72.00	549.30
2020/2	36.00	14.50	26.00	76.50
2021	70.80	29.00	0	99.80
2022	70.80	29.00	10.00	109.80
2023	70.80	29.00	0	99.80
2024/1	36.00	14.50	10.00	60.50
New funding period	284.40	116.00	46.00	400.40

Besides the above mentioned funds from University and Fraunhofer ISIT, the staff of the competence center nanosystems technology will support the work within the CRC 1261.

2.1.2 Overview of existing staff

Category	Number of persons	
	at the applicant university/universities	at other participating institutions
Professors	12	6
Junior research group leaders	8	5
Postdoctoral researchers	2	4
Doctoral researchers	1	0
Other research staff	0	0
Non-research staff	13	4
Student and graduate assistants	25	3

2.1.3 List of existing instrumentation

Project	Description of instrumentation	Year of purchase	Cost of purchase	Source of funding
A1	Kepco bi-polar power supply	2005	10	DFG
A1	MOKE microscope (Nikon)	2011	30	Helmholtz Zentrum Dresden Rossendorf
A1	BH Looper SHB108	2002	Donation	IBM
A1	20GHz sampling oscilloscope	2012	30	DFG
A1	MOKE microscope (Zeiss)	2012	100	University
A1	MOKE microscope	2019	70	University & DFG

A1	Large view MOKE microscope	2012	13	DFG
A1	Magnetic force microscope	2012	45	DFG
A1	Time-Bandwidth psec Laser	2012	80	DFG
A1	Solid-State-Laser	2016	45	DFG
A1	High sensitivity CMOS camera (Hamamatsu)	2018	36	DFG
A1, A2, A3, A7, Z1	Surface Profiler Dektak XT-E, Bruker	2012	30	University
A1, A2, A7, A9, Z1	Wafer spinner wet chemistry	2013	19	University
A1, A7, A9, Z1	DC Generator	2010	22	University
A1, A7, A9, Z1	Ardenne-Sputter deposition system (second-hand, original price approx. 1,000,000)	2008	136	DFG
A1, A7, A9, Z1	Magnetic field annealing	2009	45	University
A1, A7, A9, Z1	Lock-In-Amplifier	2010	19	University
A1, A7, A9, Z1	NanoMOKE (second-hand, original price approx. 180,000)	2008	104	DFG
A1, A7, A9, Z1	X-ray diffractometer with high temperature unit (Theta-Theta)	1995	205	DFG / University
A1, A7, A9, Z1	X-ray diffractometer Seiffert (4-circle)	2001	166	DFG / University
A1, A7, A9, Z1	Cleanroom facility in Kieler Nanolabor	2007	1950	State
A1, A7, A9, Z1	Zeiss Ultra Plus Microscope (SEM)	2011	499	DFG / University
A1, A7, A9, Z1	Equipment cleanroom (FIB + E-Beam-Lithography, Maskaligner, RIE, PECVD, IBE, wet benches + Electroplating, PLD, and other tools)	2008	4046	EFRE / State of Schleswig-Holstein
A1, A7, A9, Z1	XRD Rigaku Smartlab	2018	528	DFG / University
A1, A7, A9, Z1	VSM Upgrade (Lake Shore) for high temperature and high resolution magnetometry	10/2014	97	University
A7, A9	DBLI Extension to measure the temperature dependence of piezoelectric properties (bulk)	2017	41	University
A1, A7, A9, Z1	Sputter deposition Cluster System CS 400S (von Ardenne)	2017	1404	EFRE / State of Schleswig-Holstein
A1, A7, A9, Z1	Upgrade of Cluster system CS 400S for DC- and HF sputtering at further target positions	2017	43	University
A1, A7, A9, Z1	Confocal Laser scanning microscope (Keyence)	2016	131	EFRE / State of Schleswig-Holstein
A2	XPS-spectrometer (Full-Lab Omicron)	1996	450	HBFG

A2	XPS spectrometer (Prevac Multichamber system)	2019	685	State/DFG
A2	Measurement setup for Electrical Properties (Keithley Instr.)	2006	15	University
A2, A4, B7	3 UHV Deposition Systems	2004	100	University
A2, A5	Optical microscope	1992	10	University
A2, A5	Microscope and equipment	1992	32	University
A2, A5	Thin film measuring setup	1993	45	University
A2, A5	Lock-In-Amplifier	1997	10	University
A2, A5	Current/voltage measurement unit and source 230V	1999	11	University
A2, A5	Illumination unit	2006	14	University
A2, A5	Potentiostat/ Galvanostat	2006	13	Industrial Projects
A2, A5	Electrochemical measurement station	2007	16	DFG
A2, A5	2'' Sputterdeposition chamber	2010	70	DFG / University
A2, A5	Setup for electromechanical measurements	2011	15	University
A2, A5	WiTec Confocal Raman and AFM	2011	200	University
A6	TEM Tecnai F30 ST G ²	2005	2000	University / State
A6	TEM JEOL JEM-2100	2012	799	DFG / State
A6	UHV sputter device	2012	50	University
A6	TEM-preparation device PIPS	2010	62	University
A6	TEM etching device	2003	13	University
A6	Device for precession electron diffraction	2008	61	University
A6	Video microscope with micromanipulator	2011	15	State
A6	Microfocus rotating X-ray anode and diffractometer	2012	230	DFG/State
A6	LAMBDA X-ray detector	2016	180	BMBF
A6	High precision heavy duty tilt table for X-ray diffraction	2017	117	BMBF
A6	Upgrade of LISA X-ray diffractometer at PETRA III including 2-D detector	2011	865	BMBF
A6	Interface Physics Microfocus X-ray rotating anode with 2 experimental hutches	2012	400	DFG / State
A6	Interface Physics 2D solid-state x-ray detector (Dectris, Pilatus)	2015	35	University
A7, A9	Double beam laser interferometer (DBLI) / 4-point-bending sample holder (4PB)	2009 / 2014	165 / 39	University
A8	Server Qpro 2xE5-2697Av4/8x32GB/1TB "3HE Rack-Server"	2016	10	DFG

A9, Z1	Cleanroom equipment of Fraunhofer ISIT, esp. LPCVD, PECVD, epitaxy, ALD, sputtering (esp. AlN, AlScN, PZT), spray coating, RIE of Si, Si-compounds, piezoelectric materials, CMP, XeF2 release etch, Si-enriched TMAH release etch, electroplating (Au, Cu, Sn, In), wafer bonding	2002 - 2015	15000	Partially funded by EC, BMBF and State Schleswig-Holstein
A9, Z1	Wafer Level Double beam laser interferometer (DBLI)	2018	240	BMBF
A9, Z1	Setup for ultra-sensitive characterization of magnetic field sensors	2017	100	Fraunhofer ISIT
B1	2 x high performance computing server for integrated circuit design (Cadence IC Design) (12 & 24 core, 192 GB RAM)	2017	20	DFG
B1, Z2	Network analyser, 4 port	2015	450	DFG / University
B1, Z2	Network analyser, 2 port	2007	181	DFG / University
B1, Z2	Spectrum analyser, LF	2009	15	University
B1, Z2	Phase noise analyser	2018	69	DFG
B1, Z2	Network analyser, 4 port	2017	68	University
B1, Z2	Spectrum analyser	2017	48	University
B1, B2, B9, B10, T1, Z2	EM shielding chamber	2010	20	University
B2, B9, B10, Z2	Kognitives MIMO-SONAR-System	2019	125	DFG
B7	Spinning Disc Confocal Microscope	2010	250	DFG
B7	Light Microscope Olympus IX 81	2012	40	DFG
B7	Light Microscope Olympus BX73	2013	20	University
B7	General Bio / Chemistry Lab Equipment	2010-2015	135	University / State
B7	AFM JPK Nanowizard	2012	250	DFG / University
B7	AFM JPK CellHesion	2013	250	EU
B7	Bioprinter CellInk+	2018	25	DFG / University
B9	Mobility Lab	2016	20	University
B9	Qualisys Stationary Camera system	2017	170	University
B9	Noraxon (wireless IMU system)	2017	40	University
T1	EEG system EGI 256 channel with MRT unit	2010	160	University
T1	Software CURRY and BESA pro	2010	32	University
T1	EEG-caps / EEG-nets for all ages (children, adults) n = 12	2005 - 2015	22	DFG / University
T1	Noraxon (wireless multichannel-EMG)	2016	30	University

(All figures in k€)

2.2 Previous and requested funds

2.2.1 Overview

(All figures in k€)

Financial year/ funding period	Funding for					Total
	Staff	Direct costs	Instrumentation	Fellowships	Global funds	
2016/2	967.40	200.70	234.60	11.30	91.50	1505.50
2017	1934.60	304.90	15.00	22.50	190.00	2467.00
2018	1934.60	306.90	0	22.50	175.00	2439.00
2019	1934.60	284.70	0	22.50	185.00	2426.80
2020/2	967.40	125.20	0	11.30	88.50	1192.40
Ending funding period	7738.60	1222.40	249.60	90.10	730.00	10030.70
2020/2	1129.50	220.80	209.90	11.30	91.50	1663.00
2021	2259.00	329.70	0	22.50	191.50	2802.70
2022	2259.00	303.90	0	22.50	199.50	2784.90
2023	2259.00	309.40	0	22.50	194.50	2785.40
2024/1	1129.50	136.10	0	11.30	95.50	1372.40
New funding period	9036.00	1299.9	209.90	90.10	772.50	11408.40

2.2.2 Overview of funds requested for staff

Project	2020/2					2021					2022					2023					2024/1				
	Postdocs	Doctoral researcher	Other research staff	Non-research staff	Student assistants	Postdocs	Doctoral researcher	Other research staff	Non-research staff	Student assistants	Postdocs	Doctoral researcher	Other research staff	Non-research staff	Student assistants	Postdocs	Doctoral researcher	Other research staff	Non-research staff	Student assistants	Postdocs	Doctoral researcher	Other research staff	Non-research staff	Student assistants
A1		2					2					2					2					2			
A2		2					2					2					2					2			
A4		2					2					2					2					2			
A5		1					1					1					1					1			
A6	1	0.75				1	0.75					1	0.75			1	0.75				1	0.75			
A7		1					1					1					1					1			
A8	1	1				1	1				1	1				1	1				1	1			
A9		2					2					2					2					2			
A10		2					2					2					2					2			
B1		2					2					2					2					2			
B2		1					1					1					1					1			
B7		2					2					2					2					2			
B9	0.25	1	0.25			0.25	1	0.25			0.25	1	0.25			0.25	1	0.25			0.25	1	0.25		
B10		1	0.5	0.25			1	0.5	0.25			1	0.5	0.25			1	0.5	0.25			1	0.5	0.25	
T1		1	0.25				1	0.25				1	0.25				1	0.25				1	0.25		
Z1	2					2					2					2					2				
Z2	1					1					1					1					1				
Z3				1	28				1	28				1	28				1	28				1	28
IRTG	0.5					0.5					0.5					0.5					0.5				
SOP		0.65		0.15			0.65		0.15			0.65		0.15			0.65		0.15			0.65		0.15	
Total	5.75	22.4	1	1.4	28	5.75	22.4	1	1.4	28	5.75	22.4	1	1.4	28	5.75	22.4	1	1.4	28	5.75	22.4	1	1.4	28

In the individual projects, funding is requested for 22.4 positions for doctoral researchers.

2.2.3 Overview of funds requested for instrumentation

Project	Description of instrumentation	Funds requested for				
		2020/2	2021	2022	2023	2024/1
A1	Multi-beam optical sensor for installation into cluster deposition tool CS 400 - Model: ksa-MOS, Manufacturer: <i>k-Space Associates</i> , Michigan, USA	83.70	0	0	0	0
A10	ONEFIVE KATANA HP HIGH POWER PICOSECOND LASER	76.20	0	0	0	0
B10	MEDTRONIC Cardioinsight	50.00	0	0	0	0
Total		209.90	0	0	0	0

(All figures in k€, including VAT, transportation, etc.)

3.1 General information about research project A1

3.1.1 Project title: Magnetostrictive Multilayers for Magnetoelectric Sensors

3.1.2 Research areas:

406-02 Synthesis and Properties of Functional Materials
406-03 Microstructural Mechanical Properties of Materials

3.2 Project leaders

McCord, Jeffrey, Prof. Dr.-Ing.
06.10.1965

Meyners, Dirk, Dr.
22.05.1973

Nanoscale Magnetic Materials – Magnetic Domains
Institute for Materials Science
Christian-Albrechts-Universität zu Kiel (CAU)
Kaiserstr. 2, D-24143 Kiel

Inorganic Functional Materials
Institute for Materials Science
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Do any of the abovementioned persons hold fixed-term positions? No.

3.2.1 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.3 Summary

The project focuses on the aspects of deposition, structuring, and advanced characterization of novel magnetostrictive multilayers deployed as the piezomagnetic phase for advanced magnetoelectric (ME) sensor structures with the aim of advancing the limit of detection of current and future ME sensor approaches. Within the project, we will therefore investigate concepts to individually tune effective multilayers' properties to the various ME sensors employed in CRC, differing in utilized substrate, sensor size and thickness, as well as operating magnetic excitation characteristics. For the specific sensor types, diverse strategies will be investigated. The challenge hereby is to achieve the effective lateral magnetic properties on device level including magnetic domain control. For this, different concepts using ferromagnetic and antiferromagnetic layers, inter-layer exchange coupling, lateral patterning, and magnetic hard bias will be combined. Magnetic anisotropy alignment and strength induced during film growth and the control thereafter play a decisive role, influencing the ME sensor performance. To achieve the goals of the project, a new sputter deposition cluster tool with nine sputter sources has been put into operation which will enable us to adjust uniaxial and unidirectional magnetic anisotropy alignments already during thin film deposition.

On the basis of established magnetostrictive layer structures, the interplay between deposition conditions characterized by energy flux measurements, optional post-deposition treatment, magnetic properties, patterning, and resultant sensor performance will be explored. *In situ* stress measurements will reveal the important stress condition during magnetostrictive multilayer growth. Post processing of the multilayered piezomagnetic phase will be assisted by *in situ* magneto-optical measurements for further establishing the

aimed magnetic material properties for the various sensor concepts, including electrically modulated (**A7**) and surface acoustic wave (SAW) based ME sensors (**A9**). Overall, combining material selection, multilayering, processing, and structuring will lay the foundations for achieving ultra-sensitive ME sensors. Reducing magnetic domain-induced noise with advanced magnetic multilayer structures, taking magnetic properties, structural and processing effects into account, and thereby keeping and improving sensitivity is the main focus of the investigations. With this we plan to obtain a detailed understanding of an optimally designed piezomagnetic phase and thus a vast improvement in the sensors' limit of detection. The results of the research will lead to distinct ME composites with much improved sensing behavior for the discrete sensor concepts employed within the CRC.

3.4 Project progress to date

3.4.1 Report and current state of research

Reduction of noise contributions of magnetic origin is of major interest for any kind of high sensitivity magnetic field sensors. Depending on the sensor concept, various measures have been applied to lower the noise originating from magnetic domain activity. Among them are single domain concepts based on shape anisotropy [Di89] and biasing by permanent magnet material [Ts84]. However, a specialty of magnetoelectric composite sensors [A1-3] arises from the integration of magnetostrictive material that results in strong magnetic sensitivity of magnetic anisotropy to stress [Mc04, Ur14]. Accordingly, the control of residual mechanical stress has been identified as a prerequisite for successful ME sensor applications [Ma13, Be17].

In the past funding period, **A1** concentrated on the research of novel magnetostrictive phases for magnetic-modulated cantilever sensors, with the aim of elimination of current limitations in the detection of low frequency signals through magnetic domain activity [A1-10, Ur14]. The main challenge of this project was to solve the antagonism between quasi noise-free magnetic domain behavior and large magnetic susceptibility in structures with high piezomagnetic coefficients. One suggested solution was to tailor the unidirectional anisotropy (exchange bias) through multilayering with advanced post-annealing, thereby preventing multi-domain states even under the application of varying magnetic or elastic fields. The validity of this approach was proven within the last funding period. A large fraction of work was focused on sensors utilizing magnetic frequency conversion (MFC) [Ja12]. MFC is one way to transfer the mechanical resonance effect of cantilever sensors to the needed lower frequencies by application of strong modulating magnetic fields. At the beginning of the last funding period, MFC yielded a limit of detection (LOD) around 800 pT/Hz^{1/2} at 10 Hz for ferromagnetic single layer sensors [A1-6]. The limitations were identified to be due to magnetic domain effects [Ur14, A1-8]. In the millimeter-sized ME sensor structures, limited magnetic domain control is achieved by exchange biased (EB) antiferromagnetic/ferromagnetic (AF/FM) laminates [La12]. EB is usually set in a magnetic field in an annealing step in magnetic saturation, which introduces an equivalent aligned parallel exchange bias (PEB) to the ferromagnetic layers, where also the exact alignment of anisotropy is critical [A1-7]. Yet, due to demagnetization effects, magnetic domains still form with greater magnetic layer thicknesses [La14], which limits sensor performance. A LOD around 500 pT/Hz^{1/2} at 10 Hz for an exchanged biased sensor with a ferromagnetic layer thickness of 2 μm and above [A1-6] was obtained. We were able to overcome this limitation by the introduction of an antiparallel exchange biasing (APEB) scheme [A1-2]. The investigated layer stack consisted of up to 20 repetitions of the magnetic building block Ta(5)/Cu(3)/MnIr(8)/(Fe₉₀Co₁₀)₇₈Si₁₂B₁₀(90)/Ta(5)/Cu(3)/MnIr(8)/(Fe₉₀Co₁₀)₇₈Si₁₂B₁₀(110) (thicknesses in nm). In order to prevent substrate heating during layer deposition, idle intervals were introduced to keep the temperature below 80°C. The film stacks with layer-by-layer single domain magnetic structure and antiparallel alignment of magnetization were then set in a post-setting procedure with a required support by *in situ* magnetic domain observation. The approach for achieving the setting of APEB during the post-annealing steps requires multiple magnetic field sequences to set the magnetization in an AP configuration. We could show that in the resulting structure the magnetization responds by foremost coherent and reversible magnetization rotation to varying applied magnetic fields along the sensing direction of the ME sensors. As a result, the sensors demonstrate drastic improvements of sensor noise [A1-2, A1-5] and the noise level was reduced by more than one order of magnitude (Fig. A1-1). This resulted in an improvement of LOD at low frequencies by one order of magnitude, down to 60 pT/Hz^{1/2} at 10 Hz [A1-5]. For this sensor structures, noise density spectra showed a nearly flat noise floor that did not change with added magnetic activity in the magnetic sensing layer. This clearly shows that sensor performance was not limited by magnetic noise contributions anymore.

With the shown APEB biasing scheme, magnetic domain activity can also be prevented for an increased ferromagnetic thickness. The use of APEB for electrical frequency conversion [Ha16, A1-1] has been further

demonstrated (in coop. with **A7**). With an adapted APEB system, a drastic improvement of LOD at 10 Hz even down to $30 \text{ pT/Hz}^{1/2}$ was obtained. The examples demonstrate the significant progress achieved during the last funding period. At the time of writing, work on layer integration into bulk-micromachined ΔE -effect [Za16] sensors is ongoing.

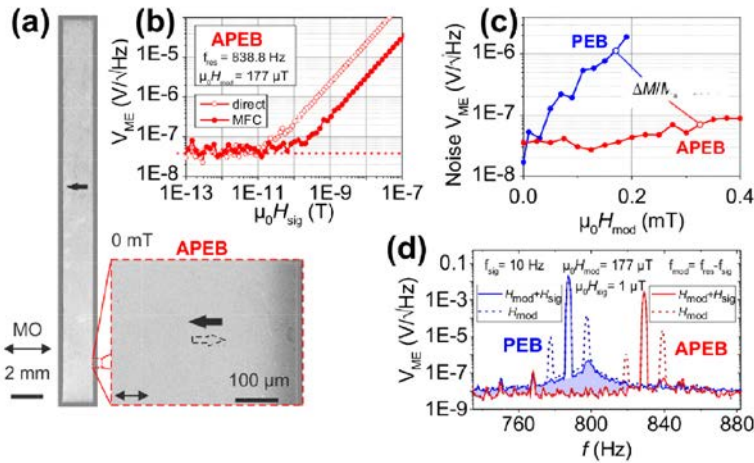


Figure A1-1: (a) Single magnetic domain state of the whole sensor and close to an edge. No closure domains are visible. (b) ME voltage versus magnetic signal H_{sig} for direct and MFC application. (c) Change of noise density with modulation field amplitude H_{mod} , showing the difference between PEB and APEB behavior field. (d) Frequency spectra of voltage noise density V_{ME} for APEB and PEB sensors at the same magnetic modulation field H_{mod} and signal field H_{sig} [A1-2].

Yet, existing limitations are due to the still existing presence of magnetic or magnetoelastic edge effects from stress relaxation at the edges with the annealed tensile stressed magnetic films, leading to an unwanted magnetic anisotropy alignment at the edges. As stated above, the process further needs to be controlled by *in situ* magnetic domain observation to ensure the AP setting above the blocking temperature of the AF layer. The annealing step further involves inducing a uniaxial anisotropy in the ferromagnetic layer of the system, where the amount of achievable anisotropy is directly connected to the saturation magnetization of the amorphous magnetic phase at the annealing temperature. As a result, limitations on achievable uniaxial anisotropy and a modulated magnetization structure in the APEB structures occur.

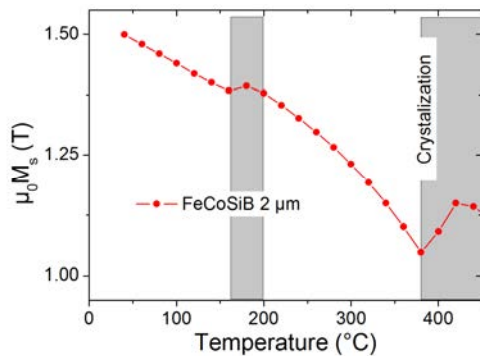


Figure A1-2: Relative change of saturation magnetization of a $2 \mu\text{m}$ thick FeCoSiB layer recorded by vibrating sample magnetometry. An in-plane saturating magnetic field $\mu_0 H_{ext} = 150 \text{ mT}$ was applied during the temperature sweep.

Fig. A1-2 displays the trend of FeCoSiB magnetization as a function of temperature T within the range of applied annealing procedures. Clearly, a lowering of the saturation magnetization by about 20% at 300°C in comparison to room temperature is seen. As the amount of induced anisotropy scales with M_s^2 , this is of high relevance for the setting of anisotropy at higher temperatures.

Together with influences of magnetoelastic self-energy [Ur14], the achievable modulated magnetic domain state for thick magnetic films may set limitations to the achievable ME sensor performance. Temperature-dependent magnetic investigations are also important to check for the occurrence of (partial) onset of recrystallization of the amorphous magnetic phase with the annealing above $T = 300^\circ\text{C}$, influences of which have already been seen from magnetic domain investigations that would lead to a degradation of the excellent soft magnetic properties of the amorphous piezomagnetic phase. Above $T = 150^\circ\text{C}$ an unexpected plateau in saturation magnetization with temperature is observed. As the strength of induced anisotropy depends on the magnetization during annealing, an understanding of the effect for a precise anisotropy setting in future layer concepts based on post-deposition treatment is of relevance. The cause of the unusual magnetization behavior and crystallization issues will be explored with **A6** for structural and chemical analysis.

Setting of induced magnetic anisotropies in a non-collinear fashion for the individual magnetic layers is not easy to obtain through the post-annealing procedure. Experiments to vary the angle of magnetization in a controlled way by post processing were only partially successful. An alternative route of setting anisotropy, EB in PEB and APEB, is introducing EB already during film deposition. Such a procedure would also allow for layer-wise and non-collinear setting of directions of magnetic film anisotropies and exchange bias for further improved response characteristics. Example results from a proof-of-concept study comparing single layer (SL), PEB and APEB are displayed in Fig. A1-3.

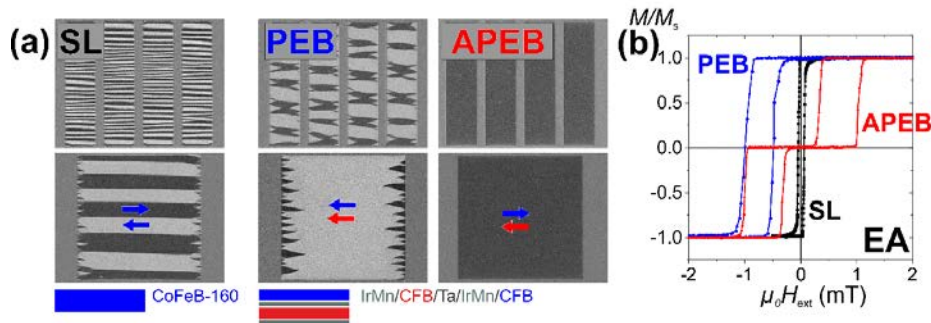


Figure A1-3: (a) Magnetic domain structure for single layer (SL), exchange biased bilayer with parallel (PEB) and antiparallel (APEB) alignment of exchange bias together with corresponding magnetization loops along the magnetic easy axis (EA) and hard axis (HA) (as indicated). The total $\text{Co}_{40}\text{Fe}_{40}\text{B}_{20}$ (CFB) layer thickness is 160 nm in all cases. Single domain states are obtained for the APEB structures. (b) The APEB state is proven by the two step magnetization reversal with two individually shifted partial magnetization loops.

Magnetic domain control is achieved without annealing. This route of preparation offers certain advantages in terms of anisotropy control and stress management and will be followed as an alternative. Therefore, a novel field deposition tool has been established in cooperation with **Z1**. The new deposition tool (clustertool CS 400 from *von Ardenne*) is equipped with 9 magnetron sputter sources and was installed in the cleanroom of the Kiel's Nanolab in 12/2017. Film deposition is performed under substrate rotation on maximum 8 inch wafers. A rotatable permanent magnet ring was developed in a cooperation project between *von Ardenne* and CAU. It enables the deposition under a magnetic field about 10 mT in field strength and stationary at the substrate level. A complementary routine for wafer mapping of magnetic anisotropy has been introduced in **A1**. Fig. A1-4 shows example outcomes of depositions with and without a magnetic field. From the magnetic domain alignment, the effective magnetic anisotropy distribution present in the layer is identified. As a result of substrate rotation, the magnetic anisotropy runs in a circle when the deposition is done without magnetic bias field (Fig. A1-4(a)). In contrast, deposition with magnetic bias generates a nearly parallel anisotropy alignment with an angular error of less than 15° (3°) across a 6 (4) inch diameter wafer (Fig. A1-4(b)). In deposition experiments varying the deposition conditions, the anisotropy field could be tuned from $\mu_0 H_k = 7.5$ mT down to 3 mT. Further lowering of anisotropy strength is expected based on the investigation of the plasma conditions during sputtering (see WP3).

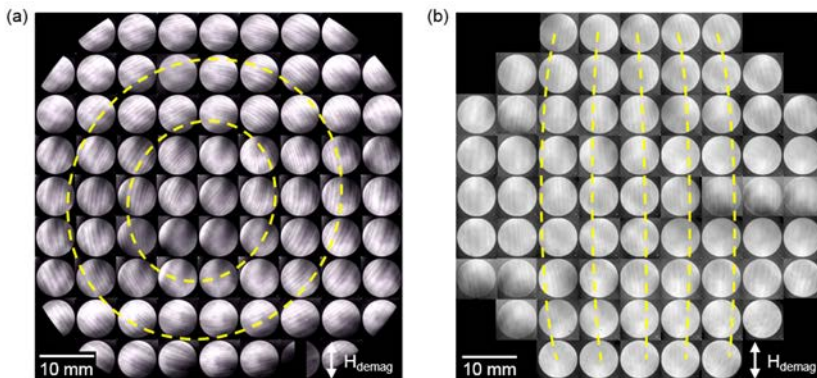


Figure A1-4: Series of magneto-optical images of FeCoSiB discs with 150 mm^2 area recorded after demagnetization on six inch wafers, (a) $1 \mu\text{m}$ thick layer deposited without magnetic field, (b) 850 nm thick layer deposited under magnetic field ($\mu_0 H_{bias} = 10 \text{ mT}$). The orientation of the axis of anisotropy is indicated.

An additional promising concept of magnetic domain stabilization is based on manipulating the magnetization states at the edges of sensor elements by reducing demagnetization effects at the sample edges. The magnetic edge state is especially important because this is the region where possible closure or spike domains form which exist even for the APEB [A1-1] structure. The boundary areas of magnetostrictive structures further play a decisive role, because stress relaxation and stray fields arising at the edges influence the effective magnetic anisotropy and magnetization distribution [Mc04]. The effect scales with the total thickness of magnetic layers. Therefore, the edge profiles formed during lithography and etching are of further importance. The state-of-the-art processing combines ion beam etching with negative resist application by spray-coating (for a detailed discussion see **Z1** project proposal). Most promising for controlling the edge magnetization is pinning the edge magnetization with an integrated permanent magnet hard bias at the edges (see WP5). The general concept is shown Fig. A1-5(a). Matching modelling and experimental data that demonstrate the concept are shown in Fig. A1-5(b). Corresponding experimental data of an integrated NdFeB powder magnet [Ni19] is given. The data demonstrate the potential of local magnetic edge biasing. Investigating the influence of integrated permanent magnets into the sensor structures will be part of the research in the next funding period (embedded permanent magnet structures based on powder magnets solidified by atomic layer deposition will be provided by **Z1**).

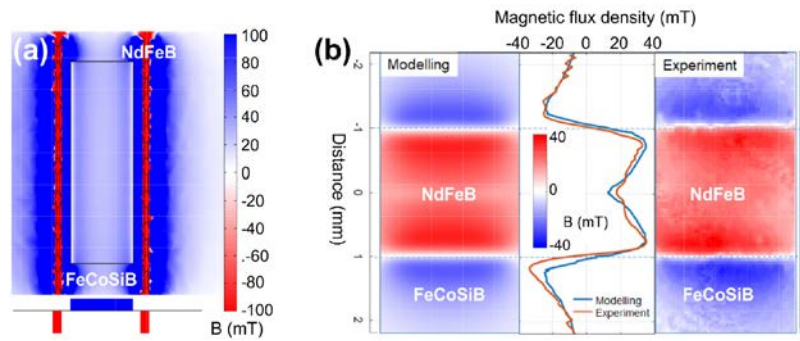


Figure A1-5: (a) Calculated magnetic field distribution of a permanent magnet together with an FeCoSiB structure. (b) Modeled and experimentally derived lateral magnetic field distribution around a permanent magnet structure. The magnetic field is experimentally derived through magneto-optics by high resolution magnetization loop analysis.

In the previous funding period, most of the investigated magnetostrictive layers and fabricated ME sensors were based on amorphous $(\text{Fe}_{90}\text{Co}_{10})_{78}\text{Si}_{12}\text{B}_{10}$ because of its remarkable characteristic of combining comparatively soft magnetic properties with significant magnetostriction. As an alternative, sputter deposited FeGaB [Lo07] layers of various compositions have been investigated and compared to FeCoSiB layers within the framework of a master thesis [Sc17]. Pronounced sensitivity to boron content of magnetic properties such as coercivity, anisotropy field and saturation magnetization in FeGaB layers was proven in good qualitative agreement with [Lo07]. However, the reported piezomagnetic coefficient being larger than for FeCoBSi could not be obtained. From this perspective, a changeover to FeGaB-based multilayers provided no added value to the CRC's ME sensor research. Furthermore, FeCo/TiN multilayers deposited at the Karlsruhe Institute of Technology have been investigated as a high temperature stable alternative to the amorphous FeCoSiB. Yet, the multilayers consisting of ultra-thin FeCo and TiN layers show strongly reduced magnetoelastic coupling. High resolution transmission electron microscopy (A6) revealed a variation of c-lattice parameter inside the FeCo layers, which probably causes the reduction. Further research in this regard is ongoing.

Overall, during the last funding period we had strong and productive cooperation with other projects in the CRC that resulted in numerous common publications, none of them solely based on our own results. The progress during the last funding period has only been possible with the interaction with our partners within the CRC. To be highlighted in this context is the common work with **A7** [A1-1], **B1** [A1-5, A1-7, A1-8, A1-9], and **Z1** [A1-6] on magnetic layer deposition, magnetic domain imaging, and noise measurements, respectively. In the last funding period, research in **A1** was mostly focused on magnetically activated ME cantilever sensors. By combining complex multilayer growth with new routes of post-processing, the fabrication of micron thick multilayer systems with layer-wise controlled exchange bias was enabled. This led to a strongly improved LOD. We could show that enabling better and more flexible control of the magnetic properties, like uniaxial and unidirectional anisotropy of individual layers in the piezomagnetic phase under consideration, is key for improvement in sensor properties. Based on these results, the setting of also other magnetic properties for individual layers would enable additional progress towards achieving an even lower LOD. Understanding the requirements, investigating the tailoring options, defining individual magnetic properties, and incorporating them in magnetic multilayer stacks provided significant impact for achieving the overall goals of the CRC. Combining research on preparation and characterization with a perception of ME operations is the key for obtaining novel piezomagnetic multilayers paving the way to the measurement of biomagnetic signals.

References

- [Be17] S. P. Bennett, J. W. Baldwin, M. Staruch, B. R. Matis, J. LaComb, O. M. J. van 't Erve, K. Bussmann, M. Metzler, N. Gottron, W. Zappone, R. LaComb, P. Finkel, Magnetic field response of doubly clamped magnetoelectric microelectromechanical AlN-FeCo resonators. *Appl. Phys. Lett.* **111**, 252903 (2017).
- [Bo13] S. Bornholdt, N. Itagaki, K. Kuwahara, H. Wulff, M. Shiratani, H. Kersten, Characterization of the energy flux toward the substrate during magnetron sputter deposition of ZnO thin films. *Plasma Sources Sci. Technol.* **22**, 25019 (2013).
- [Di89] U. Dübbern, "Magnetoresistive Sensors" in *Sensors: Magnetic Sensors*, R. Boll, K. J. Overshott, Eds. (Wiley-VCH, Weinheim, 1989), **5**, 341-380.
- [Ga19] S. Gauter, F. Haase, H. Kersten, Experimentally unraveling the energy flux originating from a DC magnetron sputtering source. *Thin Solid Films.* **669**, 8–18 (2019).
- [Ha16] P. Hayes, S. Salzer, J. Reermann, E. Yarar, V. Röbisch, A. Piorra, D. Meyners, M. Höft, R. Knöchel, G. Schmidt, E. Quandt, Electrically modulated magnetoelectric sensors. *Appl. Phys. Lett.* **108**, 182902 (2016), doi:10.1063/1.4948470.

- [Ja12] R. Jahns, H. Greve, E. Woltermann, E. Quandt, R. Knöchel, Sensitivity enhancement of magnetoelectric sensors through frequency-conversion. *Sensors and Actuators A: Physical*. **183**, 16–21 (2012).
- [La12] E. Lage, C. Kirchhof, V. Hrkac, L. Kienle, R. Jahns, R. Knöchel, E. Quandt, D. Meyners, Exchange biasing of magnetoelectric composites. *Nature materials*. **11**, 523–529 (2012).
- [La14] E. Lage, N. O. Urs, V. Röbisch, I. Teliban, R. Knöchel, D. Meyners, J. McCord, E. Quandt, Magnetic domain control and voltage response of exchange biased magnetoelectric composites. *Appl. Phys. Lett.* **104**, 132405 (2014).
- [Lo07] J. Lou, R. E. Insignares, Z. Cai, K. S. Ziemer, M. Liu, N. X. Sun, Soft magnetism, magnetostriction, and microwave properties of FeGaB thin films. *Appl. Phys. Lett.* **91**, 182504 (2007), doi:10.1063/1.2804123.
- [Lu09] D. Lundin, M. Stahl, H. Kersten, U. Helmersson, Energy flux measurements in high power impulse magnetron sputtering. *J. Phys. D: Appl. Phys.* **42**, 185202 (2009).
- [Ma13] S. Marauska, R. Jahns, C. Kirchhof, M. Claus, E. Quandt, R. Knöchel, B. Wagner, Highly sensitive wafer-level packaged MEMS magnetic field sensor based on magnetoelectric composites. *Sens. and Actuators, A* **189**, 321–327 (2013).
- [Mc04] J. McCord, Irregular domain patterns in structured magnetic thick films, *Journal of Applied Physics* **95**, 6855 (2004).
- [Ni19] F. Niekkel, J. Su, M. T. Bodduluri, T. Lisec, L. Blohm, I. Pieper, B. Wagner, F. Lofink, Highly Sensitive MEMS Magnetic Field Sensors with Integrated Powder-based Permanent Magnets. *Sensors and Actuators A* **297**, 111560 (2019).
- [Sc17] G. Schönweger, Master thesis, Christian-Albrechts-Universität zu Kiel (2017).
- [St10] M. Stahl, T. Trottenberg, H. Kersten, A calorimetric probe for plasma diagnostics. *The Review of scientific instruments*. **81**, 23504 (2010).
- [Ts84] C. Tsang, Magnetism of small magnetoresistive sensors (invited). *Journal of Applied Physics*. **55**, 2226–2231 (1984).
- [Ur14] N. O. Urs, I. Teliban, A. Piorra, R. Knöchel, E. Quandt, J. McCord, Origin of hysteretic magnetoelastic behavior in magnetoelectric 2-2 composites. *Appl. Phys. Lett.* **105**, 202406 (2014).
- [Za16] S. Zabel, J. Reermann, S. Fichtner, C. Kirchhof, E. Quandt, B. Wagner, G. Schmidt, F. Faupel, Multimode delta-E effect magnetic field sensors with adapted electrodes. *Appl. Phys. Lett.* **108**, 222401 (2016).

3.4.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [A1-1] P. Hayes, M. Jovičević Klug, S. Toxvaerd, P. Durdaut, V. Schell, A. Teplyuk, D. Burdin, A. Winkler, R. Weser, Y. Fetisov, M. Höft, R. Knöchel, **J. McCord**, E. Quandt, Converse Magnetoelectric Composite Resonator for Sensing Small Magnetic Fields. *Scientific reports* **9**, 16355 (2019).
- [A1-2] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. D. Toxværd, M. Höft, R. Knöchel, E. Quandt, **D. Meyners**, **J. McCord**, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors. *Appl. Phys. Lett.* **114**, 192410 (2019).
- [A1-3] D. Viehland, M. Wuttig, **J. McCord**, E. Quandt, *Magnetoelectric magnetic field sensors*, MRS Bulletin **43**, 834 (2018).
- [A1-4] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, **D. Meyners**, N. X. Sun, **J. McCord**, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, F. Faupel, E. Quandt, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Scientific reports*. **8**, 278 (2018).
- [A1-5] S. Salzer, V. Röbisch, M. Klug, P. Durdaut, **J. McCord**, **D. Meyners**, J. Reermann, M. Höft, R. Knöchel, Noise Limits in Thin-Film Magnetoelectric Sensors With Magnetic Frequency Conversion. *IEEE Sensors J.* **18**, 596–604 (2018).
- [A1-6] V. Röbisch, S. Salzer, N. O. Urs, J. Reermann, E. Yarar, A. Piorra, C. Kirchhof, E. Lage, M. Höft, G. U. Schmidt, R. Knöchel, **J. McCord**, E. Quandt, **D. Meyners**, Pushing the detection limit of thin film magnetoelectric heterostructures. *J. Mater. Res.* **32**, 1009–1019 (2017).
- [A1-7] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, **J. McCord**, **D. Meyners**, E. Quandt, G. Schmidt, R. Knöchel, M. Höft, Improved Magnetic Frequency Conversion Approach for Magnetoelectric Sensors. *IEEE Sens. Lett.* **1**, 1–4 (2017).
- [A1-8] S. Salzer, P. Durdaut, V. Röbisch, **D. Meyners**, E. Quandt, M. Höft, R. Knöchel, Generalized Magnetic Frequency Conversion for Thin-Film Laminate Magnetoelectric Sensors. *IEEE Sensors J.* **17**, 1373–1383 (2017).

- [A1-9] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, P. Hayes, A. Piorra, **D. Meyners**, E. Quandt, G. Schmidt, R. Knöchel, M. Höft, Thermal-Mechanical Noise in Resonant Thin-Film Magnetoelectric Sensors. *IEEE Sensors J.* **17**, 2338–2348 (2017).
- [A1-10] N. O. Urs, B. Mozooni, P. Mazalski, M. Kustov, P. Hayes, S. Deldar, E. Quandt, **J. McCord**, Advanced magneto-optical microscopy: Imaging from picoseconds to centimeters - imaging spin waves and temperature distributions (invited). *AIP Advances*. **6**, 55605 (2016).

b) Issued Patents

[A1-P1] Lage, E.; **Meyners, D.**; Quandt, E.: Magnetostruktives Schichtsystem, EP 11171354.1 – 2216

3.5 Project plan

Objectives

The overarching goal of **A1** is to obtain magnetostrictive phases with the highest sensitivity and lowest contribution to ME sensor noise. It pursues this target with research on magnetic materials individually tuned to the most promising ME sensor concepts. The type and frequency of stimulus of excitation differs strongly for the different concepts. They may also differ in the applied magnetic layer thickness. Due to the various modes of operation, the magnetostrictive phase must fulfill different and tailored requirements as compared to the demands in ME sensors based on strain-mediated ME effect and classical cantilever design. The following ranges of operating frequencies and excitation schemes are identified:

- Up to 10 kHz – magnetic excitation: resonant sensors (**Z1**)
- Up to 3 MHz – electrical excitation: ΔE -effect sensors (**Z1**, **A4**)
- 100 kHz to 10 MHz – electrical excitation: converse magnetoelectric sensors (**A7**)
- 100 MHz to 2 GHz – electrical excitation: surface acoustic wave (SAW) sensors (**A9**)

The overall research within the CRC will focus on advanced concepts of converse magnetoelectric (**A7**), ΔE effect (**A4**), and SAW sensors (**A9**). These methods all have in common that the magnetic layer is externally activated like in MFC. In project **A7**, the converse ME sensors are strongly excited by the piezoelectric substrate at comparatively high frequencies to exotic vibrational modes [A1-1]. In these modes and by the inverse magnetostrictive effect, the magnetization changes continuously, which is detected by a pick-up coil. Depending on the stress distribution, the magnetostrictive response must be tuned to the maximum coil signal, while simultaneously avoiding erratic magnetization changes. As with resonant sensors, this concept requires a large magnetostrictive volume for maximal sensor output. The best results so far were achieved for 4 μm thick magnetic multilayers. This is in contrast to SAW sensors (**A9**). Here, a trade-off is needed between magnetostrictively induced wave velocity changes and insertion losses. In preliminary work on SAW sensors exhibiting single layer FeCoSiB coatings, the best SAW sensor performance was achieved with a FeCoSiB thickness of about 400 nm. In addition, the piezoelectric substrates pose a challenge for the magnetostrictive layer deposition, as thermal expansion coefficients depend on the wafer cut used, can be anisotropic, and are very different in magnitude to those of Si and FeCoSiB. Due to the interplay between thermally induced stress and magnetoelastic properties, low-temperature deposition is required during magnetostrictive layer growth. Furthermore, post-deposition thermal treatment is rather limited for the same reason. **A4** pursues the goal of miniaturizing ΔE -effect sensors, which requires low stress deposition on thin cantilever substrates and consideration of size-dependent demagnetization effects. As a consequence, resonant, ΔE -effect (**A4**), converse ME and SAW sensors with their different modes of operation possess different challenges in terms of magnetic layer requirements and available processing options. To maximize sensor performance for each concept, different individual strategies for the magnetic layer properties have to be used to obtain the lowest LOD. This also involves layer stack structure and, if needed, additional patterning to achieve the possible lowest limit of detection. All measures have to be investigated in combination.

The overarching aim of project **A1** is to achieve a significant improvement over current sensors in the limit of detection through magnetic design that removes current limitations due to magnetic noise.

Based on the results on MFC sensors, the working hypothesis is that obtaining a stable single domain behavior by domain engineering will eliminate the magnetic noise in excited sensors (**A4**, **A7**, **A9**), essentially in full. Magnetic noise contributions can be controlled by introducing new magnetic multilayer concepts. Single domain magnetic layer concepts that maintain high sensitivity should provide a significant step forward towards significantly lower LOD of ME sensors. The requirements for the diverse sensor structures are very different due to differences in materials used, accordingly leading to differences in terms of processing options, different sizes with different ratios of edge length to sensor area, differences in optimum magnetic ma-

terial thickness, differences in operating frequency, and differences in utilized signal-generating magnetoelectric conversion. Thus, each sensor requires the investigation of individual magnetic structures to minimize magnetic noise and concurrently keep increasing sensor sensitivity. To achieve the overall goal of the project, the research concentrates on the following objectives:

The **first objective** is to obtain magnetic thin film materials with controllable effective magnetic properties and magnetic domain control. Achieving nearly exact induced magnetic anisotropy control in the as-deposited state, exchange bias without heat treatment, and well-defined antiferromagnetic interlayer coupling in combination with the important control of film stresses are the major challenges (WP1, WP3).

The **second objective** is to identify the requirements and possibilities for improving the magnetic phase of the individual sensor designs, considering magnetic design, dimensions, connecting processing considerations, as well as sensor signal generation (WP2).

The **third objective** is to incorporate the magnetic thin film materials into more complicated multilayer structures, involving patterning and additional supporting (magnetic) structures (WP4, WP5).

The **fourth objective** is the incorporation of individual multilayer and structuring concepts into the actual sensor designs. Here, the challenge is to match the requirements for layer and structure preparation with the processing tolerances of the individual sensors for the various concepts applied (WP6).

To accomplish the objectives, complementary methods of preparation and characterization ranging from advanced thin film deposition combined with energy flux and *in situ* film stress measurement, magnetic annealing, layer structuring, stress characterization, magnetometry, magnetic domain imaging, and ME characterization including supporting electrical measurements will be applied. All aspects have to be considered in conjunction to achieve the principal goal of the project.

Proposed research methods

Film deposition and patterning - Two cluster tools with nine magnetron sputter sources each are available for magnetic film deposition, which are designed for the deposition of multilayer systems by RF and DC sputtering. In addition, a pulsed-DC generator can be connected to one of the sputter sources. For inducing of magnetic anisotropy, a magnetic field can be applied with permanent magnets during layer growth. Whereas one tool (*von Ardenne* CS 700) has been intensively used for the depositions in the previous funding period, a continuous changeover to the new tool (*von Ardenne* CS 400) is expected. It was installed recently and the deposition of single FeCoSiB layers exhibiting well-defined anisotropy alignment has already been established (Fig. A1-4). The tool enables superior homogeneity of layer thickness (5% across 6 inch wafers) by using substrate rotation and angled sputter sources. Furthermore, substrate cooling is more efficient as compared to the passive cooling of the CS 700. In comparison to the CS 700, the CS 400 allows needed deposition variability by adjusting source to substrate distance as well as substrate rotation speed. To achieve the ambitious goals of the **A1** project, the installation of advanced characterization tools is planned for *in situ* measurements of film stress and energy flux from source to substrate (WP1). Structuring of magnetostrictive layers will be preferably conducted by soft ion beam etching, as previous work showed that wet chemical etching and lift-off techniques are not applicable to complex multilayers. Yet, the two techniques will still be available as alternatives for the structure transfer to simple and thin magnetostrictive coatings.

Annealing - *In situ* magnetic field annealing of magnetic film model structures will be performed on a heating stage at temperatures up to 400 °C with *in situ* magnetic imaging and magnetometry. A vacuum furnace with an electromagnet is provided for the post-annealing of individual cantilever substrates and wafers. In addition, a rapid thermal annealing system is available. Post-deposition annealing offers an alternative for magnetic property tailoring of those ME sensors, which are not prone to thermally induced layer stress.

Structure investigation - Structural analysis is performed by standard and advanced synchrotron based X-ray diffraction techniques and transmission electron microscopy with **A6**. Radial distribution function analysis will provide knowledge about structural and compositional perturbations in the amorphous phase.

Magnetic characterization and imaging - Magnetic properties of magnetic films and structures will be determined by complementary measurements of magnetization loops by vibrating sample magnetometry (VSM), BH-looper, and/or magneto-optical (MO) magnetometry. VSM and MO magnetometry can be performed at elevated (annealing) temperatures. Magnetostriction behavior $\lambda(H)$ is measured by a cantilever deflection method. Ferromagnetic resonance frequencies f_{res} and effective magnetic damping parameters α_{eff} relevant for the high-frequency applications will be extracted by pulsed inductive magnetic magnetometry (PIMM). From this, values for the saturation magnetization M_s , the magnetic anisotropy K_u , and exchange bias and interlayer exchange coupling will be derived. The magnetic domain behavior will be investigated by quasi-static and time-resolved MO imaging techniques. MO imaging will be carried out at operation

frequencies for ME device structures. Imaging of magnetic sensor responses over the whole frequency range of applications is achievable with altogether six MO imaging setups. Bandwidth limitations to match the resonance frequencies of SAW devices will be overcome by the installation of a low repetition-rate laser (A10). Combined magnetic domain imaging and ME response measurements are possible. The magnetoelectric properties and achieved limit of detection are measured in an acoustically and magnetically shielded setup (together with Z2 and B1).

Modeling - Modeling of the fundamental magnetization and ME behavior will be accomplished by a macro-spin model with all the relevant magnetic properties as input, solving the fundamental energy equations. Magnetic and ME response of magnetic multilayer structures will be calculated by taking fundamental magnetic contributions like anisotropy, interlayer coupling, and shape effects into account. Finite element modeling is used for the calculation of magnetic field distributions within the sensor for the magnetic hard bias. If needed, additional modeling will be conducted together with A8 and A10.

Work plan

The research is organized in correlated work packages with contributions from both principal investigators. In WP1 the existing experimental methods will be extended to fulfill the technical requirements demanded by the other work packages. *In situ* stress measurements and energy flux determination will facilitate understanding and precise control of magnetostrictive layer deposition. A large view magnetooptical microscope will be retrofitted for time-resolved imaging of complete sensor structures. By taking into account the new ME sensor concepts and application scenarios, the purpose of WP2 is the formulation of requirement lists and corresponding concepts for the magnetic phase. In the next step, the fabrication and characterization of novel magnetic multilayers is subdivided into interconnected packages (WP3, WP4, WP5). WP3 investigates elementary magnetic building blocks, providing a toolbox for WP4 and WP5. The scaled up magnetic layer concepts under consideration in WP4 differ in complexity, number of layers, and total magnetic layer thickness. In WP5 specific patterning concepts will be utilized to further improve the resulting magnetic properties of the stacks investigated in WP3 and WP4. Finally, integration related issues will be explored on the basis of real sensor structures in WP6. The achieved improvements in noise behavior and detection limit will constantly serve as a feedback for WP2. The scheduling of work packages is shown in Table A1-1.

Table A1-1: Work schedule - Main work done by group Meyners (red) and group McCord (blue)

	2020		2021				2022				2023				2024	
	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP1: New experimental methods																
WP2: Sensor requirements																
WP3: Magnetic building blocks																
WP4: Advanced magnetic multilayers																
WP5: Hybrid lateral structures																
WP6: Incorporating layer and lateral patterning schemes in sensor structures																

WP1: New experimental methods

The ME sensors under consideration within the CRC consist of several layers for electrodes, piezoelectric, and magnetostrictive elements. Also the substrates of bulk- and surface-micromachined sensors possess a complex layer structure. Therefore, determining the dominating origin for layer stress in the magnetostrictive phase is difficult to obtain from inspecting complete ME sensor structures. Our results show the applied magnetic materials are very sensitive to mechanical stress and its local variation. In addition, small deviations from the desired magnetic properties lead to more pronounced performance degradation of high sensitivity ME sensors. As a consequence, *in situ* stress measurements, allowing the determination of layer stress during deposition, will be used to understand and control the acting mechanisms. The deposition tool CS400 will be equipped with a multi-beam optical sensor (ksa-MOS from *k-Space Associates*, Michigan, USA) to measure arising substrate bow with the necessary very high sensitivity. To detect possible changes in the deposition conditions during long-lasting processes, the optical sensor provides an extra growth rate monitor. The stress measurements will be complemented by measurements of the energy flux from sputter

source to substrate. Such a method has been developed in the Plasma Technology Workgroup at CAU in the Institute of Experimental and Applied Physics by Prof. Kersten. It is based on a calorimetric probe [St10] which can be moved across the chamber to enable locally resolved energy flux measurements. This technique has been applied to magnetron sputter deposition in DC-, RF- and HIPIMS mode [Ga19, Bo13, Lu09]. At the time of writing, design, calibration, adaption to the CS 400 deposition tool, and installation are ongoing and conducted in cooperation with Prof. Kersten.

For the magnetic characterization, in the last funding period a unique large-view magnetooptical microscope setup has proven to be very useful (e.g. [A1-01, A1-02]). The microscope will be equipped with pulsed illumination sources to allow for time-resolved imaging of full sensor structures. For this, two different types of laser sources will be integrated in the microscope, enabling overview characterization of sensors across the whole frequency range of application in one go. In a first configuration level, we will integrate a solid state laser for frequencies up into the MHz regime. In a second step, we will integrate a model-locked laser for frequencies into the GHz regime. The integration of the high-speed illumination schemes together with the needed electronics will enable for the first time time-resolved imaging of complete sensor structures.

WP2: Sensor requirements

This work package will be conducted in close exchange with the projects on sensor concepts, in particular but not exclusively with **A7** and **A9**. Excitation modes, operation frequencies, substrate properties such as thermal expansion and roughness as well as targeted lateral dimensions of sensor structures are described for each sensor concept. Moreover, the various application scenarios addressed in the **B** projects require further sensor adaption. Thus, for each sensor concept specific requirements must be fulfilled by the piezo-magnetic phase, including sensitivity and magnetic domain control. The conditions will be determined in conjunction with magnetic response modeling and connected ME sensitivity behavior. Together with the individual boundary conditions identified for the fabrication of the magnetostrictive phase, the attainable best magnetic properties are identified. Based on the identified preferred material properties, concepts are investigated with attention paid to the structure and fabrication of the targeted magnetostrictive structures (WP3 to WP5). Our already existing concepts will serve as a starting point and will be further extended to the differing and developing sensor concepts. As the concepts advance in the course of the studies, the specifications will be constantly adapted. WP2 will provide essential input for the work packages WP3 to WP6.

WP3: Magnetic building blocks

Applying the characterization methods established in WP1 to the magnetic film deposition, this work package acquires deposition conditions prerequisite for the fabrication of magnetostrictive layer units used to build up the more complex layer structures for WP4 and WP5. A possible “toolbox” of magnetic layer elements is shown in Fig. A1-6. The figure is also of importance to WP4 and WP5)

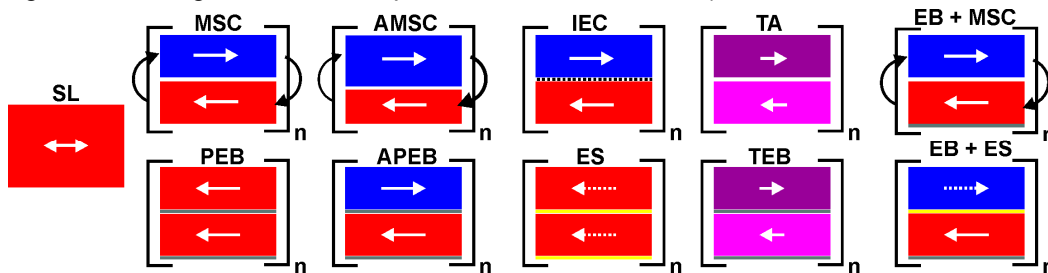


Figure A1-6: Possible layer structure elements providing a toolbox for the magnetostrictive phase for advanced sensor structures. Structures may include layer elements as single layer (SL) with defined anisotropy axis and strength and multilayers involving magneto-static coupling (MSC), also in asymmetric layer configurations (AMSC), systems based on interlayer exchange coupling (IEC) or artificial antiferromagnets, systems with tilted anisotropy (TA). Exchange bias can be parallel (PEB), antiparallel (APEB), or at a tilted configuration (TEB). Variable biasing can be induced by applying exchange spring (ES) structures. Possible combinations include single layer exchange bias together with magneto-static coupling (EB+MSC), exchange bias with exchange spring (EB+ES), and others. Arrows show the possible alignment of net magnetization inside the individual layers. In WP3 the number n of repetitions is limited to $n = 1$. (Higher numbers of n and combinations of the elements will be used in WP4 and WP5).

We will investigate elementary structures that will provide high sensitivity and magnetic domain stabilization to obtain minimum LOD. Because of its excellent material properties, the layer concepts will first be based on $(\text{Fe}_{90}\text{Co}_{10})_{78}\text{Si}_{10}\text{B}_{12}$. Concepts such as single layer (SL), parallel exchange biased (PEB) [La12], and antiparallel exchange biased (APEB) layers have already been successfully applied to modulated ME sensors [A1-1]. Yet, SAW substrates and few of the concepts themselves involve a fabrication route which do not allow post thermal treatment to adjust the magnetic properties. As pointed out before, control of induced magnetic

anisotropy with regard to alignment and strength is of major concern for constructing the advanced multilayers investigated in WP4 and WP5, e.g. stacks with layer-wise tilted anisotropy (TA) and non-collinear unidirectional anisotropy (TEB). Thus, in WP3 one focus is on deposition of magnetic layers in magnetic fields to *in situ* set the magnetic anisotropies. Furthermore, the methods for measuring stress and energy flux developed in WP1 are applied to identify and evaluate thermally and mechanically induced effects of in-field deposition on the magnetostrictive layers. For the sensor concepts, where thermally induced stress is not an overriding issue, anisotropy manipulation by deposition will provide more flexibility in the tailoring of the magnetostrictive phase. In view of the building blocks shown in Fig. A1-6, the following intermediated steps will be taken.

- (a) In exchange biased layers the established seed-layer Ta/Cu is to be replaced by a thin magnetic layer to enable well-defined unidirectional anisotropy already by magnetic field deposition.
- (b) As an alternative approach to EB, a hard magnetic layer in exchange spring (ES) systems will be prepared with thin MnIr/NiFe bi-layers. It combines the low magnetostriction of NiFe combined with the high anisotropy induced by the antiferromagnet. It can be reset without temperature treatment.
- (c) Interlayer exchange coupling (IEC) systems using a Ru interlayer exhibiting a layer thickness close to the thickness for the second antiferromagnetic coupling maximum will be introduced. The project work will benefit from the layer homogeneity and moderate deposition rate of the CS 400.
- (d) For magnetostatically coupled layers (MSC), either Ru layers with increased thickness or non-conducting interlayers will be introduced.

As an essential part of WP3, the fabricated single and bilayers are tailored and magnetically characterized with special attention to the magnetic properties relevant to the intended specific sensor operation. The locally resolved magnetic properties as characterized by magnetooptics are correlated to the results of layer stress, energy flux measurements, and structural investigations (**A6**) for further adjustment of deposition conditions. The stacks and deposition conditions will be individually adapted to the specific sensor concepts. In particular, magnetic properties relevant to the high-frequency operational modes, such as ferromagnetic resonance frequencies and effective magnetic damping parameters α_{eff} , are of relevance. In preparation for WP5 and WP6, the magnetic properties are evaluated as a function of temperature in order to determine upper limits for thermal load in layer and sensor processing after magnetostrictive layer deposition.

WP4: Advanced magnetic multilayers

Based on the fundamental layer structures, route of preparation, and layer properties which were achieved in WP3, we will investigate complex magnetic multilayers for high sensitivity and low noise density. With changing sensor requirements (WP2), we will adapt and reinvestigate aspects of layer preparation and relevant magnetic layer properties. Depending on the mode of application, different magnetic layer elements from the toolbox will be combined and stacked to the required film thicknesses. As an example, whereas SAW sensors (**A9**) currently require comparatively thin layers, e.g. converse ME sensors (**A7**) demand magnetostrictive layers with a total thickness in the micrometer range. Keeping the magnetic properties across the entire cross section, we will investigate scaled up magnetic multilayer systems. Possible multilayers with targeted modes of stacking are shown in Fig. A1-6 ($n > 1$). Recently investigated multilayers consisted of up to $n = 20$ building blocks [A1-2]. Supporting magnetic modeling of magnetic, magnetostrictive, and ME response will be used to predict the general sensor behavior. Systems will be characterized in terms of magnetic response, lateral magnetic domain behavior and effective magnetic properties, magnetostriction, ME response, and noise (in cooperation with **B1**). For this we will also rely on cantilever based resonant ME sensor structures from **Z1**. Yet, the investigated structures will directly relate to the sensor concepts of relevance. Layer properties will be evaluated under conditions as close as possible to sensor operations.

Based on the results of WP3, layers will be deposited, including single layer structures, layers stacked with non-magnetic (isolating) intermediate layers for magnetostatically coupled (MSC) layers or for the minimization of eddy current effects in high frequency sensor structures. Magnetic domain effects will become more relevant for the increased thicknesses scaling up the building blocks of WP3. Magnetic domain investigations on structured samples will be used to gain understanding of film stress influence (WP2) for the thicker layers and will provide input for readjusting individual layer thicknesses in WP3 and supply a foundation for WP5. The minimal magnetic interlayer coupling (IEC) elements for magnetic domain stabilization will be investigated. Exchange biased layers, depending on the targeted sensor schemes in a PEB, APEB, or TEB configuration, will be characterized with the focus on obtaining the intended characteristics up to high magnetic thicknesses. Adjusting magnetic anisotropies, e.g. layer-wise tilted anisotropy (TA), with the as-deposited state will allow for setting the magnetic properties for individual layers of the multilayer structure for shaping of magnetic response curves. Combined systems could consist of a combination of exchange bias and magnetostatic coupled devices (EB+MSC), enabling magnetic domain stability without reducing the sensitivity in the magnetic field sensing layer due to exchange bias. A combination of magnetostrictive and non-magneto-

strictive magnetic layers allows for decoupling of magnetoelastic layer response while still controlling demagnetization effects for some of the magnetic multilayer concepts. The examples shown in Fig. A1-6 are not complete but do provide insight into possible magnetic arrangements. Depending on the applied sensor concepts and the required processing of the devices, e.g. post-annealing and packaging, the ways of improving or preservation of magnetic properties with temperature treatment will be investigated. Here, the stability of the pre-adjusted magnetic anisotropies with temperature is of relevance. Local stress effects related to the temperature treatment will be investigated. Relaxation effects occurring in the magnetostrictive phase scale with the overall layer thickness, depending on the actual stress state of the films (see WP3). The effects are less relevant for thinner magnetic structures but are likely to have a strong influence on thicker layer stacks relevant to sensor applications such as in **A7** and smaller sized sensor structures. Further investigations will focus on the control and limit of magnetic layer deposition and magnetic layer properties over the entire multilayer thickness, which will restrict the application of certain concepts to thinner layer structures. Evaluating and stretching the limits of the proposed layer structures in terms of thickness is an important subject of this work package. Structural properties will be evaluated with **A6**.

By comparing the magnetic, magnetostriction, and ME response behavior with the structural parameters and magnetic domain behavior, a complete understanding of the connections of the aspects of layering will be derived. Limitations for the incorporation of magnetic building blocks into complex multilayers in sensor structures will be estimated and layer systems will be accordingly modified. If this work package should lead to new findings regarding the achievable magnetic behavior of the piezomagnetic layers, modified magnetic building blocks will be reinvestigated in WP3. Based on the knowledge gained, selected approaches will be directly transferred to real sensors (WP6) and combined with lateral structures (WP5).

WP5: Hybrid lateral structures

Patterning effects play a major role in the resulting effective magnetic properties and domain structures. In addition to pure magnetostatics, stress relaxation effects are significant and add laterally distributed magnetic anisotropies. The hybrid anisotropy effects have to be considered as they might influence the layer magnetizations. Magnetoelastic effects of the piezomagnetic phase also provide the opportunity to further tailor the effective magnetic properties of the piezomagnetic sensor layers. WP5 will address this issue for the incorporation of the magnetic building blocks of WP3 and WP4 into real sensor structures (WP6). We will also investigate patterning to further improve the effective magnetic film properties in terms of noise and sensitivity by tailoring the effective magnetic anisotropy, by ensuring single domain response, and by providing (local) magnetic bias fields. As an example, stress-induced anisotropies occurring at the edges will be used to tailor the effective anisotropy and to align the magnetization in a (now) intended way. An overview of possible contributions and approaches to influence the ME sensor properties is displayed in Fig. A1-7.

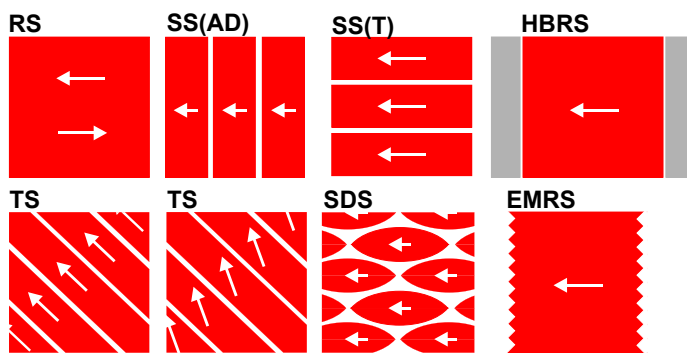


Figure A1-7: Examples of possible patterning effects of a regular structure (RS). Depending on the stress state of the film, stripe structures (SS) help to align the magnetization along certain directions including along independent directions for tilted stripes (TS). Individual elements (see also **A9**) can be used to obtain single domain structures (SDS). Hard bias (HB) (shown for regular structures – HBRS) or edge modifications (EM) (shown for regular structures – EMRS). Arrows indicate the direction of magnetization.

Layer structures to be applied are based on the results of WP3 and WP4. For structuring the magnetic layers, we access the established combination of optical lithography and ion beam etching. Depending on the actually desired effect, rather vertical or flattened profiles are to be produced by adjusting the impact angle of incident Ar ions, whose influence on the effective demagnetization field will be investigated. Based on the requirements defined in WP2 and the options provided in WP3 and WP4, we will investigate methods of further tailoring the ME response by patterning. Effective magnetic anisotropy can be modified by patterning the sensor structures, e.g. into stripes. Not only shape anisotropy effects but also developing magnetoelastic magnetic anisotropy contributions developing at edges play an important role here. For the magnetostrictive layer structures, stress relaxation effects manage to overcome magnetostatic interactions. Depending on the stress state of the films, an additional anisotropy perpendicular to the stripe axis (SS(AD)) or parallel to the stripes (SS(T)) can be obtained. The additional anisotropy will be needed to balance the existing magnetic anisotropies in the films. Depending on the direction of anisotropy, additive or subtractive contributions will allow tailoring of the effective anisotropies and thus the magnetic response to external stimulus. The effec-

tive control of mechanical stress achieved by the *in situ* stress measurements in WP3 and the understanding of such are an important prerequisite for reliable application of the proposed measures.

In addition, we will investigate compensating for anisotropy stress contributions, e.g. relevant for SAW-based sensor devices (**A9**), by patterning. This might also include partial anisotropic patterning of the film surface. We will further explore how non-collinear alignments of stripes and anisotropy (e.g. tilted stripes (TS)) can be utilized to further customize magnetic response. The general response will be modeled in advance to predict and also gain insight into the magnetic behavior. Magnetic domain behavior will always be considered and checked experimentally, as will the magnetic response characteristics. Adhered permanent magnetic structures (HBRS, see also Fig. A1-7, together with **Z1** for powder magnets) will be employed to apply a local magnetic bias field to the structures. This includes hard biased single layer structures and parallel exchange biased structures. This will be first investigated to minimize magnetic domain effects in the structures but will also be investigated to influence effective magnetic susceptibility in the sensors and to adjust the working point of sensors. Partial compensation of effective anisotropy as an external measure to tune the magnetic anisotropy beyond film properties is another aspect of hard bias. Elements of the supporting structures will be first investigated independently and parallel to WP4. In a second step, structures will be merged with each other and also combined with elements of WP4 for the targeted utilizations. It is obvious that some structures of the toolbox of WP3 and WP4 will not be compatible with the structures pursued in this work package (for instance AP structures with hard bias HB). Therefore, investigations will always be carried out in conjunction with meaningful targets. The hybrid structures will again be investigated by analyzing overall magnetic, magnetostriction, ME response, and magnetic domain characteristics with a focus on low noise and high sensitivity for the resulting ME sensors. It is expected that layer complexity will increase in the course of the work package. All investigations will be performed with the subsequent work package in mind, as the hybrid film structures form the basis for WP6.

WP6: Incorporating layer and lateral patterning schemes in sensor structures

From previous work, it is known that special attention has to be paid to the integration of the advanced multilayers and hybrid lateral structures. Sensor specific integration related issues are considered in close cooperation with projects on sensor concepts (**A4**, **A7**, **A9**), project **B1**, as well as service projects **Z1** and **Z2**. Whereas magnetic layer deposition is conducted by **A1**, actual sensor fabrication and characterization regarding sensor sensitivity, noise, and LOD is within the responsibility of the collaborating projects. Laterally resolved magnetic characterization, magnetic property characterization, and magnetic domain imaging are performed to reveal potential magnetic property changes of the integrated magnetic structures due to sensor processing. The achieved sensor performance is evaluated and correlated to the outcome of magnetic characterization. This might lead to a reevaluation of the layer concepts of WP2 and investigated design options in WP3 to WP5. If required, layer deposition, multilayering and structuring will be adapted with the new insights.

Prospects

With the developing focus of ME sensors within the CRC, we expect developments in sensor concepts that lead to altered requirements of the piezomagnetic phase and that will provide new challenges to the applied magnetic layers. Research on adaption to the concepts, meaning investigating magnetic building blocks, overall layer structure, patterning layout, and stress effects to increase sensor sensitivity and minimizing magnetic noise will continue. With improved sensors, additional possible sources of magnetic noises not related to magnetic domain behavior will become a focus of attention.

3.6 Role within the Collaborative Research Centre

A1 plays a central role within the CRC to achieve an improved limit of detection, which is essential to the measurements of the targeted biomagnetic signals. We will collaborate closely on the sensor fabrication and magnetic characterization with the groups in research area **A**. Magnetic characterization and domain imaging is planned particularly with **A4**, **A7** and **A9**. A strong cooperation on integration issues will be conducted with **Z1**. A1 will contribute to the focus group "Magnetic Layers" on issues of the magnetostrictive phase for ME sensors and to the focus groups "Comparison of Sensor Concepts", "Concepts based on ΔE -effect", and "ME Sensors". Collaborations with the following projects are planned:

- A4:** Research on advanced magnetic multilayers for ΔE -effect sensor. Assistance with deposition and magnetic characterization of ΔE -effect sensors will be provided.
- A6:** Amorphous and structural properties (radial distribution function analysis, chemical composition)
- A7:** Research on advanced magnetic multilayers for converse magnetoelectric sensors. Cooperation on time-resolved investigations of the magnetic domain evolution of electrically modulated ME sensors.

- A8:** Cooperation on modeling regarding optimal magnetic film properties.
A9: Research on advanced magnetic layers for SAW sensors. Cooperation on time-resolved imaging.
A10: Cooperation on magnetic noise effects in ME sensors. Magnetic layers for stress initiated effects.
B1: Noise studies and tailoring the ME response with regard to the frequency modulation technique and simultaneously controlling the magnetic domain states.
Z1: Integration of novel magnetostrictive multilayers into ME devices. Cooperation on powder magnets for hard bias and sensor integration. Wafer-cut ME sensors for advanced magnetic multilayers.
Z2: Supportive ME measurements regarding noise density and limit of detection.

3.7 Differentiation from other funded projects

None of the other funded projects of the PIs deals with magnetostrictive or magnetoelectric materials.

3.8 Project funding

3.8.1 Previous funding

Funding of this project within the Collaborative Research Centre started in 07/2016.

3.8.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral researcher, 100 %	2	66.3	2	132.6	2	132.6	2	132.6	2	66.3
Total										
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables	14.75		15.5		13.5		13		5.25	
Total	14.75		15.5		13.5		13		5.25	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation above k€ 50	83.7		-		-		-		-	
Total										
Grand total	164.75		148.1		146.1		145.6		71.55	

(All figures in k€)

3.8.3 Requested funding for staff for the new funding period

	Se- quen- tial no.	Name, academic degree, position	Field of research	Department of university	Project commitment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	McCord, Jeffrey, Prof. Dr.-Ing. Head of Research Group	Magnetic materials	IMS	4		Core support
	2.	Meyners, Dirk, Dr. Senior Researcher	Functional materials	IMS	4		Core support
	3.	Dr. Kornel Richter	Magnetic materials	IMS	4		Core support

	4.	Dr. Antonio Malavé	Functional materials	IMS	2		Core support
Non-research staff	5.	Robien, Sandra, Dipl.-Ing., Technician		IMS	1		Core support
Requested staff							
Research staff	6.	Elizaveta Golubeva, Doctoral Researcher	Magnetic materials	IMS		E13	
	7.	Lars Thormählen / N.N., Doctoral Researcher	Functional materials	IMS		E13	

Job description of staff (supported through available funds):

1. Prof. Jeffrey McCord represents project A1 with regard to magnetic layer design and characterization including magnetic domain investigations of magnetostrictive multilayers. He supervises the doctoral researchers and supports the planning and execution of magnetic modeling and annealing experiments and the interpretation of magnetic analysis results. He oversees the investigations on hybrid structures. He provides input for the development and implementation of concepts for improved magnetic response in ME composites. He coordinates the cooperation with other relevant projects of the CRC.
2. Dr. Dirk Meyners represents project A1 with regard to magnetic layer design, film characterization, and film deposition of magnetostrictive multilayers. He supervises the doctoral researchers and supports planning and execution of deposition and structuring experiments. He organizes the collaboration with Prof. Kersten's group for energy flux measurements. He coordinates the cooperation with other projects of the CRC and in particular the cooperation with project **Z1** on MEMS ME sensor manufacturing.
3. Dr. Kornel Richter supports the doctoral researchers with the magnetic characterization.
4. Dr. Antonio Malave is the responsible scientist for the operation of the Kiel's Nanolab. He will support the doctoral researchers in planning and execution of lithographic and etching processes.
5. Dipl.-Ing. Sandra Robien will assist with the design of electronic components for the experiments.

Job description of staff (requested):

6. M.Sc. Elizaveta Golubeva is planned as a doctoral researcher for the studies. She has a degree in physics from the Ural Federal University with a strong background in magnetism. Since 08/2019 she has been working as a researcher on the project. She knows the experimental techniques and conducted the analysis of the hard bias shown in the proposal. She is acquainted with the use of modeling programs. She will first concentrate on the integration of the stroboscopic illumination schemes in the large view setup (WP1). She will further perform the magnetic ME modeling (WP2) and the magnetic characterization and domain analysis within WP3, WP4, and WP5. She will lead the experiments on hybrid lateral structures (WP5). She will conduct further modeling of magnetic and ME response for WP4 to WP5. She will investigate time-resolved magnetic domain behavior on complete ME structures (WP6).
7. M.Sc. Lars Thormählen/N.N. At present Mr. Thormählen conducts the experiments on the preparation of magnetostrictive multilayers. He will support the installation of the equipment for stress and energy flux measurements (WP1). Using these methods he will investigate the deposition of magnetostrictive single layers and basic coupled multilayers (magnetic building blocks) according to WP3. Furthermore, he will continue the research on depositing advanced multilayers. He will collaborate with the projects on sensor concepts in area **A**, **B1**, and service projects to investigate sensor performance and integration related problems. He is expected to finish his Ph.D. studies in the first stage of the next funding period. He will instruct the new researcher, who will take over the research.

3.8.4 Requested funding for direct costs for the new funding period

(All figures in k€)

	2020/2	2021	2022	2023	2024/1
Existing funds from IMS	3.0	6.0	6.0	6.0	3.0
Sum of existing funds	3.0	6.0	6.0	6.0	3.0

Sum of requested funds	12.25	13	13.5	13.0	5.25

Equipment up to k€ 10, software, consumables for 2020/2

Cleanroom costs (photoresist, developer, solvents, etching solution, consumables)	k€	1.25
Si wafers	k€	1.50
Lithography masks	k€	1.00
Sputter deposition targets (FeCoSiB, NiFe, Ta, MnIr)	k€	2.50
Optics for large view-microscope laser integration	k€	3.00
Parts for time-resolved optical setup incl. electronics, LED, and power supplies	k€	2.00
Consumables (microscope, electronic and optical replacement parts)	k€	1.00

Equipment up to k€ 10, software, consumables for 2021

Cleanroom costs (photoresist, developer, solvents, etching solution, consumables)	k€	2.50
Si wafers	k€	2.00
Lithography masks	k€	3.00
Sputter deposition targets (FeCoSiB, Ta, MnIr)	k€	3.50
Consumables (microscope, electronic and optical replacement parts)	k€	2.00

Equipment up to k€ 10, software, consumables for 2022

Cleanroom costs (photoresist, developer, solvents, etching solution, consumables)	k€	2.50
Si wafer	k€	2.00
Lithography masks	k€	3.00
Sputter deposition targets (FeCoSiB, Ta, MnIr)	k€	4.00
Consumables (microscope, electronic and optical replacement parts)	k€	2.00

Equipment up to k€ 10, software, consumables for 2023

Cleanroom costs (photoresist, developer, solvents, etching solution, consumables)	k€	2.50
Si wafer	k€	1.50
Lithography masks	k€	3.00
Sputter deposition targets (FeCoSiB, Ta, MnIr)	k€	4.00
Consumables (microscope, electronic and optical replacement parts)	k€	2.00

Equipment up to k€ 10, software, consumables for 2024/2

Cleanroom costs (photoresist, developer, solvents, etching solution, consumables)	k€	1.50
Si wafer	k€	0.50
Lithography masks	k€	0.50
Sputter deposition targets (FeCoSiB, Ta, MnIr)	k€	1.75
Consumables (microscope, electronic and optical replacement parts)	k€	1.00

3.8.5 Requested funding for instrumentation for the new funding period

Instrumentation above k€ 50 for financial year 2020

Multi-beam optical sensor for installation into cluster deposition tool CS 400 - Model: ksa-MOS, Manufacturer: <i>k-Space Associates</i> , Michigan, USA	k€	83.70
Control and minimization of layer stress is a key factor for the deposition of the desired magnetostrictive layer systems exhibiting low and controlled effective magnetic anisotropy. According to our preceding project work, a measurement of total stress after deposition is not adequate to unambiguously identify the processing steps leading to stress formation. The requested optical sensor enables <i>in situ</i> measurement of arising substrate bow during film deposition with outstanding sensitivity (minimum detectable stress in a 1 µm metallic layer on a 100 µm substrate (E = 100 GPa): 0.1 MPa). Thereby, stress monitoring during long-lasting multilayer processes is possible, enabling adjustment and updating of deposition conditions. In combination with the energy flux measurements and structural investigations (A6), the <i>in situ</i> stress measurements will lead to a much better understanding of the interplay between deposition conditions and resulting magnetic multilayer properties. The optical sensor setup is adapted for implementation into the existing deposition tool.		

3.1 General information about Project A2

3.1.1 Project title: Hybrid magnetoelectric sensors based on mechanically soft composite materials

3.1.2 Research areas

406-02 Synthesis and Properties of Functional Materials

408-01 Electronic Semiconductors, Components, Circuits, Systems

3.1.3 Project leaders

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Do any of the abovementioned persons hold fixed-term positions? No.

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

The project aims to develop novel magnetoelectric (ME) sensors that are not based on conventional magnetostrictive and piezoelectric materials but involve new material concepts for the efficient conversion of the magnetic field change into an electric signal. We use composite cantilevers and pursue two key strategies: 1) Reduction of passive materials and components, in particular the substrate is eliminated or the substrate effect is drastically reduced by a minimalistic sensor design; 2) The energy for bond stretching is minimized by employment of very soft materials for the magneto- and electroactive components. In the current funding period, both strategies were successfully implemented. Clamp-free mechanically soft magnetostrictive composite cantilevers with a bending at saturation of almost 5° and an order of magnitude higher piezomagnetic coefficient (compared to, e.g. conventional metglas) were developed, and the potential of soft and non-clamped materials as an alternative magnetostrictive component was clearly demonstrated. Moreover, the piezoelectric material was completely removed in the sensor design and replaced by an electret generator/transducer setup, which enabled very compact and simplified cantilever sensors. Here, we also introduced a new approach to soften the vibrating beam by reduction of the restoring force through the attractive electrostatic electret potential. This approach increases the oscillation amplitude while reducing the resonance frequency and simultaneously gaining bandwidth. Accordingly, the electrostatic interaction enables direct detection of magnetic fields with a large bandwidth.

In the second funding period, we plan to extend our demonstrated electret generator/transducer principle for the development of hybrid ME sensors based on mechanically soft composite materials. Emphasis will now

shift from first feasibility studies to advanced designs and low limits of detection. In order to increase the sensitivity, we intend to maximize the total chargeable electret surface by using highly porous materials as templates. In this approach, a thin film dielectric fluoropolymer will be deposited onto the porous template by initiated chemical vapor deposition (iCVD) combined with a subsequent corona discharge treatment. iCVD in conjunction with corona discharge already turned out to enable unique deposition of ultra-stable fluoropolymer electret thin films. Especially the growth characteristics typical for CVD and low process temperature of iCVD permit the deposition on the complex and temperature sensitive substrates envisioned here. A custom-made setup based on syringe pumps allows 3D printing of complex resonator geometries, which are made up of mechanically soft composites, e.g. silicone, filled with magnetic micro- and nanoparticles. Thus, the unique combination of sensor fabrication methods provides design freedom for the individual components with micro scale precision in 3D for the optimum tailoring of the potential energy landscape of the ME resonators by the targeted employment of non-linearities like progressive characteristics or attractive potentials. The developed sensors will allow direct measurements with a large bandwidth, particularly in the range of 10 - 40 Hz for applications in magnetocardiography.

3.3 Project progress to date

3.3.1 Report and current state of research

The focus of **A2** is on the development of novel low-frequency ME sensors that are not based on conventional magnetostrictive materials (based on spin-orbit coupling) and piezoelectric materials. Instead, hybrid material concepts are pursued for efficient conversion of the magnetic field change into an electric signal. In the conventional inorganic bending beam sensors, work is not only performed to separate charges but also to stretch bonds in the magnetostrictive and piezoelectric materials and substrates. Consequently, one of the main ideas of **A2**, in addition to eliminating passive components, is to develop hybrid sensors that consist of mechanically soft composite materials. In general, the envisaged mechanical softening of the sensor components can be achieved by incorporating organic materials and/or voids such as micro- and nanopores or larger air gaps into their matrix structure. Here, two different softening routes were chosen for the magnetostrictive and piezoelectric components:

- (A) The magnetostrictive part was realized by a mechanically soft elastomer containing magnetic microparticles or the addition of an attractive Coulomb potential to effectively soften conventional metallic glass materials.
- (B) For the piezoelectric part, the classical piezoelectric material was replaced by an electret thin film compliant with the mechanically soft magnetostrictive material and containing permanent electric charges as an alternative quasi-piezoelectric component, i.e. the electret produces mirror charges in the vibrating electrode of a variable plate capacitor. The charge density increases with increasing deflection of the vibrating electrode towards the electret surface.

(A) Soft magnetoactive composites

Concepts for soft magnetoactive composites in the literature include magnetorheological fluids [Ku17], gel magnets [An12], and soft magnetic elastomers [St19]. Much progress has also been made in the theoretical understanding of these materials [El18]. The addition of nanoparticles to mechanically soft magnetic materials was investigated for various types of particles [Do18][Ha11] [Wa17] to tailor the magnetic properties.

Within the current funding period, various mechanically soft magnetostrictive composite materials were fabricated and characterized by the Adelung group. The investigated methods and materials included dip coated elastomer film stacks, casted bulk elastomers, mixed magnetorheological fluids, printed magnetic ink structures and infiltrated aeromagnets. Fig. A2-1 shows some examples. In contrast to conventional magnetostrictive materials, the present composites do not need to contain a magnetostrictive material. The magnetostrictive properties arise from the forces between the ferromagnetic microparticles in the polymer matrix. When applied to a cantilever beam as commonly used for ME sensors, the figure of merit does not only contain the magnetostriction but also includes the elastic moduli of both magnetostrictive material and substrate material as well as their layer thicknesses [Sm91]. Accordingly, a low elastic modulus of the substrate and a relatively thick magnetostrictive layer will cause a large deflection of the cantilever, which is needed for a large effect. Due to the absence of mechanical clamping to a piezoelectric layer or a substrate, the coupling can be assumed to be ideal, and the measured signal of a capacitive sensor is directly related to the deflection. Consequently, the figure of merit when developing soft magnetic composites for capacitive sensors is rather the deflection than the magnetostriction. It could be demonstrated that the highest deflections for a given magnetic field are obtained when using a soft matrix material filled with aligned magnetic particles (see Fig.

A2-1d). Besides the nano- and microscale structure, it turned out that the overall shape of the composite is of great importance in making the composites usable in sensors. A high flexibility in fabrication can be achieved via the 3D-printing and laser-cutting processes developed in the current funding period (see Fig. A2-1b, c for example).

Magnetoactive polymer composites were produced by molding and 3D printing different polymer matrixes filled with 20 wt% ferromagnetic particles. The samples were cut into cantilevers and a thin metallic film was sputtered onto one side in order to induce beam bending during the sample characterization. The magnetoactive tip displacement was calculated from measurements performed in the magnetostriction setup constructed in the framework of this project. Note that the common magnetostriction measurements in this CRC are based on thin ferromagnetic films deposited onto non-magnetic cantilever substrates and typically represent the piezomagnetic coupling coefficient (see i.e. [Gr10]). However, in the frame of electret based sensing, the tip displacement (see geometrical sketch in Figure A2-5) represents the decisive physical quantity. Fig. A2-1d demonstrates the superiority of the magnetoactive polymer cantilevers if compared to the conventional thin film metallic glasses deposited onto Si cantilevers in terms of the piezomagnetic coefficient of the tip displacement at higher magnetic bias fields. Since the strong magnetoactive straining of the composites arises from the displacement of the distributed hard magnetic particles within a soft matrix [Ka07] no saturation deformation is reached at moderate external magnetic fields. Consequently, the magnetoelectric sensitivity of a soft composite cantilever keeps increasing at higher bias fields whereas the magnetostrictive thin film reaches a saturation value. In the next funding period, the possibility of self-biasing via mechanical pre-straining of the composite will be investigated. Hereby, a direct increase of the sensor sensitivity and simultaneous reduction of the necessary bias field can be expected. [Zh16]

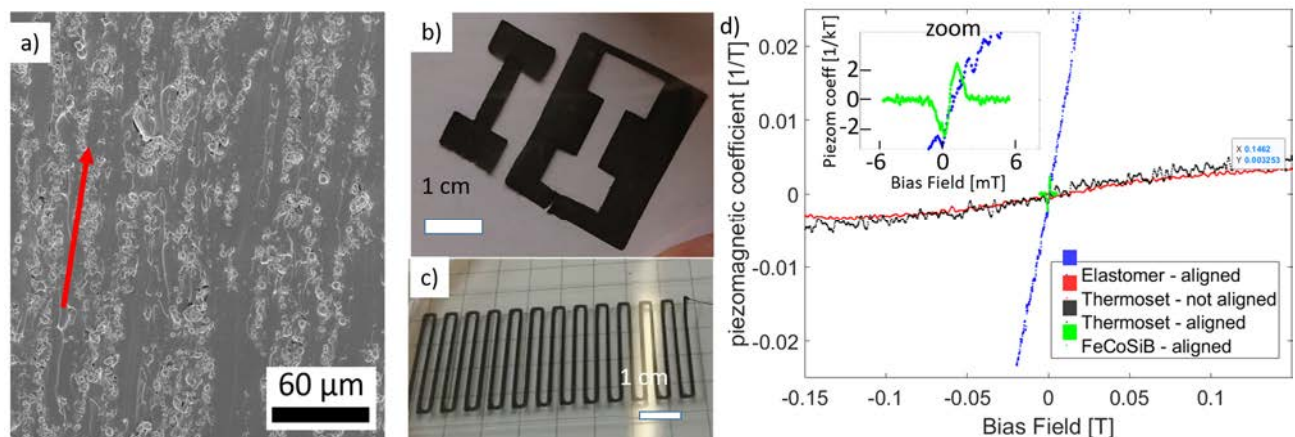


Fig. A2-1: (a) SEM image of magnetostrictive bulk elastomer. One notes the alignment of the magnetic particles in the direction of the magnetic field (red arrow.) (b) Casted PVB film filled with Fe particles and shaped by laser cutting. (c) Meander-shaped polymer, 3D printed using a direct ink writing technique. (d) Piezomagnetic coefficient of tip displacement as response to static magnetic fields normalized to cantilever length. The largest effect (blue) was observed when using a mechanically soft elastomer matrix with aligned particles, which is at least an order of magnitude larger than conventional magnetostrictive materials (FeCoSiB, zoom). The absolute maximum could not be detected because the measurement exceeded the capabilities of the device used. The effect of alignment was investigated using the thermoset polythiourethane (marked red and black). The alignment of magnetic filling particles improved the piezomagnetic coefficient by ~50%. Compared to conventional materials such as FeCoSiB (green), the required bias fields are higher.

(B) Soft piezoelectric component: Electret-capacitor replaces piezoelectric material

As described in the introduction, we have applied the electret generator/transducer principle to replace the piezoelectric layer which transforms the deformation of the magnetostrictive material into an electric signal. Bulk polymer electrets, which have been used almost exclusively so far [Se87] [Zo19], cannot be used for this purpose. A precise thickness control as well as a conformal surface is inevitable with regard to the air gap control of the sensor device, which can only be obtained by thin film electrets. Much effort has been put into the development of electret thin films so far [Ka97] [Am92] [Mo73] [He78]. However, their performance was not competitive with bulk electrets, particularly with respect to charge stability. In this project, for the first time, we used iCVD to fabricate ultra-stable thin film electrets [A2-6].

iCVD enables a solvent-free synthesis of pinhole-free organic thin films with precise film thickness control on the nanometer to micrometer scale [A2-4]. The underlying free radical polymerization can be precisely tuned

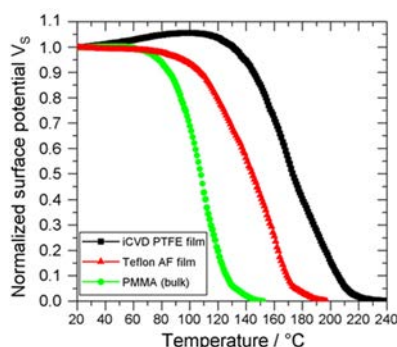


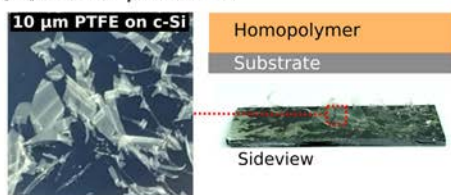
Figure A2-2: *Thermally stimulated discharge curves reveal that iCVD PTFE thin film electrets have a higher charge stability than Teflon AF thin film electrets. PMMA is shown as a representative for the performance of non-fluoropolymers.*

by the synthesis parameters, and the process can be easily scaled up to large size substrates due to the growth characteristics typical of CVD. We used polytetrafluoroethylene (PTFE) thin films for the project because PTFE typically shows the best properties for electret applications. A new iCVD chamber was set up for this purpose, operating in a continuous flow mode. The deposition rate of the PTFE films was

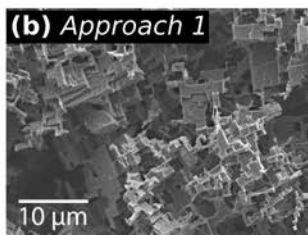
increased after trying different monomer and initiator combinations in order to obtain high rates for μm -thick film deposition, which are required for electret films, regarding the breakdown strength. Our iCVD PTFE exhibited a very low defect density that resulted in an extremely high breakdown strength. After charging in a corona setup, our electret films were even more stable than commercial Teflon AF films (Fig. A2-2) [A2-6] [A2-5] [A2-8]. The achievable surface charge of these films is very high ($V_s = -800\text{ V}$) and results in an effective change in potential per change in electrode spacing of $\Delta U/\Delta d = 187 \times 10^6\text{ V/m}$ at the moment.

However, the electret films also showed the typical low adhesion originating from the low surface energy of PTFE (which is also well-known from, e.g. frying pans). The films tended thus to delaminate from the substrate. Here, the phase transitions in the crystalline regions of PTFE at approximately $19\text{ }^\circ\text{C}$ and $30\text{ }^\circ\text{C}$ [Br05], which induce stress in the film, was identified to play a crucial role (Fig. A2-3a).

(a) Initial problem



(b) Approach 1



(c) Approach 2

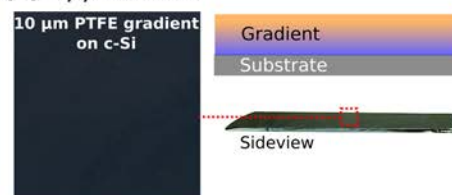


Fig. A2-3:(a) iCVD homopolymer thin films delaminate on flat surfaces (b) Nanosculptured Al substrates increase the adhesion significantly due to mechanical interlocking. (c) Gradient films feature 100% fluoropolymer functionality at the surface and 100% organosilicon functionality at the polymer-substrate interface due to the gradual change in composition, thus increasing the compatibility between film and substrate. Such films can also be applied on ultraflat surfaces, like Si wafers, without any sign of delamination, as shown in the photograph that exhibits no visible surface features.

The challenge of delamination was first solved by nanosculptured aluminum substrates (Fig. A2-3b) provided by the Adelung group. The aluminum is etched in a special procedure to fabricate small “anchors” at the aluminum surface. The mechanical interlocking between the PTFE film and the etched substrate surface is easily achieved due to the growth characteristics typical of CVD, leading to significantly increased adhesion. Another way to increase the adhesion became available when switching from homopolymers to copolymers. New gradient copolymer materials have been recently developed by the Faupel group (Fig. A2-3b) [A2-3]. They are inspired by natural structures (e.g. mussel byssus), where a gradient in Young’s modulus is used to stick soft materials (e.g. the mussel body) to hard surfaces (e.g. a jetty or rocks in the ocean). This biologically inspired approach was transferred to the polymer materials. The composition of the gradient polymer changes gradually from 100% polymer A to 100% polymer B on a scale of only 30 nm. On the top, PTFE was used to provide the electret properties of excellent charge storage, and on the bottom, an organosilicon monomer was used to form a highly cross-linked thermoset. It provides excellent adhesion to the substrate, also on extremely flat surfaces such as Si wafers, e.g. via bonds to the native oxide layer, without any sample pretreatment (Fig. A2-3c). In this way, also flexible organic substrates can be coated, as intended in the next period of this project. The novel nanoscale gradient concept developed in the current project, which was reported in [A2-3], can be not only applied to solve challenging adhesion problems but also applied in many fields ranging from biomimetic optical films to anti-icing coatings. The reaction kinetics during the free radical polymerization in iCVD have been observed by in situ mass spectrometry to obtain more precise control of the process and understand the underlying reaction kinetics. This technique is thus also available for the next period, where

new multifunctional copolymer materials are planned that require precise control of the deposition process. Addition of a suitable porogen during the reaction has shown to force a phase separation during the adsorption process of the monomer and porogen vapor. The reaction rates were correlated to the Cahn-Hilliard phase field model and enabled synthesizing thermoset thin films with sub 2 nm pore sizes, which can be used for tuning the dielectric film properties as well as increasing the effective surface area.

(C) Low frequency ME sensors by softening of mechanically hard resonators with electrets

During the present funding period, a novel design concept for ME sensors, the electret generator/transducer principle, was developed in joint work of the Adelung and the Faupel groups. Usually, damping an oscillator leads to a lower resonance frequency together with a lower amplitude. Here, the external electric field generated by an electret film is used to effectively reduce the spring constant of the cantilever but simultaneously increase the amplitude of the resonance. This, together with the broadening of the resonance curve, enables broadband measurements in the passive, low frequency mode. Fig. A2-5 shows the schematic and realization of the concept together with the modelling results. Modelling was carried out by modifying the harmonic oscillator differential equation and adding an attractive coulomb potential arising from electrostatic force caused by the electret:

$$\frac{d^2x}{dt^2} + 2\zeta\omega_0 \frac{dx}{dt} + \omega_0^2 x - \frac{1}{2m} \cdot \frac{\varepsilon_0 A V_S^2}{(d_0 - x)^2} = \frac{B}{m} \sin(\omega t)$$

Electrostatic force
Applied magnetic field

with deflection x , time t , eigenfrequency ω_0 , damping factor ζ , mass m , area A , potential V , gap size d_0 , and excitation amplitude B with a frequency ω . Amplitude and resonance frequency of the model fit qualitatively very well with the measurement values at different distances (gap sizes) of the electret, see Fig. A2-4c and d. The novel electret generator/transducer concept was published in [A2-1].

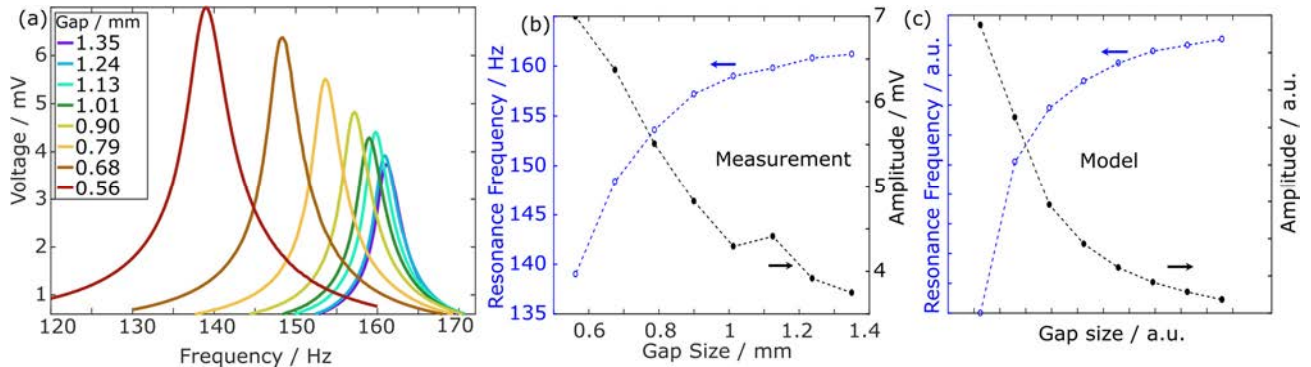


Fig. A2-4: Novel sensor based on “softening” of a cantilever by adding an attractive coulomb potential with an electret. (a) Average frequency response of an electret-based sensor for different gap sizes (in mm). The resonance is shifted to lower frequencies, but at the same time the peak gets higher and broader. (b) Measured (average) and (c) calculated changes from numerical solver for the mentioned differential equation, in resonance frequency (blue) and signal amplitude (black) with respect to the gap size. [A2-1]

Recent work on multi-resonant cantilevers for energy harvesting [Bo19] that could be frequency tuned by an external magnetic field confirmed our hypothesis and showed a reduction of stiffness for small distances to the external magnet. A tunable multi-resonant sensor will be part of the proposed work package WP5.

(D) Soft hybrid sensor

Soft hybrid sensors combining both electrets with soft magnetostrictive composites and resonance frequencies in relevant biomagnetic frequency regions were originally the focus of the current funding period. After the discovery of the electret generator/transducer sensors (see Sect. (C)), emphasis was put on the investigation of those systems. Meanwhile, first feasibility studies were also performed with the original soft hybrid sensors. Fig. A2-6(b) shows a cantilever with a resonance frequency around 60 Hz. The electret-induced mirror charge can be read out from a conductive gold film deposited on the cantilever. Both current and voltage signals are accessible and permit the use of the sensor in a passive mode. When comparing the capacitive hybrid sensor with a conventional sensor (index p for piezoelectric), the generated voltage depends on the constant charge of the electret Q and is therefore directly defined by the capacity C of the setup by $U = Q/C$, which depends

on the distance between cantilever and electret $d = (d_0 - x)$ and the area A (see Fig. A2-5). Neglecting the change in area upon bending, one obtains:

$$\frac{\partial U}{\partial H} = \frac{\partial U}{\partial d} \cdot \frac{\partial (d_0 - x)}{\partial H} = \frac{\partial U}{\partial d} \cdot \frac{\partial d}{\partial H} = \frac{1}{\epsilon_0 \epsilon_r} \frac{Q}{A} \cdot \frac{\partial d}{\partial H}$$

$$\frac{\partial E}{\partial H} = \frac{\partial E}{\partial \lambda} \cdot \frac{\partial \lambda}{\partial H} = \frac{1}{\epsilon_0 \epsilon_r^p} \cdot \frac{\partial \left(\frac{Q}{A}\right)^p}{\partial \sigma^p} \cdot \frac{\partial \sigma^p}{\partial \lambda} \cdot \frac{\partial \lambda}{\partial H}$$

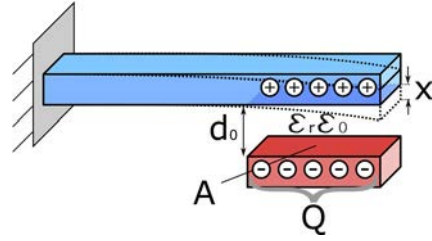


Figure A2-5: Sketch of a capacitive sensor. The magnetoactive cantilever (blue) is mounted facing an electret (red).

Different from the piezoelectric coefficient, the corresponding number for the electret-based sensor is not a material constant; it depends on the geometry of the sensor. Accordingly, the change in distance or deflection of the cantilever directly defines the magnitude of the sensor response and should be maximized. As shown in Fig. A2-6d, the deflection of the realized magnetoactive polymers already exceeds the deflection of conventional magnetostrictive cantilevers. The corresponding change in potential per change in distance that is currently achievable in the sensors is $\Delta U/\Delta d = 187 \times 10^6$ V/m. In general, the first non-optimized hybrid composite sensor turned out to represent a very flexible concept with great potential for improvement and will be exploited in the next funding period (see work plans for details). Hereby, one important aspect will be the advancement of the design in terms of the electrode position and the stiffness of the resonating composite material being specifically adjusted to produce the desired oscillation profile (see WP5). Another aspect will be the development of an adapted low frequency, low-noise signal processing. A direct comparison of the current and voltage signal implies that a current measurement could be more promising than the voltage measurements conventionally used for most of the other sensor types investigated in this CRC. This is why in the next funding period, an alternative measurement setup will be explored in collaboration with **A5** (related to the current measurements) and **B1** (see WP4).

(E) Noise Considerations

To enable the detection of small magnetic fields, a large signal-to-noise ratio is desired. By following the model presented in section C, an increase in the effective piezoelectric effect can be achieved by decreasing the distance between the cantilever and electret. As a comparative investigation, a cantilever consisting of magnetostrictive Metglas was measured with a piezoelectric thin film of PVDF and an electret-capacitive read out at a distance of 1 mm facing the cantilever. This relatively large gap was chosen to have a small effect on the resonance frequency, as shown in Fig. A2-4, and thus allows comparable measurements. The cantilever had a resonance frequency of 322.5 Hz in the absence of an electret and a resonance frequency of 321 Hz in the presence of one. Sensitivity measurements were performed and are depicted in Fig. A2-6(a). The electret-capacitive measurement yielded a larger ME coefficient (2959 V/T) compared to the PVDF-based measurement (506 V/T) with almost 6 times higher voltages at the same magnetic fields. The noise floor was also increased by a factor of 6, leading to almost identical LOD values of $96 \text{ pT/Hz}^{1/2}$ for the piezoelectric measurement and $73 \text{ pT/Hz}^{1/2}$ for capacitive readout. This demonstrates that the strong increase in signal by using the capacitive readout is coupled to the same increase in noise level. A possible explanation for this unchanged signal-to-noise ratio is the existence of a noise source in the magnetic cantilever. When changing to a capacitive readout, the deflection of the cantilever is detected with higher sensitivity. Accordingly, if a deflection occurs due to noise, which can be magnetic, thermally induced, or acoustic, it is detected with the higher sensitivity, and the signal-to-noise ratio remains unchanged. It can be concluded that a capacitive readout with an electret is an excellent method to detect a cantilever deflection with a greatly increased sensitivity, but new cantilever materials and thus new magnetostrictive materials are required to increase the signal-to-noise ratio. One possibility is porous materials, which offer a higher surface-to-volume ratio that could result in large magnetostriction and low noise. To elucidate possible noise sources, a capacitive sensor (see Figure A2- 7b) was excited with magnetic fields and acoustics with the same shielding to external influences, see Figure A2- 7c. It can be clearly seen that the noise level for both measurements is identical, and thus it can be stated that the magnetic field for the measurement is not a source of the noise.

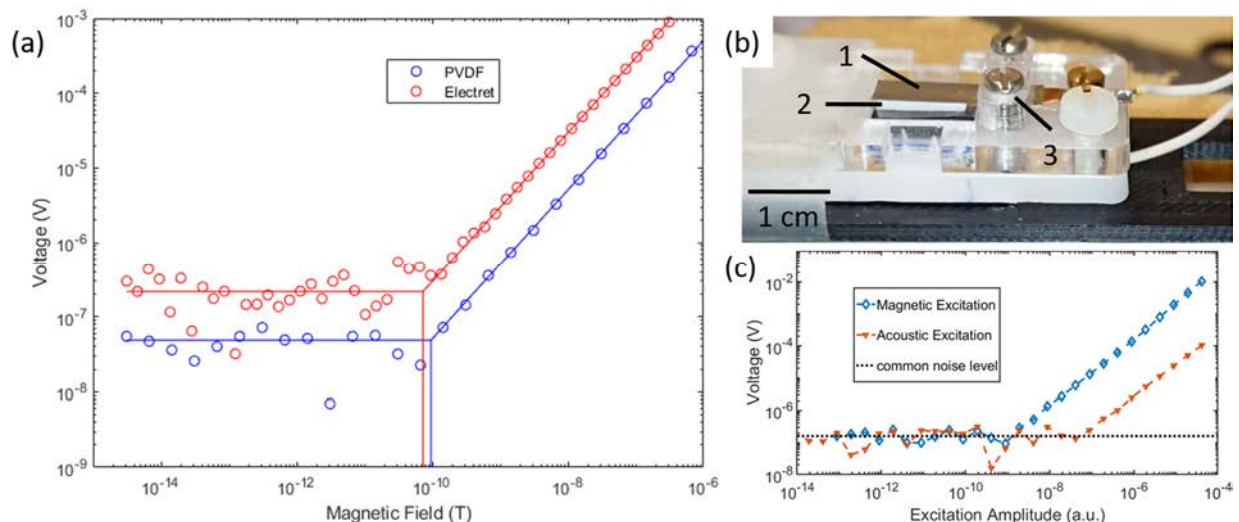


Figure A2- 7: (a) Comparison of piezoelectric measurement with PVDF and capacitive measurement with an electret, both done with the same sensor. ME coefficients (piezo: 506 V/T; electret: 2959 V/T), LOD (piezo 96 pT/Hz^{1/2}, electret 73 pT/Hz^{1/2}). The electret increases the ME coefficient compared to piezoelectric measurement, but the signal-to-noise ratio is unchanged. (b) Photograph of the sensor setup, showing magnetostrictive cantilever (1) and the electret (2) mounted on a custom holder (3). (c) Linear response measurement of an electret-based sensor at a frequency of 191 Hz when using magnetic fields (blue) as well as acoustic waves (red) to excite the sensor. Both excitations exhibit the same noise level.

References

- [Am92] N. Amyot, J. E. Klemberg-Sapieha, M. R. Wertheimer, Y. Segui, M. Moisan, Electrical and structural studies of plasma-polymerized fluorocarbon films. *IEEE Trans. Elect. Insul.* **27**, 1101–1107 (1992).
- [An12] H. An, S. J. Picken, E. Mendes, Nonlinear rheological study of magneto responsive soft gels. *Polymer*. **53**, 4164–4170 (2012).
- [Bo19] S. Bouhedma, Y. Zheng, F. Lange, D. Hohlfeld, Magnetic Frequency Tuning of a Multimodal Vibration Energy Harvester. *Sensors (Basel, Switzerland)*. **19**, 1149 (2019).
- [Br05] E. N. Brown, D. M. Dattelbaum, The role of crystalline phase on fracture and microstructure evolution of polytetrafluoroethylene (PTFE). *Polymer*. **46**, 3056–3068 (2005).
- [Do18] Y. Z. Dong, S. H. Piao, K. Zhang, H. J. Choi, Effect of CoFe₂O₄ nanoparticles on a carbonyl iron based magnetorheological suspension. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. **537**, 102–108 (2018).
- [El18] R. Elhajjar, C.-T. Law, A. Pegoretti, Magnetostrictive polymer composites: Recent advances in materials, structures and properties. *Progress in Materials Science*. **97**, 204–229 (2018).
- [Gr10] H. Greve, E. Woltermann, H.-J. Quenzer, B. Wagner, E. Quandt, Giant magnetoelectric coefficients in (Fe₉₀Co₁₀)₇₈Si₁₂B₁₀-AlN thin film composites. *Appl. Phys. Lett.* **96**, 182501 (2010).
- [Ha11] M. J. Hato, H. J. Choi, H. H. Sim, B. O. Park, S. S. Ray, Magnetic carbonyl iron suspension with organoclay additive and its magnetorheological properties. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. **377**, 103–109 (2011).
- [He78] U. Hetzler, E. Kay, Conduction mechanism in plasma-polymerized tetrafluoroethylene films. *Journal of Applied Physics*. **49**, 5617–5623 (1978).
- [Hs70] S. T. Hsu, R. J. Whittier, C. A. Mead, Physical model for burst noise in semiconductor devices. *Solid-State Electronics*. **13**, 1055–1071 (1970).
- [Ka97] R. Kacprzyk, J. Ziąja, Properties of corona charged plasma vapour deposited PTFE film. *Journal of Electrostatics*. **40-41**, 319–323 (1997).
- [Ka07] M. Kallio, T. Lindroos, S. Aalto, E. Järvinen, T. Kärnä, T. Meinander, Dynamic compression testing of a tunable spring element consisting of a magnetorheological elastomer. *Smart Mater. Struct.* **16**, 506–514 (2007).
- [Ku17] M. Kubík, O. Macháček, Z. Strecker, J. Roupec, I. Mazurek, Design and testing of magnetorheological valve with fast force response time and great dynamic force range. *Smart Mater. Struct.* **26**, 47002 (2017).
- [Me12] M. Mecklenburg, A. Schuchardt, Y. K. Mishra, S. Kaps, R. Adelung, A. Lotnyk, L. Kienle, K. Schulte, Aerographite: ultra lightweight, flexible nanowall, carbon microtube material with outstanding mechanical performance. *Advanced materials (Deerfield Beach, Fla.)*. **24**, 3486–3490 (2012).
- [Mo73] D. T. Morrison, T. Robertson, R.F. sputtering of plastics. *Thin Solid Films*. **15**, 87–101 (1973).

- [Pe12] T. Peter, O. Polonskyi, B. Gojdka, A. Mohammad Ahadi, T. Strunskus, V. Zaporozhchenko, H. Biederman, F. Faupel, Influence of reactive gas admixture on transition metal cluster nucleation in a gas aggregation cluster source. *Journal of Applied Physics*. **112**, 114321 (2012).
- [Se87] G. M. Sessler, *Electrets* (Springer Berlin Heidelberg, Berlin, Heidelberg, 1987).
- [Si19] L. Siebert, O. Lupan, M. Mirabelli, N. Ababii, M.-I. Terasa, S. Kaps, V. Cretu, A. Vahl, F. Faupel, R. Adelung, 3D-Printed Chemiresistive Sensor Array on Nanowire CuO/Cu₂O/Cu Heterojunction Nets. *ACS applied materials & interfaces*. **11**, 25508–25515 (2019).
- [Sm91] J. G. Smits, W. Choi, The constituent equations of piezoelectric heterogeneous bimorphs. *IEEE transactions on ultrasonics, ferroelectrics, and frequency control*. **38**, 256–270 (1991).
- [St19] O. V. Stolbov, Y. L. Raikher, Magnetostriction effect in soft magnetic elastomers. *Arch Appl Mech*. **89**, 63–76 (2019).
- [Ts04] Y. Tsori, F. Tournilhac, L. Leibler, Demixing in simple fluids induced by electric field gradients. *Nature*. **430**, 544–547 (2004).
- [Wa17] G. Wang, Y. Ma, M. Li, G. Cui, H. Che, J. Mu, X. Zhang, Y. Tong, X. Dong, Magnesium ferrite nanocrystal clusters for magnetorheological fluid with enhanced sedimentation stability. *Solid State Sciences*. **63**, 70–75 (2017).
- [Zh16] Y. Zhou, D. Maurya, Y. Yan, G. Srinivasan, E. Quandt, S. Priya, Self-Biased Magnetoelectric Composites: An Overview and Future Perspectives. *Energy Harvesting and Systems*. **3**, 1–42 (2016).
- [Zo19] H. Zou, Y. Zhang, L. Guo, P. Wang, X. He, G. Dai, H. Zheng, C. Chen, A. C. Wang, C. Xu, Z. L. Wang, Quantifying the triboelectric series. *Nature communications*. **10**, 1427 (2019).

3.3.2 Project-related publications by participating researchers

Peer-reviewed articles and books

- [A2-1] M. Mintken, M. Schweichel, S. Schröder, S. Kaps, J. Carstensen, Y. K. Mishra, T. Strunskus, F. Faupel, R. Adelung, Nanogenerator and piezotronic inspired concepts for energy efficient magnetic field sensors. *Nano Energy*. **56**, 420–425 (2019), doi:10.1016/j.nanoen.2018.11.031.
- [A2-2] L. Siebert, O. Lupan, M. Mirabelli, N. Ababii, M.-I. Terasa, S. Kaps, V. Cretu, A. Vahl, F. Faupel, R. Adelung, 3D-Printed Chemiresistive Sensor Array on Nanowire CuO/Cu₂O/Cu Heterojunction Nets. *ACS applied materials & interfaces*. **11**, 25508–25515 (2019).
- [A2-3] Schröder, O. Polonskyi, T. Strunskus, F. Faupel. Nanoscale gradient copolymer films via single step deposition from the vapor phase. **submitted to Materials Today ("minor revisions") 2019**.
- [A2-4] O. C. Aktas, S. Schröder, S. Veziroglu, M. Z. Ghorri, A. Haidar, O. Polonskyi, T. Strunskus, K. Gleason, F. Faupel, Superhydrophobic 3D Porous PTFE/TiO₂ Hybrid Structures. *Adv. Mater. Interfaces*. **6**, 1801967 (2019), doi:10.1002/admi.201801967.
- [A2-5] M. Scharnberg, S. Rehders, Ö. Adiyaman, S. Schröder, T. Strunskus, F. Faupel, Evaporated electret films with superior charge stability based on Teflon AF 2400. *Organic Electronics*. **70**, 167–171 (2019), doi:10.1016/j.orgel.2019.04.016.
- [A2-6] S. Schröder, T. Strunskus, S. Rehders, K. K. Gleason, F. Faupel, Tunable polytetrafluoroethylene electret films with extraordinary charge stability synthesized by initiated chemical vapor deposition for organic electronics applications. *Scientific reports*. **9**, 2237 (2019), doi:10.1038/s41598-018-38390-w.
- [A2-7] V. Postica, A. Vahl, J. Strobel, D. Santos-Carballal, O. Lupan, A. Cadi-Essadek, N. H. de Leeuw, F. Schütt, O. Polonskyi, T. Strunskus, M. Baum, L. Kienle, R. Adelung, F. Faupel, Tuning doping and surface functionalization of columnar oxide films for volatile organic compound sensing. *J. Mater. Chem. A*. **6**, 23669–23682 (2018), doi:10.1039/C8TA08985J.
- [A2-8] R. E. Hirschberg, M. Scharnberg, S. Schröder, S. Rehders, T. Strunskus, F. Faupel, Electret films with extremely high charge stability prepared by thermal evaporation of Teflon AF. *Organic Electronics*. **57**, 146–150 (2018), doi:10.1016/j.orgel.2018.02.040.
- [A2-9] Y. K. Mishra, R. Adelung, ZnO tetrapod materials for functional applications. *Materials Today*. **21**, 631–651 (2018), doi: 10.1016/j.mattod.2017.11.003
- [A2-10] O. Lupan, V. Postica, J. Gröttrup, Y. K. Mishra, N. H. de Leeuw, R. Adelung, Enhanced UV and ethanol vapour sensing of a single 3-D ZnO tetrapod alloyed with Fe₂O₃ nanoparticles. *Sensors and Actuators B: Chemical*. **245**, 448–461 (2017), doi:10.1016/j.snb.2017.01.107.

3.4 Project plan

Objectives

The goal of the project is to develop novel sensors similar to magnetoelectric cantilevers, where the conventional magnetostrictive and piezoelectric components are replaced with new material concepts for the efficient conversion of the magnetic field change into an electric signal. For the magnetostrictive component,

the deformation in a magnetic field does not arise from spin-orbit coupling but from the interaction of ferromagnetic particles in a mechanically soft matrix. Instead of the piezoelectric readout, a contact free, capacitive readout from a highly charged electret film is applied to detect the beam deflection. In addition, the substrate is eliminated completely. This approach promises a minimization of the energy for bond stretching and ensures efficient signal conversion. In addition to using soft matrixes for the magnetostrictive layer, we will also pursue the second novel approach, developed in the current funding period, to soften a conventional stiff magnetostrictive cantilever by tailoring its potential energy surface via the attractive electrostatic potential of thin film electrets.

In the current funding period, emphasis has been placed on new approaches and feasibility studies. The second funding period will focus on concepts that enhance the limit of detection, particularly for applications in magnetocardiography and in deep brain stimulation (DBS), where direct broadband measurement is required. The design freedom provided by the methods described below allows tailoring of the individual components with microscale precision. With targeted use of non-linearities, such as progressive characteristics or attractive potentials, the potential energy landscape of the ME resonators can be shaped. This approach increases the oscillation amplitude while reducing the resonance frequency and simultaneously gaining bandwidth. These objectives are based on the following hypotheses:

- The sensitivity (ME-coefficient) of our sensors can be increased by using highly porous electret materials with a much higher charge density, by decreasing the distance between the cantilever and the electret, and by increasing the induced deflection of the cantilever.
- The distance between electret and cantilever can also be used to tune the resonance frequency to lower frequencies. This allows an adoption of the sensor to measure exactly in resonance, e.g. for applications in DBS (see below).
- Together with the sensitivity, the noise level of the sensor defines the LOD of the sensor. Noise sources in our new sensors are thermal noise, acoustic noise, and electric noise. Internal magnetic noise can be neglected because the sensor is operated in the direct mode without active excitation.
- Sources for electric noise are compensation currents and the resulting ohmic losses in the moving electrode. Smaller electrode areas or intermittent electrodes will reduce the electric noise of the sensor.
- A high stability of the electrets reduces the shot noise since the charges are tightly bound.
- Anisotropy can help to increase the sensitivity of the sensor in one desired direction. The sensitivity to all other directions is reduced, which will cause a noise reduction in the sensor. Anisotropy can be achieved by orientation of particles in chains or fibers, by introduction of pre-strain in the matrix, and by the use of semi-crystalline polymers or polymer blends.
- In a capacitive sensor, the signal is defined by the deflection of the cantilever, which is caused by a magnetic interaction of the filler particles and limited by the elastic properties of the matrix material. Both depend on geometric constraints and can be modified by utilization of porous materials which will mechanically soften the matrix and define the ultimate configuration for the filler particles.
- The resonant detection of signals containing multiple frequencies, such as signals from a deep brain stimulator, can be achieved either by exciting different harmonics of a single cantilever or by designing a sensor geometry that contains multiple oscillators for the different frequencies. The use of higher harmonics is expected to eliminate the $1/f$ noise problem.
- A prediction of sensor signal and noise is possible for non-harmonic oscillation and can be modelled and simulated with numerical solvers.
- Porosity in magnetoactive polymers offers a possible solution by decoupling the magnetic response from the noise sources. Tuning the porosity will reduce the noise from acoustic or thermal excitation.

Proposed research methods

(1) Processing

Fabrication of the magnetoactive polymers will be performed with wet chemistry techniques in the Adelung group. Direct ink printing and laser cutting are also available for integration into the sensor design. Fabrication of t-ZnO networks is an established method in the Adelung group and can be used in several furnaces to fabricate t-ZnO and t-ZnO networks of different geometries for the intended aeropolymers, which are polymers with a very large porosity in analogy to aerographite [Me12]. The electret thin film component of the sensor will be fabricated with the iCVD technique, as established in the current funding period. The Faupel group runs three iCVD setups, one of which is dedicated to this project. The CVD-typical growth characteristics and low process temperature of iCVD turned out to be ideal for the deposition on highly porous substrates. Charging of the porous electrets will be performed by a subsequent corona discharge treatment in a special setup. A centrifugal melt spinner built in-house is available in the Adelung group and will be used to prepare fibers containing magnetic particles.

(2) Functional and structural characterization

The magnetic measurements can be conducted in a custom setup in the Adelung group. The sensors can be magnetically and electrically as well as acoustically shielded in this setup. Homogeneous AC and DC fields can be applied by low-noise Keithley instrument devices (Sourcemeter 2400 & Current Source 6221). The sensor response will be measured with a Stanford research lock-in amplifier (SR830) and dual channel low pass filter (SR640). Recording the time-resolved data is performed by a 16bit adc with 1 MHz maximum sampling rate (Measurement Computing USB-2537) controlled by National Instruments Labview software. The characterization of the electrets can be investigated by an electrostatic voltmeter and a programmable heating plate in the Faupel group. Furthermore, Fourier-transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) can be used in the Faupel group for the chemical characterization and identification of functional groups in the polymer samples. Scanning and transmission electron microscopy (TEM) will be used for the structural characterization in close cooperation with **A6** with advanced TEM.

Work plan

The work planned for the next funding period is bundled into five work packages (WPs) shown in a Gantt chart in Table A2-1. As before, each group continues to develop new materials and components separately. While the soft magnetostrictive composite materials will be examined in the Adelung group within WP1, the electret materials will be investigated in the Faupel group within WP2. Nonetheless, the project is based upon three conjoint WPs dealing with the development of new, specifically porous materials (WP3), sensor theory (WP4) and the fabrication and characterization of new soft hybrid sensors (WP5). The overall strategy is twofold, which means that new materials and an adapted sensor theory for soft ME hybrids will be developed at the same time. This process will not likely take place in a strict linear fashion but in a dynamic way characterized by several parallel and interactive development iterations.

Table A2-1: Work schedule

		2020		2021				2022				2023				2024	
		3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2
WP 1	Soft-magnetostrictive composites																
WP 2	New multifunctional electrets materials																
WP 3	New, porous magnetostrictive composites and electrets																
WP 4	Sensor modelling and theory																
WP 5	Sensor fabrication and characterization																

AG Adelung

AG Faupel

Both groups

WP1: Soft magnetostrictive composites

To obtain a low LOD of the sensors, new concepts will be applied to the mechanically soft magnetostrictive composites to allow a large deflection of the cantilever in a magnetic field and low magnetic noise. One concept to reduce the noise is to realize a strong anisotropy in the material, which will result in a strong effect and strong deflection when the magnetic field is applied in the sensitive direction and a reduced effect to magnetic fields in all other directions. This anisotropy can be achieved by using a desired orientation of the particles in chain or fibers and by using a matrix with anisotropic mechanical properties. The magnetostrictive properties will be investigated with a newly developed device for soft composites that has a large deflection and will be correlated with simulation results from **A10**. The existing measurement setup is designed for relatively stiff cantilevers which bend only by small angles, whereas magnetostrictive polymers have similar magnetostrictive coefficients combined with softer cantilevers. Accordingly, the current setup does not allow a measurement of the saturated material, and a new setup will be developed to adapt to the special requirements of the sensors. The orientation of the magnetic particles in chains or fibers will be realized by applying strong magnetic fields during solidification of the matrix or embedding polymer fibers that contain magnetic particles. Such fibers can be synthesized by centrifugal melt spinning or electrospinning. One advantage of embedded fibers is the combination of two polymers, e.g. a stiff polymer for the fibers and a soft matrix. Additionally, the mechanical anisotropy can be achieved by using non-miscible polymer blends where a desired phase separation will be performed in an external magnetic field to align the particles and to embed them in an anisotropic matrix. The large magnetic bias field for sensor devices will be realized with powder magnets in collaboration with **Z1**.

WP2: New multifunctional electret materials

This work package is dedicated to the development of new electret materials via iCVD. Based on the findings from the previous funding period, it is inevitable to use copolymer materials to solve problems like film delamination, low deposition rates, etc. The use of copolymers also allows adding additional functional groups to the electret material to tune the crystallinity within the thin film to avoid the abovementioned phase transitions. Furthermore, the aim is to deposit an additional protective layer on top of the electret films by iCVD to enable use in harsh environments, in particular humid environs, which is currently of great interest in the field of electret research. Here, the iCVD technique enables a unique way to achieve this aim due to its mild deposition conditions, which will not eliminate the surface charge of the electret. These protected electrets will then be tested in high humidity environments as well as by mechanical stresses (e.g. cleaning of the electret surface with tissues and alcohol), which are typical procedures where electrets lose their surface charge immediately. The protective coating will furthermore shield the electrets from attracted ions from the ambient air which would compensate the surface charge. These ions are typically one of the main reasons for the fast decay of the electret surface charge in unshielded environments.

Accompanying the synthesis of these new electret materials via iCVD, a detailed study will be conducted on how different chemical groups, like methyl groups, ester groups, or amide groups, influence the electret charge storage properties, something that has not been reported in the literature so far. The release of charge carriers from the electret can generate burst noise in the sensor [Hs70]. The aim is thus to minimize the number of charge carriers released from the electret material and to increase the surface potential V_s . For this purpose, different comonomers will be used for synthesizing the thin films. They will add repeating units with different functional groups between the CF_2 repeating units. A systematic study of these new copolymers will yield electrets with minimized spontaneous charge release so that electret burst noise can be ruled out as a noise source in the sensor. Using the abovementioned copolymer, we furthermore anticipate an increase in V_s in order to increase the $\Delta U/\Delta d$ effect in this way. We aim to increase it from $187 \times 10^6 \text{ V/m}$ currently to $500 \times 10^6 \text{ V/m}$ within the next funding period in this work package. The systematic study on the functional groups, which effect the resulting surface charge, will contribute greatly to general understanding of charge storage in electret materials. The in situ mass spectrometry diagnostics, set up in the previous funding period, can also be used to support this purpose. Moreover, the preservation of the functional monomer groups in the copolymer and their charge storage properties will be investigated with FTIR and with the electrostatic voltmeter setup developed during the previous funding period, respectively.

WP3: New porous magnetostrictive composites and electrets

The aim of this work package is to fabricate porous polymeric materials with a large surface-to-volume ratio. There already exists expertise in the field of very porous, so-called “aeromaterials” in the Adelung group based on ZnO templates [A2-9]. The approach will be realized for the magnetostrictive as well as the electret components of the sensors. In general, both sensor components will benefit from increasing their softness or their effective surface charge, respectively, by introducing additional porosity into its macro- and/or microstructure.

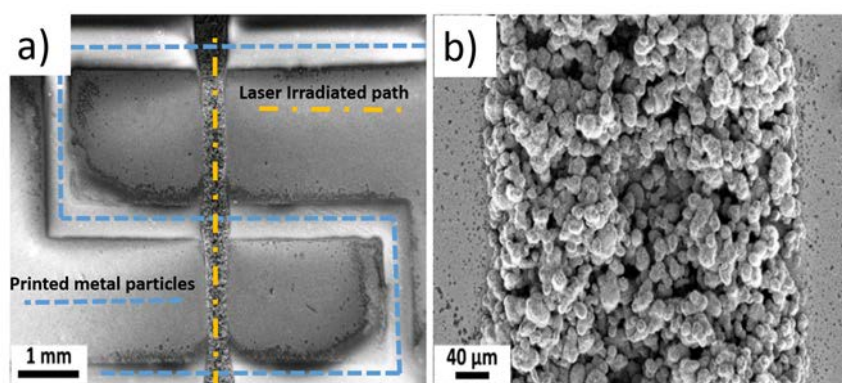


Figure A2-8: Porous material synthesis. A modified 3D printer allows direct ink writing. (a) Printed meander-shaped metal particles post-processed. (b) Zoomed image of metal oxide particles.

Two main synthesis routes have been developed in the Adelung group to fabricate magnetoactive composite materials with

porosities on the macro- and microscale:

- 1.) Composite aeropolymers, so called “aeromagnets”, can be produced by infiltrating and curing porous sacrificial templates, such as tetrapodal ZnO (t-ZnO) [A2-10] networks (Fig. A2-7) [A2-2].

- 2.) 2.) A soft polymer film containing particles is deposited on the porous template materials. This will permit the realization of geometric assemblies on much smaller dimensions compared to the methods described in WP1. First investigations have demonstrated a possible realization, as shown in Fig. A2-8a. The decoration of surfaces with nanoparticles is well established in both groups [A2-7] [Pe12].

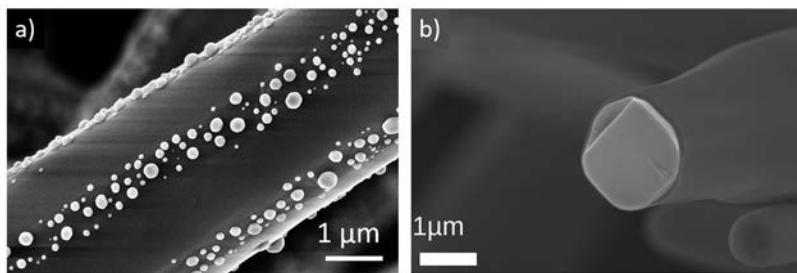


Figure A2-9: (a) Nanoparticles on porous template material. (b) Conformal poly(ethylene glycol dimethylacrylate) (PEGDMA) thin film deposited via iCVD on a highly porous t-ZnO network shows complete coverage of each single tetrapod arm.

Delicate 3D structures can be printed with magnetic ink. This method has the great advantage of being extremely versatile with respect to the feasible 3D geometries. The alignment of the particles in the matrix will be furthermore tuned with not only magnetic fields but also advanced shape-defining methods. These methods can involve direct ink printing and laser cutting. Whereas direct ink printing defines the geometry in a bottom-up process, the laser cutting permits a top-down process. These processes can be combined to allow the realization of complex shapes on different length scales.

Moreover, both of these fabrication methods can be used to prepare templates with highly porous surfaces for the electret deposition in the Faupel group. This is desirable since in the case of electret materials, an increased porosity will lead to a larger effective charged surface area and stronger electrical fields per distance inside the electret-capacitor and, thus, an increased ME signal strength. Here, one possible porous template structure can be the abovementioned t-ZnO [A2-9]. The porous template materials are the ideal platform because they have a very large surface area and do not contain closed pores. Accordingly, the complete surface can be coated by using the iCVD technique because it allows the conformal film deposition on porous structures without shadowing effects as typically observed in PVD methods. The feasibility of iCVD on ZnO template materials was already demonstrated (Fig. A2-8b). The structuring methods, e.g. 3D printing, available in the Adelung group will be used to integrate these aerostructures in the final sensor design. Besides using a porous template material for the electret deposition, we will also explore other methods of increasing the internal electret porosity directly during the synthesis. Preliminary experiments have shown that a suitable porogen can produce nanoporosity by phase separation during the iCVD synthesis of organic thin films. The resulting nanostructure was also simulated with the Cahn-Hilliard model (Fig. A2-9).

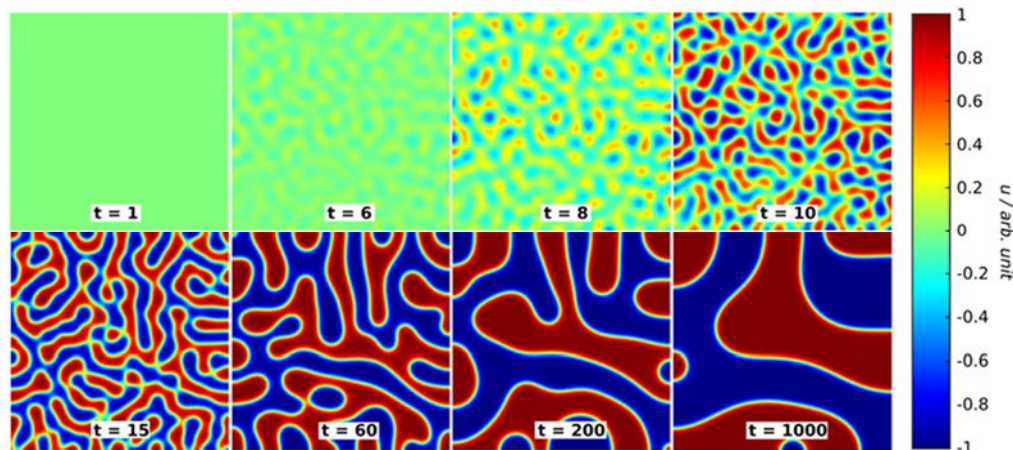


Figure A2- 10: Phase separation according to the Cahn-Hilliard phase field model at different time steps.

Here, fast reaction rates are chosen to make the monomer immobile and yield pore sizes as small as possible (e.g. timestep $t = 10$), which maximizes the effective surface area of the polymer film. Further simulations will be performed in the Faupel group in cooperation with the Wulfinhoff group (A10) with a modified Cahn-Hilliard model. Here the Cahn-Hilliard model (only for diffusion-driven kinetics) will be combined with Stokes equations to consider also the convective contribution to the phase separation for low viscous monomers/porogen. According to the findings of Tsori et al., a phase separation can also be forced in two, similar, well-mixing liquids by application of an electric field between unevenly spaced electrodes [Ts04]. This effect will be transferred to the iCVD reaction by applying an electric field during the free radical polymerization to enable control of the phase separation, e.g. of two comonomers that usually show mixing. Pores of 10 nm to 900 nm are anticipated here in the synthesis of porous materials with large effective surface areas. The experiments will also be correlated to the advanced Cahn-Hilliard-Stokes model.

The chemical properties of all polymers fabricated in this WP (magnetoactive compound as well as electret) will be characterized by XPS and FTIR. Investigation of the structure of the aeromaterials will be performed with SEM and TEM in cooperation with **A6**. The surface charge of the porous electrets will be measured with the electrostatic voltmeter setup constructed in the previous funding period.

WP4: Sensor modelling and theory

In the first period, a model describing the non-harmonic oscillation for an electret-based capacitive sensor was developed which allowed a prediction of fundamental mechanisms such as the shift in resonance frequency and the increase in bandwidth as well as amplitude due to electrostatic interactions. Based on this existing model, the sensors will be modelled with COMSOL multiphysics as well as ab initio calculations, and the results of the simulation will be compared to the data from the measurements. In addition, the model will be extended to address vibrational noise due to external effects, such as acoustics. This will permit identification of the key components and a more detailed understanding of the undamping mechanisms, the effects of the porous media, and the utilization of cantilevers with complex shapes. Within this work package, analytical descriptions will be developed wherever possible to identify efficient key parameters that determine signal strength and effect sizes, as previously done with the electret-based sensor. The design of the electrode and possible partial electric shielding will be included in the model. The results will be used as feedback for sensor development (WP 1-3) and will help achieve improved sensors in an iterative development. The tuning of the resonance frequency, as already demonstrated in the first funding period, will be developed further to allow an adoption of the sensors.

The typical biomagnetic sources as well as the artificial deep brain stimulator provide signals over a broad range of frequencies with only a small amount of energy in a single frequency. This typically requires sensors with a large bandwidth and very low LOD. A possible alternative, which will be modelled, is a multi-frequency resonator. Such a device can be made either by designing a special complex geometry (see Fig. A2-11b) or by using already observed higher harmonics to measure with a single non-harmonic sensor. The soft magnetostrictive material and the electret provide many degrees of freedom in the overall sensor design, especially as methods such as 3D printing and laser cutting can be employed. Consequently, sensors can be modelled that employ more than one electret layer. For the softening type of sensor, a significant broadening of the peak around the resonance frequency with the same signal strength can be expected if two electrets are used on both sides of the cantilever. Another option to tune the susceptibility of the material to a given magnetic frequency spectrum is to utilize sensor arrays. The modelling of the arrays allows identifying the exact shape for fabrication. Furthermore, coupling between the individual cantilevers of an array can lead to energy transfer from one cantilever to another. With the modelling, it can be understood whether weak or strong coupling is advantageous for the overall output of the sensor. Wherever the modelling effort is going beyond the abilities of a multiphysics simulation, collaboration and intense dialog with the theory and modelling groups (**B1** and **A10**) within the CRC will be essential.

WP5: Sensor fabrication and characterization

Within this work package, sensors will be assembled and characterized, based on the theoretical results from WP 4. The bandwidth will be tuned to fit the requirements of measuring the targeted biomagnetic signals. The tuning will be done by choosing a geometry that determines a certain resonance frequency and an additional broadening by undamping the sensors or cantilever arrays with different states of coupling. This can be achieved by the possibilities of soft 3D printing as an additive manufacturing step, laser cutting as an efficient subtractive step, and the freedom in positioning and charging the electrets. For the individual cantilevers, the signal strength can be increased by the aforementioned advanced magnetostrictive composites and the higher charged porous electrets as well as the design of the bending beam. For instance, wherever constraining forces have to be applied, e.g. to induce a bending moment in a beam upon expansion in the magnetic field, the substrate can be eliminated, and the bending can be induced by a thin layer that is rigid under tension but flexible upon bending. Examples would be an extremely thin pre-strained polymer foil on which the magnetostrictive material can be printed and which can be cut with micrometer precision with the layer, or even the thin metal electrode. In a post-processing step, the existing cantilevers can be modified in their geometry, and multi-resonator sensors that show a resonance at two or more desired frequencies can be realized (see Fig. A2-10b). Simultaneous detection with a multi-resonant sensor is a possible way to eliminate $1/f$ noise. The design of the electrode will be tailored according to predictions from modelling in WP4.

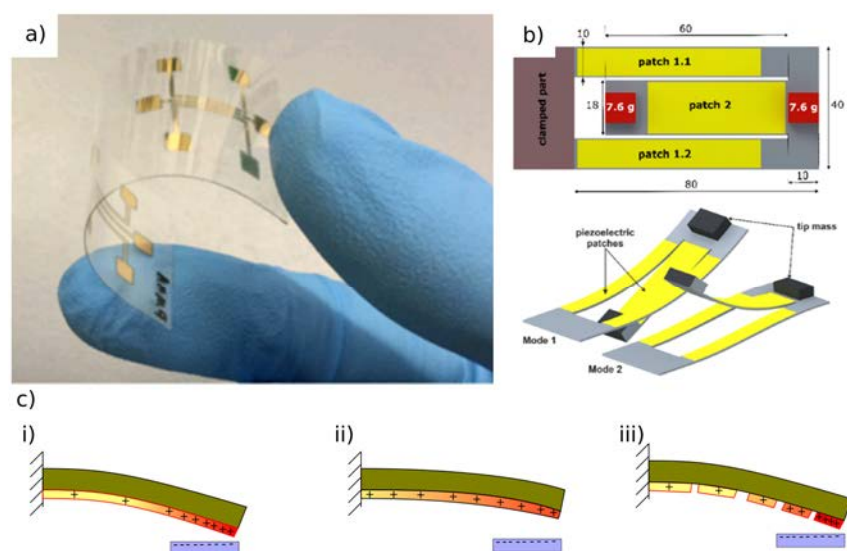


Fig. A2-11: (a) Flexible organic device with electret film [A2-6]. (b) Example for a multi-resonator [Bo19] which can be produced by laser cutting magnetoactive polymers. (c) Schematic image of the charge distribution in the electrode. A continuous electrode will change its charge distribution when approaching the electret during oscillation, see (i) & (ii). This results in the flow of compensation currents, which are a possible source of noise. An intermittent electrode will have a similar charge distribution but no compensation currents can flow and the current noise is reduced, see (iii).

For sensor noise, complete coverage of the cantilever with an electrode will cause the flow of compensation currents in the electrode to have an equipotential surface. Such currents are connected to ohmic losses and may be a dominant noise source of a sensor, see Fig. A2-11c. An intermittent electrode may help to lower the electric noise of the sensor and thus improve the LOD. The response to artificial external noise sources of acoustics and vibrations will be investigated, particularly for the porous materials, and correlated to simulations in WP4. As for the sensor readout, we will not only use the usual voltage readout but also explore current readout in cooperation with **A5**.

Since this project pursues completely novel sensor approaches, emphasis so far has been put on feasibility studies and new material concepts. We expect to reach competitive LODs in the second funding period, which should make possible addressing a broad range of applications in the third funding period. The envisioned advantage of the present approach is the tailored adoption of the selective frequency perception for biomagnetic and related signals like the deep brain stimulation device. Consequently, application to relevant medical questions and problems will be addressed in the third period in close collaboration with partners from the clinic and Faculty of Medicine.

3.5 Role within the Collaborative Research Centre

As discussed in the work plan, we cooperate with the following projects:

- A1:** Studies regarding noise analysis and reduction,
- A4:** Readout of the fabricated sensors,
- A5:** Current-based readout via electret films,
- A6:** TEM analyses of magnetoactive polymers and aeromaterials,
- A8:** Support during sensor modelling,
- B1:** Sensor noise performance,
- B7:** Template material synthesis,
- A10:** Collaboration within WP1 regarding simulations,
- Z1:** powder magnets for strong biasing,
- Z2:** Support with sensor characterization.

A2 is mainly involved in the following focus groups: "Comparison of sensor concepts" and "Modelling"

3.6 Differentiation from other funded projects

Besides the current CRC 1261 Projects **A2**, **A4**, **A5**, and **B7**, no funded project in the Faupel group or the Adelung group deals with magnetic sensors or electrets.

3.7 Project funding

3.7.1 Previous funding

This project has been funded within the Collaborative Research Centre since 06/2016. Previously, it was funded under another DFG programme from 01/2015 to 06/2016 (reference number FA 234/26-1 and AD 183/14-1).

3.7.2 Requested funding

Funding for	<2020/2>		<2021>		<2022>		<2023>		<2024/1>	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral researcher, 100%	2	68.40	2	136.80	2	136.80	2	136.80	2	68.40
Total		68.40		136.80		136.80		136.80		68.40
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables	9.20		17.20		11.20		11.20		5.60	
Total	9.20		17.20		11.20		11.20		5.60	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation	0		0		0		0		0	
Total	0		0		0		0		0	
Grand total	77.6		154.0		148.0		148.0		74.0	

(All figures in k€)

3.7.3 Requested funding for direct costs for the new funding period

	Seq uen- tial no.	Name, academic degree, position	Field of research	Depart- ment of university or non- university institution	Project commit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1	Adelung, Rainer, Prof.Dr., Head of Research Group	Nano Materials	IMS	4		Core support
	2	Faupel, Franz, Prof. Dr., Head of Research Group	Material Compounds	IMS	4		Core support
	3	Carstensen, Jürgen, Dr., Senior Researcher	Nano Materials	IMS	3		Core support
	4	Kaps, Sören, Dr., Senior Researcher	Nano Materials	IMS	3		Core support
	5	Strunskus, Thomas, Dr., Senior Researcher	Material Compounds	IMS	2		Core support
Non-research staff	6	Bahr, Jörg, Dipl.-Ing. (FH), Technician		IMS	4		Core support
	7	Rehders, Stefan, Dipl.-Ing. (FH), Technician		IMS	4		Core support
Requested staff							
Research staff	8	Lukas Zimoch, Doctoral Researcher	Nano Materials	IMS		E13	
	9	N.N., Doctoral Researcher	Material Compounds	IMS		E13	

Job description of staff (supported through available funds):

1. Prof. Dr. Rainer Adelung is principle investigator and responsible for the magnetoactive materials. He advises the scientific staff in the material development and sensor system.

2. Prof. Dr. Franz Faupel is principle investigator and responsible for the thin film electrets. He advises the scientific staff in the sensor development and measurement system.
3. Dr. Jürgen Carstensen is an expert in the field of electrical characterization and assists in the coordination and interpretation of the electrical noise investigations.
4. Dr. Sören Kaps is an experienced scientist and will be advising the experimental work in the lab, especially when designing setups for synthesis and characterization of magnetoelastic polymers.
5. Dr. Thomas Strunskus is an experienced scientist in the Faupel group and advises the PhD student in the iCVD synthesis, deposition parameters, and the analysis of polymer films.
6. Dipl.-Ing. (FH) Jörg Bahr will support the students and doctoral researchers in the project in all issues regarding the mechanical construction and maintenance of experimental setups.
7. Dipl.-Ing. (FH) Stefan Rehders is responsible for the design and construction of mechanical parts, mechanical repairs, and support with vacuum systems.

Job description of staff (requested):

8. The doctoral researcher Lukas Zimoch of the Adelung group will develop magnetoelastic polymers, assemble sensors, and characterize them. The work packages WP1 will be performed by him and he will take part in WP3, WP4, and WP5.
9. The doctoral researcher of the Faupel group will develop the advanced electret materials for the sensors and will be involved in modelling and performance testing of the sensors. She/He is responsible for the experiments in WP2 and will take care of the electret part in WP3, WP4, and WP 5.

3.7.4 Requested funding for instrumentation for the new funding period

(All figures in k€)	2020/2	2021	2022	2023	2024/1
existing funds from core support	2.50	5.00	5.00	5.00	2.50
Sum of existing funds	2.50	5.00	5.00	5.00	2.50
Sum of requested funds	9.20	17.20	11.20	11.20	5.60

Equipment up to k€10 for financial year 2020/2

Special chemicals for iCVD polymer electret synthesis (initiators, comonomers, porogens), substrates (silicon wafer, PET, PMMA)	k€	3.8
Mass flow controller Alicat M 10 sccm	k€	2.8
Swagelok valve and vacuum parts	k€	0.8
Chemicals and small parts for porous magnetic materials	k€	1.8

The mass flow controller and additional vacuum parts are needed to set up an additional gas line to the iCVD reactor, necessary for the deposition of the intended new copolymers in WP2

Equipment up to k€10 for financial year 2021

Special chemicals for iCVD polymer electret synthesis (initiators, comonomers, porogens), substrates (silicon wafers, PET, PMMA)	k€	7.6
Mechanical and electrical parts for a new magnetostriction characterization setup	k€	6.0
Chemicals and small parts for porous magnetic materials	k€	3.6

Equipment up to k€10 for financial year 2022

Special chemicals for iCVD polymer electret synthesis (initiators, comonomers, porogens), substrates (silicon wafers, PET, PMMA)	k€	7.6
Chemicals and small parts for porous magnetic materials	k€	3.6

Equipment up to k€10 for financial year 2023

Special chemicals for iCVD polymer electret synthesis (initiators, comonomers, porogens), substrates (silicon wafers, PET, PMMA)	k€	7.6
Chemicals and small parts for porous magnetic materials	k€	3.6

Equipment up to k€10 for financial year 2024/1

Special chemicals for iCVD polymer electret synthesis (initiators, comonomers, porogens), substrates (silicon wafers, PET, PMMA)	k€	3.8
Chemicals and small parts for porous magnetic materials	k€	1.8

3.1 General information about Project A3(E)

3.1.1 Project title: Resonant Magnetolectric Sensors

3.1.2 Project leaders

Quandt, Eckhard, Prof. Dr.-Ing.
05.04.1960

Inorganic Functional Materials

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3.2 Project history

3.2.1 Report

Objectives and original planning

The aim of this project was to improve the performance of resonant magnetolectric (ME) sensors in terms of an increase in effect size and a decrease in cross-sensitivities, respectively, of the noise floor. These resonant sensors are attractive due to their effect enhancement being proportional to the quality factor Q . As their bandwidth is limited, they can be either used in combination with frequency conversion techniques, the ΔE -effect or for synthetic sinusoidal signals (e.g. **B7**). The investigations include concepts related to bending mode resonant sensors, coupled resonators, lateral bulk mode resonators, and tunable resonators. Research is carried out on large-scale sensors with a length of 22 mm, on bulk micromachined (BMM) sensors with 3 mm length and surface micromachined (SMM) sensors with lengths down to 1 mm. For the fabrication of these sensors, silicon micromachining, quartz processing, and techniques involving metallic substrates are used. Special approaches include measures to increase the quality factor by using quartz and silicon substrates or lateral bulk mode resonators, to reduce acoustic cross-sensitivity by using high frequency resonances or anti-symmetric vibrational modes. Frequency tuning, which is important for small bandwidth applications to match the signal frequency as in deep brain stimulation, is investigated by two approaches: first, coupled resonator structures with piezoelectric actuators are explored. Based on these systems, continuous real-time frequency sweeps are studied. Second, NiTi-based shape memory alloys are investigated as substrate materials. Here, a short temperature pulse that changes the stiffness of the shape memory alloy sets the sensor resonance frequency.

Research plan changes

In the original planning of the CRC, resonant bending ME sensors were considered to be one of the key components for ME sensors dedicated to biomagnetic applications. In combination with frequency conversion techniques (magnetic frequency conversion, **A1**; electric frequency conversion, **A7**) or by utilizing the ΔE -effect (**A4**), sufficient bandwidth can be obtained assuming that a higher order bending mode is employed. In this case an increase in Q was considered to be directly translated into an almost identical increase in sensitivity and limit of detection (LOD). For other applications using artificial magnetic fields (deep brain stimulation (DBS), **B5**; nerve stimulation, **B6**; magnetic particle detection **B7**), it was planned to directly use the resonant sensors – ideally tunable to match the signal frequency – and thus again gain from any improvement in signal strength.

The research in the beginning of the first funding period provided results that led to significant changes in the work program and finally to the decision to end this project after the first funding period. First, the resonant ME sensors are limited by thermal-mechanical noise in the vicinity of their resonance [A3-9], and thus the theoretical and experimental gain only scales with $Q^{1/2}$ instead of the expected increase with Q . Second, applications

with fixed frequencies but non-sinusoidal signals (in the CRC: DBS, **B5/T1**) will also benefit from broad-band detection, as the signal at the fundamental frequency (or at one of the multiples) only contains about 3% of the total energy. As a consequence, a very broad-band sensor based on the propagation of surface acoustic waves (SAW) and the employment of the ΔE -effect was added as an additional work package instead of the WP 1(b) “High Q Bending Resonators”. This new sensor concept was very successful, yielding a LOD of 70 pT/Hz^{1/2} at 10 Hz and a bandwidth of 50 kHz. These SAW magnetic field sensors will be continued in the new project **A9**. Details of the obtained results are summarized in **A9**, published in [A3-3], [A3-5] and [A3-6], as well as patented [A3-P1]. Fabrication of resonant ME sensors for other projects [A3-1] will be continued by **Z1**, which assures their availability after the end of project **A3**.

During the research work at Fraunhofer ISIT, it became obvious that the anti-phase modes of coupled resonators are very difficult to excite (WP 2). For this reason, the focus was shifted to a new sensor concept with integrated powder-based permanent magnets. Additionally, a comprehensive study on cantilever ME sensors was performed in order to improve the LOD by implementing the new piezoelectric material AlScN and by investigating the influence of the geometry parameters.

Results

Bending resonators

Within the previous funding period (PAK 902) we could show that an improvement of the quality factor (Q), e.g. by operation in vacuum, increased the magnetoelectric effect directly proportional to Q. With this, huge ME-coefficients of 20 kV/cmOe were achieved [Ki13]. During this funding period with the close collaboration of **B1**, we analyzed that in resonance the noise is dominated by the thermal-mechanical noise [A3-9]. This holds both for the large scale sensors of 22 mm length resonating at 800 Hz [A3-10] and the BMM sensors of 3 mm length resonating up to 7.5 kHz. Both calculations and measurements confirm hereby, that this noise scales in resonance with $Q^{1/2}$. In Fig. A3-1 this is shown as an example on a BMM sensor. The linear dependence of the signal on Q and the dominating thermal-mechanical noise result in a scaling of the signal-to-noise ratio and achievable limit of detection (LOD) with $Q^{1/2}$. In resonance at 7.5 kHz, a LOD down to 2 pT/Hz^{1/2} is achieved by operation in vacuum.

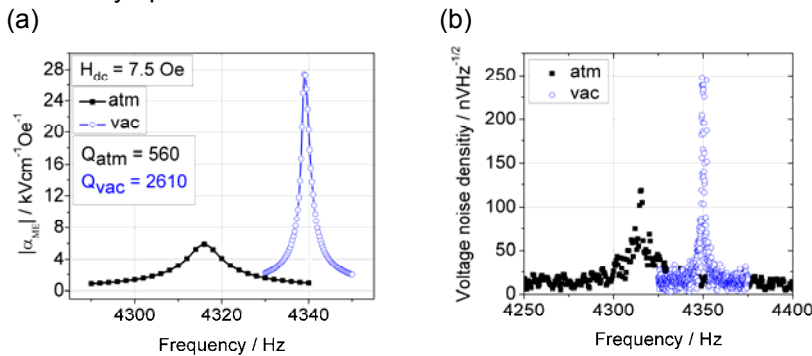


Figure A3-1: a) Magnetoelectric coefficient α_{ME} and b) noise density for a BMM Sensor with 3 mm length, 25 μ m polysilicon, 2 μ m AlN and 2 μ m FeCoSiB under (atm) atmospheric pressure and at (vac) $1 \cdot 10^{-4}$ mbar. Increase of Q and α_{ME} by factor ~ 5 increase of noise by $\sim 5^{1/2}$.

A similar trend is shown for the ΔE -effect read-out scheme, published in [A3-4]. A detailed analysis of the dependence of the sensor's admittance on the quality factor, supported by models from **A4**, shows an increase of the signal voltage by Q^2 . The noise scales in resonance again by $Q^{1/2}$, dominated mainly by the thermo-mechanical noise, see Fig. A3-2. As long as magnetic noise is not dominating, an improvement of the LOD by $Q^{3/2}$ can be achieved. From the simulations, a LOD of 10 pT/Hz^{1/2} at 1 to 10 Hz for the BMM sensors is predicted for a feasible improvement of the Q-factor from 1000 to 6000.

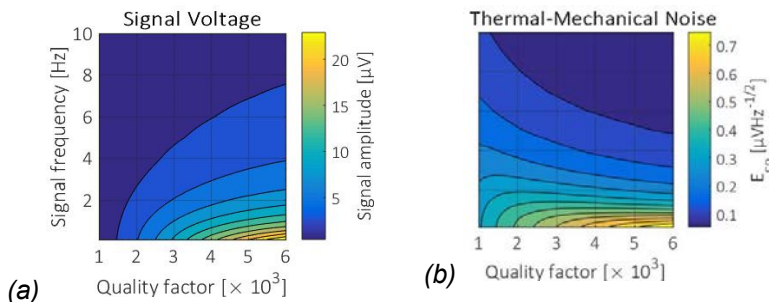


Figure A3-2 from [A3-4]: Amplitude of the signal voltage as a function of Q and the signal frequency. b) Voltage noise density for the same set of parameters, based on the noise model in [A3-9] assuming a dominant thermal-mechanical noise. BMM Sensor with 3 mm length, 50 μ m polysilicon, 2 μ m AlN and 2 μ m FeCoSiB.

The disadvantage of the decrease of the bandwidth with Q can be avoided by higher resonance frequencies, e.g. by using higher-order modes. Investigations with **A4** using the ΔE -effect on the second mode show hereby two more advantages. The thermal-mechanical noise is less dominant in the second mode and the magnetic behavior is improved. The wider bandwidth at higher bending modes and the potential to avoid or reduce the

thermal-mechanical noise motivated us to transfer the knowledge of resonating ME sensors to the surface acoustic wave (SAW)-concept. Furthermore, higher frequency resonance modes were investigated in the scope of the electrically modulated ME sensors (A7). Here, the so-called U modes at approximately 500 kHz are of great interest and will be further investigated.

Sensors with frequency tuning

For brain stimulator applications and the development of vector field sensors and sensor arrays in specific applications, resonators with either identical resonance frequencies or precisely defined frequency spacing are required. For instance, to detect the artificial magnetic signal of deep brain stimulation, the resonance frequency of ME sensors has to be tuned to the stimulus frequency of the brain pacemaker (approx. 130 Hz) or its higher harmonics. Also, tuning fork ME sensors, which are designed to reduce the acoustic and vibrational noise, require ME sensors with identical resonance frequencies. Two approaches to achieve tunability of the resonance frequency have been investigated in this project.

The first approach uses coupled resonators in combination with piezoelectric actuators. Two different tunable ME sensors with three parallel cantilevers fabricated from the same wafer have been investigated in this approach. As shown in Fig. A3-3, sensor I is a double-side clamped coupled resonator. The middle beam with a stack of 12 μm polysilicon/1 μm AlN/2 μm FeCoSiB is used as the magnetic field sensing element. The outer piezoelectric actuators consist of only polysilicon and AlN. The resonance frequency can be tuned by changing the stiffness of the structure with an applied voltage to the piezoelectric actuators. To increase the sensitivity while preserving the same frequency tuning method, sensor II is designed as a clamp-free structure consisting of three parallel cantilevers with a mechanical coupling at the free end. All three beams have the same geometry and the same stack. In resonance, a ME coefficient of 22 V/cmOe with a LOD of 4.6 nT/Hz^{1/2} and a ME coefficient of 424 V/cmOe with a LOD of 128 pT/Hz^{1/2} are measured for sensor I and II, respectively. High quality factors of more than 1600 are achieved for both sensors due to the polysilicon substrate and the vacuum encapsulation of the sensors. The resonance frequency of both sensors can be tuned as expected when a DC voltage is applied (Fig. A3-3). Sensor I has a higher frequency shift coefficient of 0.5 Hz/V than sensor II (0.2 Hz/V) due to a higher stress concentration in its double-side clamped structure. Both sensors show a linear tuning of the resonance frequency in the investigated voltage range, which is highly reversible and hysteresis-free. In conclusion, two tunable ME sensors, especially sensor II with low LOD of 128 pT/Hz^{1/2}, are demonstrated as promising candidates for the aforementioned applications.

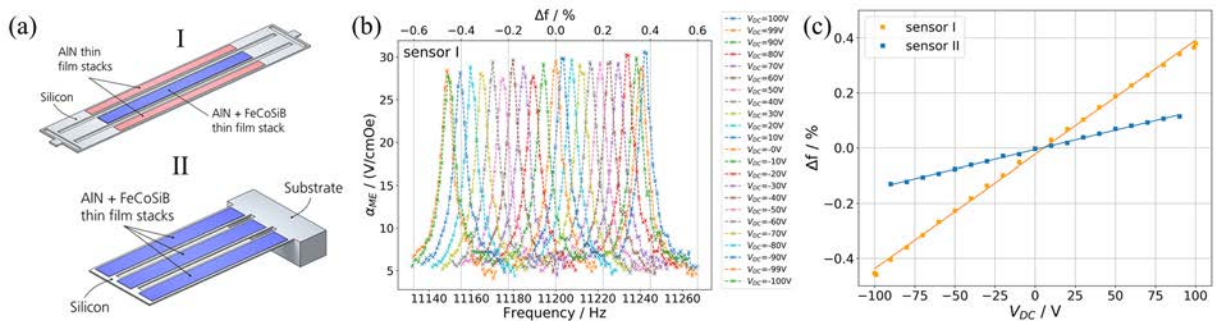


Figure A3-3: Tunable ME sensors with integrated piezoelectric actuators. a) Schematic illustration of two tunable ME sensor concepts. Sensor I contains an inner beam of $2234 \mu\text{m} \times 105 \mu\text{m}$ and two outer beams of $2234 \mu\text{m} \times 146 \mu\text{m}$. The functional layers with a length of $1500 \mu\text{m}$ are deposited in the middle of the substrate. All three beams are mechanically coupled on both sides and decoupled from the substrate by introducing a stress relaxation structure. Sensor II consists of three beams with the same size of $1500 \mu\text{m} \times 200 \mu\text{m}$ and a coupled structure of $100 \mu\text{m} \times 700 \mu\text{m}$. (b) Measured ME coefficient α_{ME} of sensor II with different applied DC voltages. (c) Resonance frequency of sensor I and II as a function of the applied voltage. Frequency shift coefficients of 0.41 % per 100 V and 0.14 % per 100 V are measured for sensor I and II, respectively.

The second frequency-tuning approach uses NiTi-based shape memory alloy (SMA) substrates for resonant ME sensors. The stiffness of this substrate can be changed with a short temperature pulse to set the sensor's resonance frequency. The first successful SMA ME sensor was a freestanding $2.5 \text{ mm} \times 15 \text{ mm}$ cantilever composed of 1 μm AlN/2 μm FeCoSiB/50 μm NiTi. By heating the entire composite to 450°C for 30 minutes, an austenite finish temperature of 84°C was achieved. Upon heating the sensor above this temperature, a change in resonance frequency by 12 % from 312 Hz to 351 Hz was observed due to the phase change of the SMA from R-phase to austenite [A3-7]. These ME sensors exhibited a sensitivity of 290 V/cmOe and a LOD of 110 pT/Hz^{1/2}. The comparable low sensitivity was expected due to heating FeCoSiB to 450°C , well above the crystallization temperature of 350°C [Hr14]. A second design approach focused on incorporating the ME onto SMA / Si substrates to benefit from the high quality factor of Si. From our analytical calculations (Fig. A3-

4a), a tunability of the resonance frequency of 0.1 % to 26.8 % can be expected. The difference in frequency between martensite and austenite phases becomes enhanced by increasing the TiNiCu film thickness or by eliminating the Si substrate. TiNiCu was chosen as the substrate because previously it has been demonstrated to undergo the transformation reversibly for up to 10 million cycles [Ch15]. Two new microfabrication schemes have been developed to allow the integration of AlN and FeCoSiB onto freestanding SMA and onto SMA/Si substrates. While in the original work plan changing to a high temperature stable magnetic composite of TiN/CoFe multilayers was planned, the new fabrication schemes allow the deposition of the magnetic layer at the end of the fabrication process. This enables depositing of the preferred FeCoSiB magnetic layer onto an atomically smooth Si surface. Furthermore, our process does not require the magnetic layer to undergo any heat treatment required by the SMA. Fig. 1b shows the tunable resonant frequency of a freestanding $1.7\ \mu\text{m}$ AlN/40 μm TiNiCu/2 μm FeCoSiB ME sensor that was heat treated at 500 °C prior to FeCoSiB deposition. In martensite at room temperature, the resonant frequency was 355 Hz with a quality factor of ~ 20 . Upon heating above the A_f temperature to 37 °C, a 12% shift in the resonance frequency to 388 Hz was observed with an increased quality factor of ~ 27 (Fig. A3-4b).

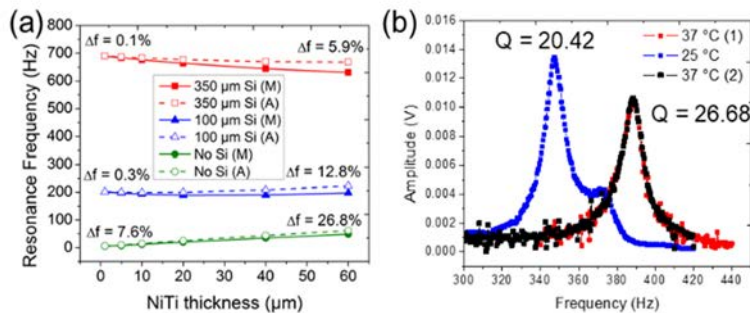


Figure A3-4: a) Analytical calculation showing influence of Si and TiNi thickness on resonance frequency tuning (Δf). b) Experimental demonstration of a freestanding $1.7\ \mu\text{m}$ AlN / 40 μm TiNiCu / 2 μm FeCoSiB ME sensor with $\Delta f = 12\%$.

ME sensors with powder-based permanent magnets

In this new sensor concept, 3-dimensional permanent magnets are integrated in silicon cantilevers. The magnets are positioned at the cantilever tip while a piezoelectric AlN layer at the cantilever base is used for read-out. This approach, originally developed for magnetic harvesters at ISIT, avoids magnetic noise in the magnetostrictive layer. The magnets are fabricated in a wafer-level technology by filling etched silicon cavities with NdFeB powder of around 5 μm particle size. Subsequently, the particles are agglomerated by an Al_2O_3 ALD layer and magnetized in the out-of-plane direction. The fabrication technology is described in more detail in Z1. Fig. A3-5 shows a photograph of a powder-magnet-based sensor together with a LOD measurement of cantilevers with 2000 μm and 1500 μm total length. LOD values below 10 $\text{pT}/\text{Hz}^{1/2}$ in resonance at frequencies of 2.2 kHz and 3.6 kHz are achieved [A3-2]. The external magnet field is applied in direction of the cantilever long axis.

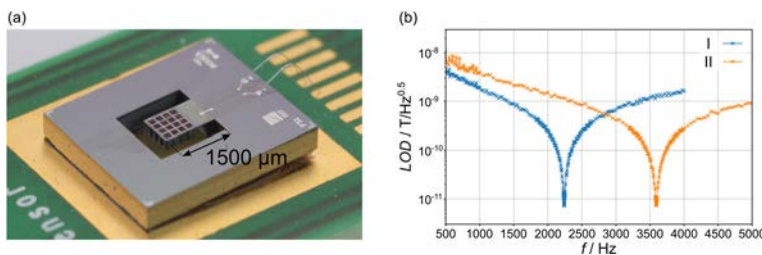


Figure A3-5: Powder-based NdFeB permanent magnets integrated into resonant MEMS magnetic field sensors. (a) photograph of a cantilever 1500 μm in length with permanent magnets at the cantilever tip and a piezoelectric AlN thin film in the bending region; (b) LOD as function of frequency of two permanent magnet MEMS sensors with cantilever lengths 1500 μm and 2000 μm , respectively, characterized in direct detection mode.

Sensors with piezoelectric AlScN layers

Resonant ME sensors with two different piezoelectric materials have been investigated, one being AlN [A3-10] and the other AlScN. So far no research has been reported on ME sensors with AlScN as the piezoelectric functional layer. As described in project A9, $\text{Al}_{1-x}\text{Sc}_x\text{N}$ ($x = 27\%$) has a higher piezoelectric coefficient that is about 2 times better than AlN [A3-8]. With the increase of Sc concentration, the stiffness of the thin film decreases and the dielectric constant increases. Two representative sensors, both having a Q of about 600, are compared in Tab. A3-1. In resonance, the ME coefficient of the AlScN-based sensor was measured to be approximately two times higher than that of the AlN-based ME sensors. However, the voltage noise density of the AlScN-based sensor is also about two times higher than that of the AlN-based sensor, as it scales linearly with the piezo-coefficient as well. This results in comparable LODs of sensors with both piezoelectric materials, when operated in direct detection. As the sensitivity is proportional to the piezoelectric coefficient and the

losses from the piezoelectric layer are not dominant for the sensor concept utilizing the ΔE -effect, these sensors are expected to strongly benefit from a change to AlScN. In addition, the decrease in Young's modulus is expected to further increase the sensitivity of the ΔE -effect sensor. An investigation is ongoing in collaboration with **A4**.

Table A3-1: Measurement results of ME sensors with AlN and AlScN operated in direct detection.

Piezoelectric layer	ME coefficient / V/cmOe	Noise density / nV/Hz ^{1/2}	LOD / pT/Hz ^{1/2}
AlN	709	45	63
AlScN	1338	82	61

References

- [Ch15] C. Chluba, W. Ge, R. Lima de Miranda, J. Strobel, L. Kienle, E. Quandt, M. Wuttig, Ultralow-fatigue shape memory alloy films. *Science* **348**, 1004-1007 (2015).
- [Hr14] V. Hrkac, E. Lage, G. Köppel, J. Strobel, J. McCord, E. Quandt, D. Meyners, L. Kienle, Amorphous FeCoSiB for exchange bias coupled and decoupled magnetoelectric multilayer systems: Real-structure and magnetic properties. *J. Appl. Phys.* **116**, 134302 (2014).
- [Ki13] C. Kirchhof, M. Krantz, J. Teliban, R. Jahns, S. Marauska, B. Wagner, R. Knöchel, M. Gerken, D. Meyners, E. Quandt, Giant magnetoelectric effect in vacuum, *Appl. Phys. Lett.* **102**, (2013), 232905.

Project-related publications by participating researchers

a) Peer-reviewed articles and books

- [A3-1] C. Tu, Z.-Q. Chu, B. Spetzler, P. Hayes, C.-Z. Dong, X.-F. Liang, H.-H. Chen, Y.-F. He, I. Lisenkov, H. Lin, Y.-H. Lin, J. McCord, F. Faupel, **E. Quandt**, N.-X. Sun, Mechanical-Resonance-Enhanced Thin-Film Magnetoelectric Hetero-structures for Magnetometers, Mechanical Antennas, Tunable RF Inductors, and Filters, *Materials* **12** (2019), 2259.
- [A3-2] F. Niekkel, J. Su, M. T. Bodduluri, T. Lisec, L. Blohm, I. Pieper, **B. Wagner**, F. Lofink, Highly sensitive MEMS magnetic field sensors with integrated powder-based permanent magnets, *Sensors and Actuators A* **297**, 111560 (2019).
- [A3-3] P. Durdaut, A. Kittmann, E. Rubiola, J.-M. Friedt, **E. Quandt**, R. Knöchel, M. Höft, Noise Analysis and Comparison of Phase- and Frequency-Detecting Readout Systems: Application to SAW Delay Line Magnetic Field Sensor, *IEEE Sensors Journal* (2019), 1-9, DOI:10.1109/JSEN.2019.2914965.
- [A3-4] B. Spetzler, C. Kirchhof, J. Reermann, P. Durdaut, M. Höft, G. Schmidt, **E. Quandt**, F. Faupel, Influence of the quality factor on the signal to noise ratio of magnetoelectric sensors based on the delta-E effect. *Appl. Phys. Lett.* **114**, 183504 (2019).
- [A3-5] P. Durdaut, A. Kittmann, A. Bahr, **E. Quandt**, R. Knöchel, M. Höft, Oscillator Phase Noise Suppression in Surface Acoustic Wave Sensor Systems. *IEEE Sensors J.* **18**, 4975-4980 (2018).
- [A3-6] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, F. Faupel, **E. Quandt**, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Sci Rep.* **8**, 278 (2018).
- [A3-7] V. Röbisch, A. Piorra, R. Lima de Miranda, **E. Quandt**, D. Meyners, Frequency-tunable nickel-titanium substrates for magnetoelectric sensors. *AIP Advances* **8**(12), 125320 (2018).
- [A3-8] S. Fichtner, N. Wolff, G. Krishnamurthy, A. Petraru, S. Bohse, F. Lofink, S. Chernitz, H. Kohlstedt, L. Kienle, **B. Wagner**, Identifying and overcoming the interface originating c-axis instability in highly Sc enhanced AlN for piezoelectric micro-electromechanical systems. *J. Appl. Phys.* **122**, 35301 (2017).
- [A3-9] P. Durdaut, S. Salzer, J. Reermann, P. Hayes, D. Meyners, **E. Quandt**, G. Schmidt, R. Knöchel, M. Höft, Thermal-Mechanical Noise in Resonant Thin-Film Magnetoelectric Sensors. *IEEE Sensors J.* **17**(8), 2338-2348 (2017).
- [A3-10] E. Yazar, S. Salzer, V. Hrkac, A. Piorra, M. Höft, R. Knöchel, L. Kienle, **E. Quandt**, Inverse bilayer magnetoelectric thin film sensor. *Appl. Phys. Lett.* **109**, 22901 (2016).

c) Issued Patents

- [A3-P1] A. Kittmann, S. Zabel, E. Yazar, F. Faupel, R. Knöchel, M. Höft, P. Durdaut, **E. Quandt**, Sensorelement für Magnetfelder mit hoher Frequenzbandbreite, DE 10 2016 123 274 B4

3.3 Funding

Funding of this project started in July 2016. It will be completed by the end of the current funding period.

3.3.1 Project staff in the ending funding period

	Se- quen- tial no.	Name, aca- demic degree, position	Field of re- search	Department of uni- versity or non-uni- versity institution	Project com- mit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	Quandt, Eck- hard, Prof. Dr.- Ing., Professor	Functional Materials	IMS	4		Core support
	2.	Wagner, Bern- hard, Prof. Dr., Professor	Microsys- tems Tech- nology	ISIT	4		Core support
	3.	Malave, Anto- nio, Dr., Sen- ior Researcher	Functional Materials	IMS	4		Core Support
	4.	Meyners, Dirk, Dr., Senior Researcher	Functional Materials	IMS	2		Core Support
	5.	Lofink, Fabian, Dr., Senior Researcher	Microsys- tems Tech- nology	ISIT	4		Core Support
	6.	Lisec, Thomas, Dr. Senior Re- searcher	Microsys- tems Tech- nology	ISIT	4		Core Support
Non-research staff	7.	Metzing, Thomas, Dipl.- Ing., Techni- cian		IMS	2		Core Support
Staff funded with approved grant money							
Research staff	8.	Anne Kittmann Sabrina Curtis Viktor Schell	Functional Materials	IMS		E 13	
	9.	Jingxiang Su	Microsys- tems Tech- nology	ISIT		E13	

Job descriptions of staff (supported through existing funds):

1. Prof. Dr.-Ing. Eckhard Quandt was responsible for the coordination and the scientific management of the CAU part of the project A3 and represents the project together with Prof. Wagner.
2. Prof. Dr. rer. nat. Bernhard Wagner was responsible for the coordination and the scientific management of the ISIT part of the project A3 represents the project together with Prof. Quandt.
3. Dr. Antonio Malave supported the doctoral researcher in the operation of the Kieler Nanolabor.
4. Dr. Dirk Meyners supported the doctoral researcher in thin film deposition and characterization.
5. Dipl.-Ing. Thomas Metzing supported the CAU doctoral researcher in issues regarding maintenance.
6. Dr. Fabian Lofink supported the ISIT doctoral researcher in MEMS design and fabrication issues.
7. Dr. Thomas Lisec supported the doctoral researcher in process technology and development.

Job descriptions of staff (funded with approved grant money):

8. The doctoral researchers Anne Kittmann, Sabrina Curtis and Viktor Schell (both in maternal leave of Anne Kittmann) were responsible for the scientific work at the CAU.
9. The doctoral researcher Jingxiang Su was responsible for the scientific work at the ISIT.

3.1.1 General information about Project A4

3.1.2 Project title: ΔE -effect sensors

3.1.3 Research area(s):

406-02 Synthesis and Properties of Functional Materials

408-01 Electronic Semiconductors, Components, Circuits, Systems

3.1.4 Project leader(s)

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Do any of the abovementioned persons hold fixed-term positions? No.

3.1.5 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

The ΔE -effect magnetic field sensor is particularly suited for measuring low-frequency AC fields. It avoids 1/f noise by utilizing the frequency shift of a high frequency electromechanical resonator from the change in the Young's modulus of a magnetostrictive component in a magnetic field. The sensor allows broadband magnetic field measurements down to the DC range and is resistant to microphony and mechanical noise. In particular, our sensor concept developed in Kiel provides full device integrability that will now be explored in the second funding period. As a final goal, we plan to develop fully integrated ΔE -effect sensors and sensor arrays including sensor electronics in a single unit. Initially, for cost savings and flexibility in design and testing, the development of the mechanical part, based on MEMS technology, and the electronics will occur on separate chips. The design of the magnetoelectric MEMS resonators will be based on the developed anisotropic magnetoelectric and electromechanical ΔE -effect models and will include the relevant losses, in particular clamping, eddy currents, and thermomechanical losses. The realization of the micromechanical design as a MEMS device is intended via Europractice, which provides prototyping and low volume production of MEMS structures separately as well as complementary metal oxide semiconductor (CMOS) technologies for integrating the sensor electronics. Especially, we plan to use the PiezoMUMPS technology of Europractice, as it already offers integration of the required piezoelectric AlN layer. The magnetic layer will be deposited as a final step in Kiel. Here, exchange biased films are also envisioned. In addition to providing robust, fully integrated magnetic field sensors with a broad bandwidth and huge dynamic range, we also plan to explore the possibility of using

sensor arrays with a large number of integrated sensors for increased resolution, noise reduction, and improved limit of detection. While, in principle, each sensor could be operated with its own electronics, total power consumption and challenges in parallel channel processing will require the development of proper grouping strategies as well as readout and excitation schemes. The already well-established larger sensors will serve as a benchmark for the miniaturized sensor elements and will also be further investigated in parallel.

3.3 Project progress to date

3.3.1 Report and current state of research

In the current funding period, emphasis was not laid on integration but rather on fundamental understanding of the complex sensor behavior and intensive modelling, which turned out to be crucial for further progress towards integration and an improved detection limit. Moreover, much effort has been put into a new type of ΔE -effect sensor, developed together with **A3**, which uses the ΔE effect to change the speed of guided surface acoustic shear waves (SAWs), so-called Love waves, in a magnetic field. For these reasons, all ΔE -effect sensors investigated by us in the current funding period were based on thin film technology and MEMS but had dimensions in the mm range and were not fully integrated. Work on multimode operation and adapted electrodes as well as on adaptive readout schemes, which started already before the reporting period, was completed and published ([A4-5], [A4-6]).

Due to its versatility, several applications of the ΔE -effect sensors even beyond the CRC were pursued concurrently. In a DARPA project (DARPA-BAA-15-19) together with **A3**, Virginia Tech (VT), Micromechatronics Inc. (MMech), Michigan Tech (MT), United Technologies Research Center (UTRC), and AVX Corp (AVX), the ΔE -effect sensor was investigated as electrical current sensor for "Tunable Energy Efficient Electronics". In the search for a ΔE -effect sensor with a very broad bandwidth in the MHz range, the Love wave SAW sensor based on shear waves was developed [A4-3] and patented [A4-P1]. On the other hand, the cantilever ΔE -effect sensor has now also been applied successfully in **B7** for cell imaging. In cooperation with **B2**, a simultaneous utilization of direct detection and ΔE detection has been investigated. The ΔE -effect sensors could also be promising for geophysical magnetic measurements which require sensors with a broad bandwidth down to DC and, unlike optical atomic magnetometers, are not saturated by the earth's magnetic field. A cooperation involving **A3**, **A4**, **B1**, **B2** and the Institute of Geosciences in Kiel has been established.

In the following, the results of the first funding period will be reported. To address the full integration of the ΔE -effect sensors in the second funding period, the Rieger group joined with its expertise, particularly in CMOS circuit design. Preliminary work of the Rieger group on integration will be presented in the second part of this report.

a) Detailed report

Sensor & system model

The work in the first period was focused on gaining a deep understanding of the ΔE -effect sensors. Understanding and identifying the influences on the sensitivity and the origin of noise was achieved with measurements combined with a detailed evaluation with a comprehensive model for the sensor system. The three main components of the model are depicted in Fig. A4-1. In the first part, the magnetic field-dependent component of the elastic stiffness tensor is calculated (ΔE effect) with a magnetoelastic sub-model. A variety of different approaches are available that have different advantages and are appropriate for different magnetic configurations. In a second step, the elastic stiffness tensor is used for an electro-mechanical model of the sensor that provides the sensor impedance $Z(f, H)$ as a function of frequency f and magnetic field H . The calculated sensor impedance $Z(f, H)$ is a decisive component in the equivalent signal and noise circuit that permits the calculation of signal, noise, and detection limit of the sensor and the setup in the last step.

The magnetoelastic models cover the full range, from quasi-static single-spin approaches to multi-spin mean-field and dynamic calculations. With these models, also the frequency dependence of the effect and inhomogeneities from the material and geometric effects can be considered [A4-1]. Specific domain configurations can be investigated with a multi-spin domain model. For μm -sized regions or the calculation of magnetostrictive self-energy effects, graphic processor-supported micromagnetic models can be used that have been developed in A4 from scratch.

The resulting stiffness tensor $C_{ijkl}(f, H(\vec{r}), \sigma(\vec{r}), \vec{r})$ of the magnetic film is a tensor field that depends on the frequency f of operation, the magnetic bias field $H(\vec{r})$, the stress tensor field $\sigma(\vec{r})$, and the spatial coordinates $\vec{r}$. It is used as input for the second part of the model, namely the electromechanical sub-model. It is based on

a finite element model (FEM) implemented in COMSOL Multiphysics and is used to calculate the electrical impedance of the sensor as a function of the frequency. With the FEM approach, complex device geometries and the spatial material properties, in particular $C_{ijkl}(H, \sigma, \bar{r})$, can be considered. Different numerical and analytical models for the quality factor have been implemented and developed that allow calculating the loss required for the electromechanical calculations. This includes all mechanisms that cannot be avoided by operation in vacuum, like thermoelastic damping, anchor loss and eddy current loss of the magnetic layer as a function of geometry, frequency, and magnetic materials parameters.

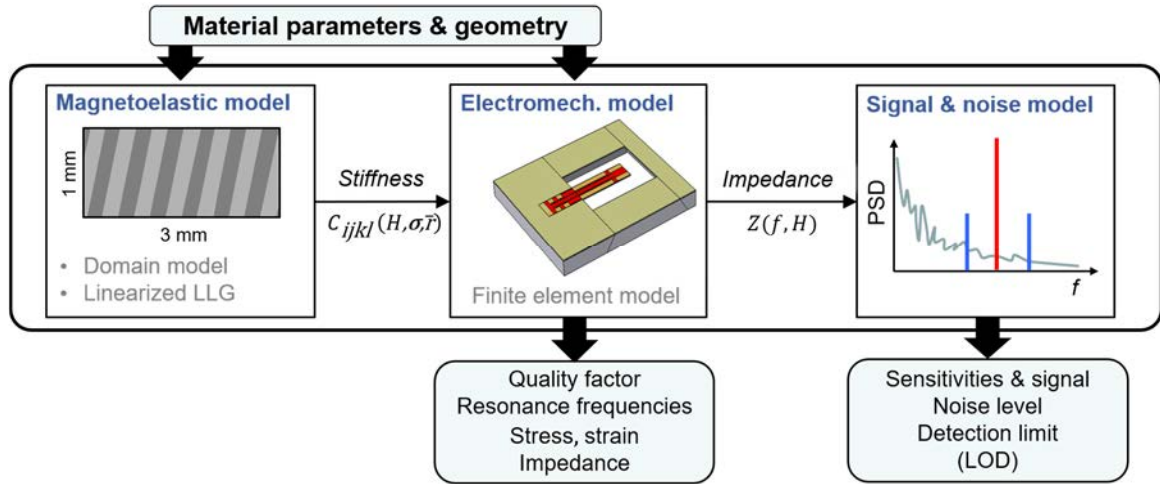


Fig. A4-1: Overview of the components of the ΔE -effect sensor model. It consists of a magnetoelastic model that provides the components C_{ijkl} of the stiffness tensor depending on the magnetic field H , the stress σ , and the location $\bar{r}$ in the sensor. C_{ijkl} is the input for the electromechanical model. This model passes the impedance on to the signal and noise model from which the sensitivities, noise level, and the detection limit (LOD) are calculated.

The sensor impedance is used as the input for a signal and noise model that has been developed in close cooperation with **B1**. With the model, sensitivities, signal, and noise levels were calculated [A4-4]. The noise model includes thermal-mechanical noise for arbitrary sensor geometries and the thermal-electrical noise of the piezoelectric layer and the measurement setup. We have used the model successfully to calculate the limit of detection (LOD) and resonance modes of our ΔE -effect sensors [A4-2].

The developed model comprises a comprehensive and advanced approach for modelling the full ΔE -effect sensor. In contrast, the available literature ([Li82], [Sq90], [Da09], [Zh14]) is mainly limited to quasi-static single-spin approaches describing only the ΔE effect and neither sensitivity nor noise.

Experimental and model results

The model has been validated in combination with measurements on different sensor designs in various studies. Deep insights into the ΔE effect and its application in magnetic field sensing were gained from comparing measurements with model results. A strong overlap between the magnetic theory and device applications has been achieved. Together with **A1** and **A3**, the best multi-layer ΔE -effect sensors have been analyzed extensively with magneto-optical imaging and impedance measurements. It is found that internal inhomogeneities have a strong influence on the ΔE effect and the sensitivity of the device. The inhomogeneity of the internal stray field is identified as an important factor for improving the sensitivity. This is well reflected by the models and explains the dependence of the sensitivity on the resonance mode utilized [A4-1]. Using an adapted electrode design to operate in the second bending mode avoids local stray field distributions and so, combined with an optimum electrical excitation, has led to a six-fold improvement in sensitivity compared to the first mode and a detection limit below 100 pT/Hz^{1/2} from 10-100 Hz [A4-5]. This study [A4-1] also emphasized the important role of the layer thicknesses for bending modes. The ideal substrate and piezoelectric layer thicknesses depend on their mechanical and electric properties. For the magnetic layer, an optimum thickness results and depends strongly on the geometry of the film and the anisotropy energy density. At the maximum, a strong sensitivity boost by a factor of 4 is estimated when compared to the current thickness. Exceeding the maximum results in a reduced sensitivity that approaches zero for increasing film thickness. The tendency is consistent with measurements performed on differently sized sensor devices. Understanding and predicting this effect is of fundamental importance for downscaling the device while keeping or increasing the existing sensitivity.

The influence of the quality factor Q on the LOD was investigated with measurements and simulations of ΔE -effect sensors in vacuum [A4-2]. It was found that the thermal mechanical noise dominates at low excitation amplitudes, but magnetic noise dominates at large amplitudes. Whereas it is known that the $LOD \sim Q^{-0.5}$ for

the direct detection, we found that $LOD \sim Q^{-1.5}$ for ΔE -effect sensors operated at their mechanical resonance frequency in the thermal-mechanical noise regime (Fig. A4-2). The results emphasize the need for magnetic noise reduction [A4-4] and the great potential of the quality factor for improving the detection limit of ΔE -effect sensors, if magnetic noise can be suppressed. The loss mechanisms that dominate the quality factor have been investigated and the models validated with different sensor designs and geometries including vacuum encapsulated resonators from the ISIT (A3).

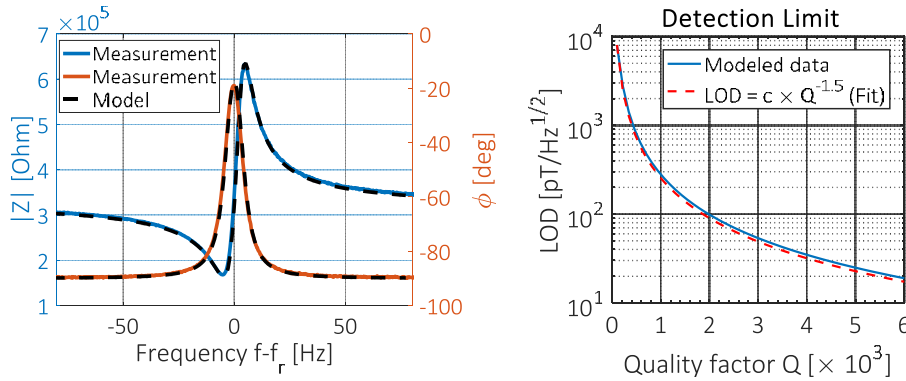


Figure A4-2: Comparison of results from the electro-mechanical FEM model with measurements on the impedance of a ΔE -effect sensor (left) and calculation of the limit of detection (LOD) for this sensor geometry as a function of the quality factor Q . A fit (red, dashed) shows the dependence of the LOD on Q [A4-2] (right).

A strong dependency of Q on the magnetization and frequency was found that is well explained by stress-induced eddy current loss (magnetoelastic loss) in the model. This loss dominates at the magnetic bias field and limits the Q -factor to about $Q = 1000 - 2000$. In magnetic saturation, the dominant loss depends strongly on the resonance mode used. Bulk and alternative modes of vacuum encapsulated plate and cantilever resonators were analyzed. These sensors are much smaller than the previously used sensors and operate at modes up to the low MHz regime. Promising modes were found with kHz bandwidths and large quality factors of $Q > 4000$ in magnetic saturation and $Q = 2000$ at the optimum magnetic bias field. The loss models are consistent with these results and open the possibility of already considering the magnetoelastic loss during the sensor design for future devices.

The frequency dependence of the magnetic properties, the ΔE effect, and the magnetic sensitivity were investigated in cooperation with the McCord group (A1). A strong dependency of the ΔE effect and the sensitivity on the frequency was found in the high MHz regime. A maximum in the sensitivity is predicted in the low GHz regime below the ferromagnetic resonance frequency. Although this frequency regime is not relevant for the cantilever sensors, it can strongly influence surface acoustic wave (SAW) resonators or nano-plate resonators operating at several hundreds of MHz. The frequency effects on the Young's modulus are supported by [Sm03].

Besides bending modes, shear resonance sensors were designed and analyzed experimentally and with the model. It was found that the shear modulus can offer a much higher sensitivity than the ΔE effect, if the magnetic properties are well controlled (Fig. A4-3). The comparison of the model with measurements points out that other components of the stiffness tensor in torsional modes of cantilever sensors have a negative effect on the sensitivity, and edge effects must be controlled precisely. Hence, the aforementioned Love wave SAW ΔE -effect sensor was explored to use the shear modulus. Fig. A4-4 shows a comparison between model results from the current project and experiments. Although the development of this sensor type is still at an early stage, a huge dynamic range of 120 dB combined with a low detection limit in the range of 100 pT/Hz^{1/2} was achieved in joint work (A3, A4, A8, B1, B2) [A4-3] and a patent was filed [A4-P1].

All aforementioned ΔE -effect sensors require a magnetic bias field for optimal operation. The bias field is usually provided by an external magnetic field generated by coils. As an alternative possibility, exchange biased magnetic multilayers [La12] can be used. Here we could show that similar minimum detection limits of about 350 pT/Hz^{1/2} (at 10 Hz) can be reached without an external magnetic field. This is of particular interest for the application projects and sensor integration.

As another way to improve the LOD, magnetic flux concentrators have been analyzed together with A8. Flux concentrators can increase the sensitivity by several factors, depending on their size relative to the magnetic layer of the sensor. Improving the sensitivity of the mm-sized cantilever design by a factor of 3 requires a large concentrator area that reduces the spatial resolution from a few mm² to several cm². Consequently, flux concentrators are only recommended and advantageous for μ m-sized sensors. For the integrated sensor arrays that will be investigated in the second funding period, the maximum number of sensor elements is expected to be limited by the electronics. Here, flux concentrators can possibly be a great way to utilize the excess volume on the chip and significantly increase the detection limit.

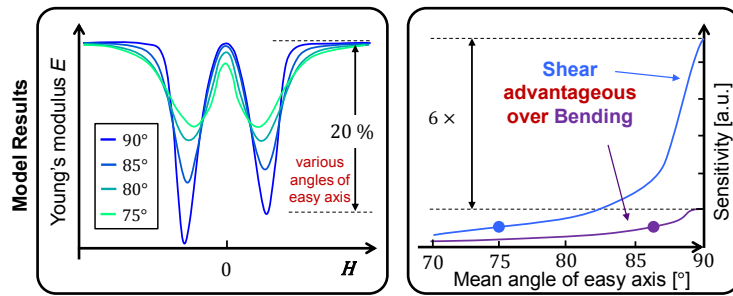


Figure A4-3: Model results for the Young's modulus for different orientations of the mean easy axis to the applied magnetic field H . A small deviation from a 90° orientation results in a significant change of the ΔE effect of the Young's modulus (left). The resulting magnetic sensitivity derived for pure bending and pure shear as a function of the mean angle of the easy axis to the applied field. At angles close to 90° , the shear mode shows a magnetic sensitivity about six-fold higher (right).

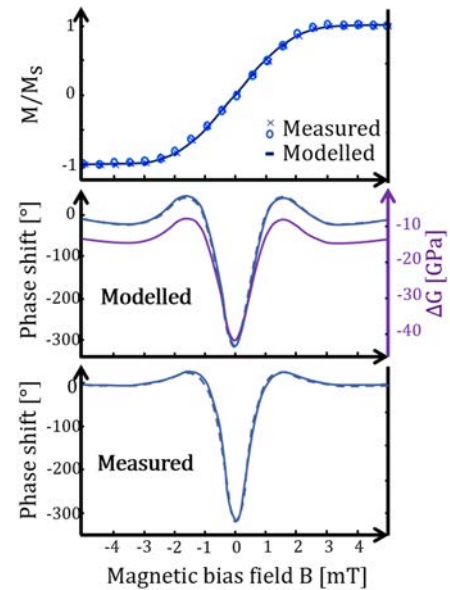


Figure A4-4: Comparison of model results with measurements on a surface acoustic wave (SAW) Love wave sensor: Comparison of modelled with measured magnetization curve (top) modelled phase shift and modelled change of shear modulus G (middle) and measured phase shift (bottom) [A4-3]

b) Preliminary work of the Rieger group

The principal expertise of the Rieger group is in the field of electronic engineering with integrated circuit design. Over the past 15 years practical experience has been gained in the design, implementation, and testing of miniaturized and low-power sub-circuits and sensing systems for biomedical applications, both in academia and industry. The realization of integrated circuits using CMOS or bipolar-CMOS (BiCMOS) application-specific integrated circuit (ASIC) technologies is accessible to us in this project via the Europractice manufacturing services based on shared multi-project-wafer runs. Since November 2018, initial work in the Rieger group with the focus on sensor concepts developed in this consortium have been supported with a CRC doctoral student grant. The measurements of ΔE -electronics reported here result from this financing.

Initial work on resonant sensor readout electronic components has been carried out in the Rieger group as reported in [A4-8]. In that work, a digitally-controlled flexural plate wave sensor readout setup was investigated to estimate the effect of quantization errors of the excitation generator (excitation frequency around 1.84 MHz, realized in $0.35 \mu\text{m}$ CMOS technology on 0.045 mm^2 of silicon) and signal sampler for application in binary screening. It was established that a frequency resolution of 1 kHz is appropriate, and a differential detection system with relatively low accuracy of 0.05% and moderate resolution is sufficient to discriminate between two sensor loading conditions. It was demonstrated that the high bandwidth selectivity of the sensor can be employed to sufficiently suppress harmonic components so that a square wave excitation signal may be used in specific applications. This considerably simplifies the read-out electronics compared to when on-chip sinewave generation is required. It also reduces the need for on-chip filtering and enables one to derive multiple frequency-locked excitation generators from a single square-wave master clock.

Since ASIC integration technology permits a high density of sensor electronics and the accommodation of a large number of parallel channels (exceeding 100 channels - the limitations will be established in this project), the power efficiency of the individual channels becomes important. Especially in applications, such as this project, which require a very low-noise input stage, the design of the front-end amplifier must be carefully considered. The design of low-noise amplifiers is a core expertise of the Rieger group [A4-P3], prominently applied in the past to the acquisition of biopotentials. Conventionally, the trade-off between the current consumption of the amplifier stage and the input-referred noise is expressed by comparing with the noise performance of an idealized bipolar junction transistor. The resulting metric, termed the noise-efficiency-factor, indicates how efficiently the circuit employs available current to minimize electronic noise. Bipolar transistors tend to be more noise efficient than their CMOS counterparts. An optimized practical design that consumes 1.3 mW may exhibit voltage noise as low as $3.3 \text{ nV/Hz}^{1/2}$ and $1.8 \text{ pA/Hz}^{1/2}$ current noise [A4-10]. Due to their lower input impedance, BiCMOS input stages are not readily applicable to high-impedance sensors, which include the ΔE structure [A4-9]. Therefore, suitable strategies for base current cancellation and impedance matching will be investigated.

In order to minimize the power consumption per detection channel, passive and active strategies will be investigated in this project. In a passive grouping strategy, sensors are electrically connected in front of the first amplification stage, so that several sensors share a common input amplifier. In the active approach, optimized front-end electronics will be investigated which reduce the power consumption per sensing channel. Preliminary studies have been carried out to validate the principal approaches. For passive grouping, two ΔE -effect sensors with similar properties were selected and connected to a readout amplifier built from discrete components in a bench setup. The amplifier is a replica of the circuit devised in Kiel to characterize the ΔE sensors in [Du17], representing the state-of-the-art. Notably, the available sensors have been selected from spare devices manufactured during the previous periods of this CRC. The designs are not optimized in any way for the integration intended here. A frequency sweep of the excitation signal is performed, and the sensor output is measured first for the individual sensors and then, in a second experiment, for the sensors connected to the amplifier input in parallel. The measured results are shown in Fig. A4-5. From the sweep results, it is observed that the resonance peak frequencies of the individual sensors differ by approximately 11 Hz. This is close enough to yield a constructive addition of the peak amplitudes when the sensors are operated in parallel. The parallel peak amplitude is higher by a factor of about 1.7 compared to the average of the individual sensor peaks. The noise measurement in Fig. A4-5 yields similar wide band noise levels for both the individual sensors as well as for the parallel connection. Although these preliminary results lack accuracy and require a further improved measurement setup, they support the general notion that passive grouping is feasible and a potential for signal-to-noise ratio improvement exists.

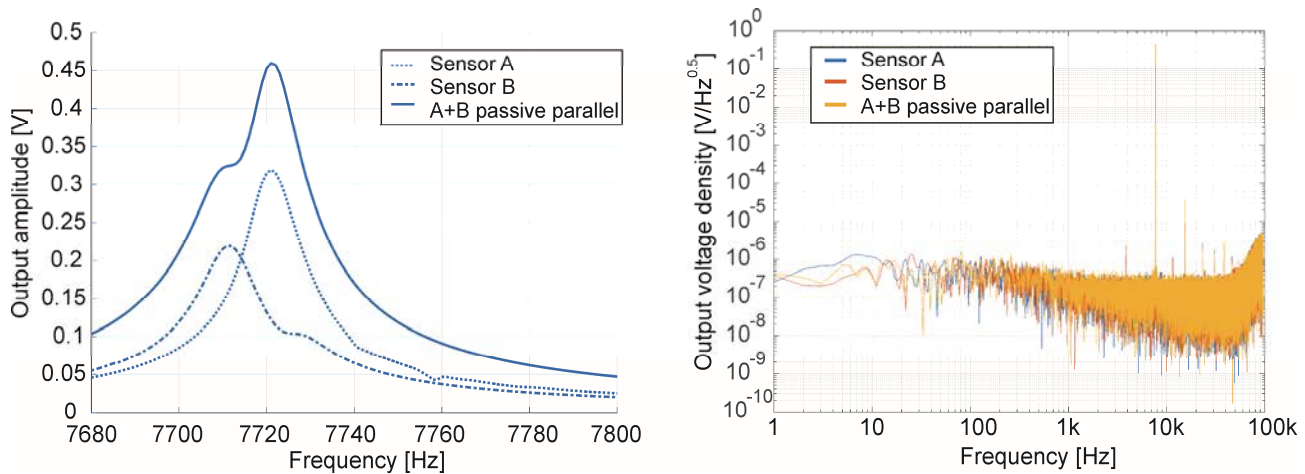


Fig. A4-5: Preliminary measured results comparing passive parallel sensor connection with individual sensor performance. Sweep of the excitation frequency (left) and noise spectral diagram while the sensors are excited at 7.72 kHz (right). The sensors were not optimized for matching and exhibit a noticeable difference in resonance frequency. Still, parallel sensor connection increased the signal amplitude more than the noise level, resulting in an improved signal-to-noise ratio.

As a candidate for active grouping, it is envisaged that the concept of orthogonal current reuse [Ja14] can be employed. Here, the current needed to bias a first differential pair amplifier is used again to also bias further amplifiers, and thus reduces the power consumption on a per-channel basis compared to a row of conventional parallel amplifiers without sacrificing amplifier noise performance. Recombining the amplifier output currents in a prescribed way individualizes the outputs and removes signal and noise contributions from the other channels. Channel crosstalk was shown in [Ja14] to remain below -46 dB. Initially, an implementation of the current reuse amplifier providing three independent sensing amplifiers is designed with the circuit parameters for the target 350nm CMOS technology by ON Semiconductor as provided by Europractice. Different versions of the test structure are considered with some using lateral bipolar transistors, which can be manufactured in the standard CMOS technology, and others using p-channel MOSFET input devices. The schematic diagram of the bipolar input stage is shown as an example in Fig. A4-6 (left), since it illustrates the stacking principle most clearly. Simulations of the complete amplifier circuit including channel separation stage have been performed. The small-signal simulation results for open-loop amplifier gain and input-referred voltage noise density are shown in Fig. A4-6 (right) for the first of three channels. The results indicate that the noise floor is reached within the targeted frequency range of the ΔE -effect sensor around 1 MHz. Also, sufficient gain is produced by the circuit in this frequency band. A first chip including this and further test structures is currently in fabrication and expected back for evaluation before the start of the new project period.

Reading out a high-impedance ΔE -effect sensor requires careful interface circuit design. Signal drift is a commonly observed problem in which undesired discharge of the interface capacitance leads to a slowly varying signal level which, when amplified with a high gain, may saturate the signal processing stages and lead to loss

of signal information. Strategies to mitigate this problem have been proposed [A4-P2]. Folding the signal by means of periodically recharging the interface capacitance to a known reference potential accomplishes the reduction of signal and drift amplitude. The resulting steps in the signal can be compensated by a digital post-processing algorithm after amplification and digitization. However, the loss of resolution due to quantization inevitably leads to additional noise in a reconstructed signal. It appears as a $1/f$ -noise component with a magnitude depending on the frequency of capacitance recharge [A4-7]. Consequently, in this noise-sensitive application, we aim to manage sensor drift to a level that requires only infrequent interface reset and does not occur during a measurement interval.

Experience with the operation of the software package for MEMS layout has been gained by the Rieger group. Sensor geometries for first MEMS test structures which also consider the layer thicknesses set by the manufacturer have been devised with the modelling expertise of the Faupel group and have been laid out by using the PiezoMUMPs design kit provided by CMP, Grenoble. The design has taped out and samples are expected back for characterization before the start of the new funding period.

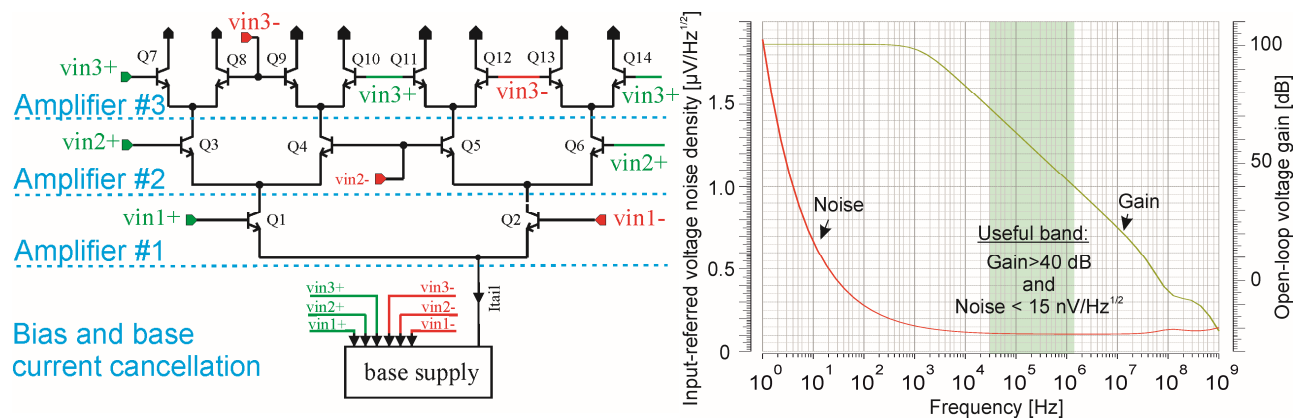


Fig. A4-6: Schematic diagram of the stacked input stages of the current reuse amplifier (left). The circuit provides three independent differential sensing amplifiers. Simulation results for input-referred voltage noise density and gain suggest a useful bandwidth at around 1 MHz (right).

References

- [Cl80] Clark, A. E.: *Magnetostrictive rare-earth-Fe compounds in Handbook of Ferro-Magnetic Materials*, (Elsevier, The Netherlands: North-Holland (1980), vol. 1).
- [Du17] P. Durdaut, V. Penner, C. Kirchhof, E. Quandt, R. Knöchel, M. Höft, Noise of a JFET Charge Amplifier for Piezoelectric Sensors. *IEEE Sens. J.* **17**, 7364 (2017).
- [Da09] L. Daniel, O. Hubert, An analytical model for the ΔE effect in magnetic materials. *Eur. Phys. J. Appl. Phys.* **45**, 31101 (2009).
- [Go11] B. Gojdka, R. Jahns, K. Meurisch, H. Greve, R. Adelung, E. Quandt, R. Knöchel, F. Faupel, Fully integrable magnetic field sensor based on ΔE effect. *Appl. Phys. Lett.*, **99**, 223502 (2011). Moving micro magnets. Nature Research Highlight, *Nature* **155**, 480 (2011).
- [Gr10] H. Greve, E. Woltermann, H. J. Quenzer, B. Wagner, E. Quandt, Giant magnetoelectric coefficients in (Fe₉₀Co₁₀)₇₈Si₁₂B₁₀-AlN thin film composites. *Appl. Phys. Lett.* **96**, 182501 (2010).
- [Hu15] J. M. Hu, T. Nan, N. X. Sun, L. Q. Chen, Multiferroic magnetoelectric nanostructures for novel device applications. *MRS Bulletin* **40**, 728 (2015).
- [Hu11] D. Hunter, W. Osborn, K. Wang, N. Kazantseva, J. Hattrick-Simpers, R. Suchoski, R. Takahashi, M. L. Young, A. Mehta, L. A. Bendersky, S. E. Lofland, M. Wuttig, I. Takeuchi, *Nat. Commun.* **2**, 1 (2011).
- [Ja14] R. Jahns, S. Zabel, S. Marauska, B. Gojdka, B. Wagner, R. Knöchel, R. Adelung, F. Faupel, Magnetic field sensor based on ΔE effect. *Appl. Phys. Lett.* **105**, 052414 (2014).
- [Ja13] R. Jahns, A. Piorra, E. Lage, C. Kirchhof, D. Meyners, J. Gugat, M. Krantz, M. Gerken, R. Knöchel, E. Quandt, Giant magnetoelectric effect in thin film composites. *Journal of American Ceramic Society* **96**, 1673 (2013).
- [Jo13] B. Johnson, A. Molnar, An Orthogonal Current-Reuse Amplifier for Multi-Channel Sensing. *J. Solid-State Circuits* **48**, 1487 (2013).
- [Ja12] R. Jahns, H. Greve, E. Woltermann, E. Quandt, R. Knöchel, Sensitivity enhancement of magnetoelectric sensors through frequency conversion. *Sensors and Actuators A: Physical* **183**, 16-21 (2012).
- [KI19] M. J. Klug, L. Thormählen, V. Röbisch, S. Salzer, M. Höft, E. Quandt D. Meyners, J. McCord, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors. *Appl. Phys. Lett.* **114**, 192410 (2019).

- [La12] E. Lage, C. Kirchhof, V. Hrkac, L. Kienle, R. Jahns, R. Knöchel, E. Quandt, D. Meyners, Exchange biasing of magnetoelectric composites. *Nature Materials* **11**, 523 (2012).
- [Lu02] A. Ludwig, E. Quandt, Optimization of the Delta E effect in thin films and multilayers by magnetic field annealing. *IEEE Transactions on Magnetics* **38**, 2829 (2002).
- [Li82] J.D. Livingston, Magnetomechanical properties of amorphous metals, *Phys. Stat. Sol. A* **70**, 591 (1982).
- [Mc15] J. McCord, Progress in magnetic domain observation by advanced magneto-optical microscopy. *J. Phys. D: Appl. Phys.* **48**, 333001 (2015).
- [Na13] T. Nan, Y. Hui, M. Rinaldi, N. X. Sun, Self-Biased 215MHz Magnetoelectric NEMS Resonator for Ultra-Sensitive DC Magnetic Field Detection. *Scientific Reports* **3**, 1985 (2013).
- [Na08] C. W. Nan, M. Bichurin, S. Dong, D. Viehland, G. Srinivasan, Multiferroic magnetoelectric composites: Historical perspective, status and future directions. *J. Appl. Phys.* **103**, 031101 (2008).
- [Os96] R. Osiander, S. A. Ecelberger, R. B. Givens, D. K. Wickenden, J. C. Murphy, T. J. Kistenmacher, A microelectromechanical based magnetostrictive magnetometer. *Appl. Phys. Lett.* **69**, 2930 (1996).
- [Ro17] V. Röbisch, S. Salzer, N. O. Urs, J. Reermann, E. Yazar, A. Piorra, C. Kirchhof, E. Lage, M. Höft, G. Schmid, R. Knöchel, J. McCord, E. Quandt, D. Meyners, Pushing the detection limit of thin film magnetoelectric heterostructures. *J. Mater. Res.* **32**, 1009 (2017).
- [Sm03] P. Smole, W. Ruile, C. Korden, a. Ludwig, E. Quandt, S. Krassnitzer, and P. Pongratz, *IEEE Int. Freq. Control Symp. PDA Exhib. Jointly with 17th Eur. Freq. Time Forum*, 2003. Proc. 2003 **4** (2003).
- [Sq90] P.T. Squire, Phenomenological model for magnetization, magnetostriction and ΔE effect in field-annealed amorphous ribbons, *J. Magn. Magn. Mater.* **87**, 299–310 (1990).
- [Zh14] H. Zhou, A. Talbi, N. Tiercelin, O. B. Matar, Multilayer magnetostrictive structure based surface acoustic wave devices, *Appl. Phys. Lett.* **104**, 0–4 (2014).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [A4-1] B. Spetzler, C. Kirchhof, E. Quandt, J. McCord, **F. Faupel**, Magnetic Sensitivity of Bending Mode ΔE -effect sensors, *Phys. Rev. App.* **12**, 064036 (2019).
- [A4-2] B. Spetzler, C. Kirchhof, J. Reermann, P. Durdaut, M. Höft, G. Schmidt, E. Quandt, **F. Faupel**, Influence of the Quality factor on the Signal to Noise Ratio of Magnetoelectric Sensors based on the ΔE effect. *Appl. Phys. Lett.* **114**, 183505 (2019). **Editor's Pick**.
- [A4-3] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, **F. Faupel**, E. Quandt, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Scientific Reports* **8**, 1 (2018). **Top 100 read articles 2018**.
- [A4-4] P. Durdaut, J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, **F. Faupel**, G. Schmidt, R. Knöchel, M. Höft, Modeling and Analysis of Noise Sources for Thin-Film Magnetoelectric Sensors Based on the ΔE effect. *IEEE Transactions on Instrumentation and Measurement* **66**, 2771 (2017).
- [A4-5] S. Zabel, J. Reermann, S. Fichtner, C. Kirchhof, E. Quandt, B. Wagner, G. Schmidt, **F. Faupel**, Multi-mode ΔE effect magnetic field sensors with adapted electrodes, *Appl. Phys. Lett.* **108**, 222401 (2016).
- [A4-6] J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, **F. Faupel**, G. Schmidt, Adaptive readout schemes for thin-film magnetoelectric sensors based on the ΔE effect. *IEEE Sens. J.* **16**, 4891 (2016).
- [A4-7] **R. Rieger**, Signal-Folding for Range-Enhanced Acquisition and Reconstruction. *IEEE T Circuits-I* **62**, 2617 (2015).
- [A4-8] Y. Y. Chen, **R. Rieger**, Evaluation of a Readout Circuit with ASIC Oscillator for Acoustic-Wave Sensor Application. *International Journal of Electronics Letters* **1**, 9 (2013).
- [A4-9] **R. Rieger**, J. Taylor, Design Strategies for Multi-Channel Low-Noise Recording Systems. *Analog Integr. Circuits Signal Process* **58**, 123 (2009).
- [A4-10] **R. Rieger**, J. Taylor, A. Demosthenous, N. Donaldson, P. J. Langlois, Design of a low-noise preamplifier for nerve cuff electrode recording. *IEEE J. Solid-State Circuits* **38**, 1373 (2003).

b) Issued Patents

- [A4-P1] E. Quandt, A. Kittmann, S. Zabel, E. Yazar, **F. Faupel**, R. Knöchel, M. Höft, P. Durdaut, Sensor-element für Magnetfelder mit hoher Frequenzbandbreite; DE102016123274B4.
- [A4-P2] **R. Rieger**, Piezo-Electric Transducer System and Signal Processing Method Thereof; TWI446134B.
- [A4-P3] **R. Rieger**, Integrated Low Noise Sampling Amplifier; TWI377782B.

3.4 Project plan

Objectives

Based on the achieved thorough theoretical understanding of the ΔE -effect sensor and the successful experimental validation, the final goal of Project A4 is now the research of fully integrated ΔE -effect sensors and sensor arrays, including sensor electronics, fabricated as a single unit in ASIC technology. From the sensor concepts pursued within the CRC 1261, the ΔE sensor is particularly suited for full integration. It is particularly well understood and can be operated at frequencies below 10 MHz, which thus keeps the electronics simple. Moreover, because it is a flux density sensor, the sensor concept itself does not limit downscaling of the device. Finally, concerning transfer to application, the ΔE sensor is robust, does not require integration of any coils, and has a broad bandwidth down to DC. Apart from the transfer to applications, the integration has many advantages, also from the fundamental point of view. Especially, the reduction in sensor size increases the local resolution, and fabrication of the sensors in a semiconductor and MEMS fabrication unit ensures very high reproducibility of the individual sensors, which is crucial for sensor arrays with a large number of sensors. In the second funding period, for cost savings and flexibility in design and testing, the development of the MEMS technology part of the sensor and the sensor electronics will occur on separate chips.

The central hypotheses are: (1) We can downscale the sensor without major loss in LOD; (2) The integration of the sensor electronics will not significantly affect individual sensor performance; (3) we can group the sensors to reduce the required electronic channels. This would lead to a strongly improved LOD of sensor arrays, scaling with $n^{1/2}$, where n is the number of individual sensors. Concerning (1), downscaling will mainly affect the magnetostrictive layer, particularly due to significantly increased edge effects on the domain structure. We expect that those effects will, inter alia, be overcompensated by the largely improved quality of the much thinner magnetostrictive layer, the elimination of anisotropy stress due to deposition on a released resonator structure, the very high quality factor of the MEMS resonators which was shown to enter with $Q^{1.5}$ in the LOD of ΔE -effect sensors, and a tailored design that especially minimizes the very detrimental stray field effects. As for (2) and (3), we refer to the details given below and the first encouraging experiments on sensor grouping, discussed above. In parallel to the miniaturization, we will continue investigations of the established larger sensors.

Proposed research methods

The magnetoelectric MEMS resonators will be designed with the developed entirely anisotropic magnetoelastic and electromechanical ΔE -effect models (see report) and will include the relevant losses, in particular clamping, eddy current, and thermomechanical losses. The realization of the micromechanical design as a MEMS device is intended to be done by Europractice, which permits prototyping and low volume production of MEMS structures separately as well as CMOS technologies for integrating the sensor electronics. We plan to use the PiezoMUMPS technology of Europractice, as it not only provides the optimum feature size and layer thickness ranges but also permits integration of the required piezoelectric AlN layer. Within the CRC 1261, AlN has turned out to be the material of choice for the piezoelectric layer in terms of signal-to-noise ratio as well as quality and reproducibility of the deposited films. The PiezoMUMPS technology of Europractice allows four designs per year, each with 15 chips that can be sub-diced to obtain a total of 60 chips per order. Europractice also provides packaging and 3D stacking of post-processed chips.

The magnetic layer will be deposited as a final step in Kiel by using external shadow-mask technology to achieve mask alignment in the μm -range and precise film structuring. The post-deposition ensures that potentially present anisotropic stress from the MEMS process cannot affect the magnetic properties. Shadow masks are not suitable for the deposition of periodic multilayer structures with a large number of periods, but in our PiezoMUMPS design the thickness of the magnetostrictive layer will only be of the order of 200 nm. Thus, we expect the number of periods to be two or even one. The very low number of periods is another big advantage of downscaled sensors because the quality of the magnetostrictive layer in larger structures turned out to decrease considerably with increasing period number. In the unexpected case that the shadow-mask approach is not feasible, the magnetic layer could be deposited without structuring to cover the whole device. Short circuits will be avoided through previous deposition of an Al_2O_3 layer and manual coverage of the comparatively large bond pads. For sensor arrays, the small area of the chip ensures very homogeneous deposition with essentially no spread between the individual cantilevers of a given array.

The size of the cantilevers is ideal for characterization by the magneto-optic Kerr effect (MOKE) technique. MOKE is extensively used within the SFB 1261 and operated by the McCord group [Mc15].

Based on the expected very high reproducibility in device fabrication via ASIC technology, plans are to explore the possibility of using sensor arrays with a large number of integrated sensors for increased resolution, noise reduction, and improved limit of detection. Sensor arrays are also interesting for vector magnetometry. For the arrays, important points to be addressed are optimum packing of the individual sensors, crosstalk, electromagnetic shielding as well as mechanical decoupling. While, in principle, each sensor could be operated with its

own electronics – at least for arrays with a large number of sensors – total power consumption and other challenges will require the development of proper grouping strategies as well as readout and excitation schemes. CMOS test structures will be fabricated on ASIC via Europractice and these chips will be characterized with standard methods of electronics measurement. This includes stimulus generation and signal acquisition using custom-programmed microprocessors, software-supported instrumentation with LabView (National Instruments Inc.) as well as Low-noise spectrum analyzers for noise and distortion measurement.

Work plan

The work plan is shown as a Gantt chart in Fig. A4-7. It is subdivided in the five work packages discussed below. An overview on the duration of the work packages is given in the following table.

Figure A4-7: Work schedule – Main work performed by the Faupel group (red) and the Rieger group (blue). Notably, electronic and mechanical design is continued while chips are in manufacture so that there are no gaps in the work flow.

	2020		2021				2022				2023				2024	
	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP 1: MEMS layout and test																
WP 2: Magnetic component																
WP 3: Single sensor elements																
WP 4: Sensor electronics																
WP 5: Sensor arrays																

WP1 MEMS layout and test

This work package is based on an established MEMS process that has stable thin-film parameters and a well-developed set of design rules. We also benefit from the existing experience with MEMS prototyping within the CRC (ISIT, **Z1**) and the development of powerful models for the ΔE effect in the Faupel group together with the experience in chip design and tapeout flow in the Rieger group. The design parameters for sensors and arrays optimized in **WP3** and **WP5** are translated into geometries suitable for MEMS fabrication in this work package. Appropriate information flow between the work packages will be ensured. This is essential, as the sensor design is constrained by the design space offered by the PolyMUMPs technology. The layout will be performed using the standard tools provided by Europractice. With an established tool and production chain, this approach ensures maximum reproducibility and allows a flexible and quick realization of new designs.

In this work package, the software tools for the MEMS design are established and first test structures are realized. The test structures are used to investigate the boundary conditions for the magnetic layer deposition in **WP2** and the design of the electromechanical resonator. Various analytical methods available in Kiel are used for a thorough characterization of the resulting structures. This includes surface roughness, underetching effects, and the geometry of layer edges. The results are also used to adjust the existing electromechanical models with structural inhomogeneities and tolerances, if necessary. The layout is then simulated again using the methods of **WP3** and **WP5** and checked against the designed target parameters.

Sensor grouping strategies will also be considered in this WP, because only a limited number of bonding pads are available (constrained by the number of bonding wires that can reasonably be attached and by the die package size). Packaged as well as bare dies will be ordered from Europractice. They provide up to 60 chips per process run, which allows us thorough experimental testing and detailed parameter studies. The various designs are inspected for geometric, mechanical, and electrical quality in our laboratories. After the chips have passed this stage of quality control, they are sent on to **WP2** in which the magnetic layer is added.

WP2 Magnetic Component

Within this work package, the magnetic thin film will be deposited, analyzed, and transferred to the MEMS geometry with a focus on high reproducibility at a sufficiently low limit of detection. The deposition will mostly be performed in the Faupel group due to the necessity of a custom-build deposition chamber. Here we benefit from longstanding experience with thin-film deposition that includes the use of magnetic materials and dedicated deposition chambers, which permit deposition from various sources and in a magnetic field.

In previous approaches, the magnetic film was deposited before the release of the resonator and structured with photolithography in Kiel. Upon release of the cantilever beam, the structure may relax and anisotropic stress can influence the magnetic properties of the film. Here, we follow a different approach and deposit the magnetic film on the released resonator and structure it with a shadow mask. As a great advantage, this method prevents the impact of anisotropic stress on the magnetic material after the release. Because the resonator structural dimensions are intended to be in the range of a few hundred μm , a crucial step for the quality and reproducibility is the alignment of the shadow mask. For this purpose, a custom-made deposition chamber has been constructed in the Faupel Group. It permits a mask alignment with micrometer precision without breaking the vacuum. Shadow masks are available with sub- μm feature size and will be ordered externally.

In close collaboration with **A1** and **A3**, we will start with the deposition of single-layer FeCoSiB films and compare them with those established in the previous funding period within the CRC. An important factor for the sensitivity is the volume fraction of the magnetic film. Because the substrate thickness of the new sensors is only about 10 μm , a thin magnetic film of 200 - 400 nm is sufficient to obtain a magnetic volume fraction similar to the previous designs. The small thickness will be beneficial for the quality of the magnetic film, despite its small in-plane area. A magnetic easy axis will be induced by depositing the magnetic layer in the presence of a magnetic field to avoid heat treatments. Measurements and simulations performed in **A3** and **A4** showed that the intrinsic stress in such thin FeCoSiB films results only in a negligible deflection of the cantilever that does not harm the functionality of the device.

In a second step, Cr-interlayers will be deposited to reduce the demagnetizing field and stabilize the magnetic domain configuration. Sensors with such interlayers have shown previously the lowest detection limit [A4-5]. As single layers, they require a magnetic bias field for optimum sensitivity. The bias field will be applied externally first, before alternative methods are established. For this purpose, we intend to transfer exchange biased multilayers to the structures which have been successfully developed and used in the first funding period by **A1**, **A3**, and **A4** [K19]. Because of the small thickness, only one or two layers will be required. This simplifies the analysis and should have a pronounced positive effect on the film quality. As a simple, alternative approach, permanent magnets can be used to provide a low noise external magnetic bias field.

Our abovementioned previous investigations showed that the main parameter to increase the sensitivity of the sensors is the homogeneity of the internal stray field. To increase homogeneity, we will implement an alternative magnetic material with a larger anisotropy energy density that is compensated by a larger saturation magnetostriction. A potential material is FeCo that has shown one order of magnitude higher saturation fields of about 10 mT with a correspondingly higher effective saturation magnetostriction of up to 260 ppm in 0.5 μm thick films [Hu11]. This approach can also serve as a countermeasure if the expected reproducibility of the magnetic layer is not attained. The envisioned magnetostrictive material with higher magnetic anisotropy would also exhibit a larger bias field for the point of operation and would be very interesting for **B7**, where ΔE -effect sensors with a larger bias field are considered to increase the sensitivity of the magnetic susceptibility particle mapping (MSPM) technique.

The deposited magnetic films will be analyzed on the μm -scale together with **A1** with regard to domain structure and magnetization behavior. The sensor dimensions have a perfect size for the advanced magneto-optical imaging techniques available. From the analyses, the magnetic properties can be extracted, which permits the estimation of a geometry- and resonance mode-dependent ideal magnetic layer thickness by using the models adjusted in **WP1**. The analysis of the real-time magnetization dynamics will drive and validate the first models for the magnetic noise behavior in cooperation with **A10**. Together with **A6**, the interlayer structure and crystallinity will be analyzed in detail to quantify and connect the micro-structural properties with the global magnetization behavior and the magnetization distribution, essential for high sensitivity.

The magnetic layer deposited in **WP2** will be passed on to **WP3** and **WP5** for the development of sensors and sensor arrays.

WP3: Single sensor elements

In this work package the development and model-based design of fully functional sensor devices is focused. This includes the resonator design, the combination with monolithically integrated electronics from **WP4**, and the principle investigation of single sensor and resonator structures to build complete sensor arrays in **WP5**.

The design, manufacturing, and characterization of single sensors will be continued in order to provide ready-to-use ΔE -effect sensors for the application projects, particularly **B7**. Besides the established designs, it includes high-frequency vacuum encapsulated devices processed in **Z1** with high quality factors and alternative

materials such as AlScN. Modification of the established magnetic layer systems and development of an advanced magnetic layer will be pursued together with **A1** and eventually transferred to **Z1**. These sensors will also be used for a benchmark of the new μm -sized sensors to validate their potential advantage in large number sensor arrays.

Simultaneously, we will address the downscaling of the resonator geometry. The aim is to achieve a similar noise and signal level compared to current sensors, but with geometries in the hundred μm -range. Hence, a similar level of detection ($< 100 \text{ pT/Hz}^{1/2}$) is targeted with a strongly increased spatial resolution. As a starting point for the design, we use a geometry predicted by the adjusted electromechanical models of **WP1** and the magnetic models from **WP2**. Geometry variations of the cantilever geometry will be made to find optimal aspect ratios and magnetic film thicknesses. For this step the quick external MEMS fabrication is a great advantage. It permits us to obtain up to 60 chips with dimensions of $5 \times 5 \text{ mm}^2$ with each production run. On each chip, up to 1000 different designs can be placed and a different magnetic layer thickness and structure can be used. Hence, systematic parameter studies can be performed easily and quickly. On this small scale, also flux guides and concentrators will be investigated for the increase of the detection limit and later for implementation in vector magnetometers and arrays in **WP5**. The noise and LOD characterization will be done in collaboration with **B1**. As soon as the single sensor element reaches a reproducible LOD below $300 \text{ pT/Hz}^{1/2}$, arrays will be developed. If, despite all expectations, the targeted LOD for a single sensor cannot be reached with sensor dimensions suitable for the PolyMUMPs technology, the well-established processes of **Z1** will be used.

WP4 Sensor electronics

Based on the existing experience in ASIC design, sensor readout electronics are investigated and manufactured by using multi-project-wafer shuttles by Europractice. The electrical sensor characteristics are modelled in parallel with the investigations in **WP1** and **WP2**. The sensor models previously developed in this CRC are used as starting points for the advance of extended models including the new design parameters. An equivalent circuit model informed by the physical sensor design choices is implemented in the Cadence design environment. Interface electronics are co-designed, tailored to the sensor in terms of impedance, resonance frequency, and noise. Testbenches are built in the simulator using the sensor equivalent circuit model and transistor models provided by the foundry. A fully integrated chip in a standard CMOS technology is targeted with a minimum of external components. Although the chip is individually characterized for its electrical performance at first, eventually it is intended to combine the electronic chip with the MEMS chip for testing. 60 standard bonding pads for external connections fit into the minimum silicon area of 4 mm^2 set by Europractice for the target technology. The number of pads can be increased by using a larger silicon area (at an extra manufacturing cost), by customizing smaller pads, or by using non-standard pad placement (e.g. a staggered layout). As a specific challenge, the readout of a large-scale array is envisioned. Here, the challenge of achieving best noise performance with adequate power consumption is addressed. Although absolute power consumption is not a primary concern, the power must be managed to a level compatible with the MOS technology (typically in the range of several tens of milliwatts with careful design).

Overall, the focus lies on the research of analogue electronics with minor on-chip digital enhancement. When integrated on a single chip, performance metrics including crosstalk, substrate coupling, and mutual heating must be considered during the design phase. The following three major groups of electronic circuits are targeted in this WP:

- Integrated electronic structures for selection of sensor groups. In close collaboration with **WP5** array grouping strategies are assessed from the electronic implementation point of view. For example, potential methods of array selection include on-chip transmission gate trees, front-end amplifier power cycling, or one-time programmable matrix networks.
- Low-noise front end for parallel readout. Here, different concepts for scaled low-noise readout are investigated, including the principle of orthogonal current reuse, power cycling, noise matching, and amplifier switching. The limitations of the approaches for this application are investigated to find an optimum combination of strategies.
- Oscillators for sensor excitation. The oscillator circuits for generating the excitation signal and for driving the sensor arrays are realized on-chip. Sensor grouping strategies also affect the design of the excitation generators. Also, the noise performance required of the generators is investigated and taken into account by low-noise design. Moreover, it is investigated how well differential measurement mitigates the excitation noise. If oscillator noise is found to be a limiting factor, an external oscillating device, e.g. a quartz crystal, is considered to provide a reference clock.

In addition, approaches for in situ circuit parameter tuning are investigated. If it is possible to measure key sensor parameters during operation or in a calibration phase, mismatch in a number of sensor parameters could be accommodated. For example, small differences in natural sensor oscillation frequency on different

dies, potentially caused by parameter variations during manufacturing, are anticipated. The electronic excitation oscillator is made tunable, so that operation at the optimum frequency is possible. Initially, tuning is accomplished using off-chip control signals to adjust the electronic parameters after the target parameter has been established in advance by measurement. Eventually, automatic measurement is desired, so that an automated control loop can be included to always operate the sensor-electronic combination at its optimum operating point.

Circuit development and verification follows the standard procedures for integrated chip design. First, a suitable technology is chosen from the available options at Europractice. The ON Semiconductor 350 nm CMOS technology is the initial choice, as it yields a good balance between tapeout frequency, cost, and performance. Moreover, electrically isolated pockets can be formed in this technology for minimum channel crosstalk. Second, circuit concepts are verified by simulation using the Spectre circuit simulator in Cadence. Layout and appropriate performance checks are carried out before tapeout. Third, the fabricated chips are characterized in our labs for functionality. They are compared to the appropriate benchmarks to demonstrate and advance the state-of-the-art. Other parameters to be identified as relevant in this project are the noise-to-power tradeoff (known as the noise efficiency), the dynamic range, signal-to-noise ratio, usable bandwidth, signal drift, channel crosstalk, and available number of parallel channels. Array structures are also compared to single sensor performance as the baseline benchmark. Moreover, the performance of the electronic readout system is compared to discrete sensor readout electronics established in **B1** currently representing the state-of-the-art as described in [Du17]. The ASICs are also made available to **A5** for testing with piezotronic sensors based on the ΔE -effect.

There are tapeout shuttles available four to five times per year. This leaves adequate room to measure manufactured chips and to complete design iterations before subsequent tapeout of a modified chip. Two tapeout runs are planned per year on average for this WP. This enables the evaluation of different electronic system strategies in combination with the different generations of MEMS sensor chips.

WP5: Sensor arrays

The previous findings are combined to design and fabricate fully functional sensor arrays with integrated electronics that are optimized with respect to different qualities. Selected sensor designs studied in **WP3** will be used to increase the capability of the sensor chip for vector magnetometry. This will be done by arranging single sensor elements with different orientations on the MEMS device to achieve the capability of 2D vector magnetometry. Our previous studies in cooperation with **B7** and **A8**, have shown that each sensor element has a sensitive axis but also provides a slight signal for other directions within the film plane. To suppress the unwanted components, two different strategies will be used and eventually combined. First, in cooperation with **B2**, post-signal processing will be used to filter out the unwanted sensitivity directions, knowing the sensitivity characteristic of each single sensor. At this point the automatic sensor characterization developed in **WP4** will be a great advantage. Second, the flux concentrators and flux guides tested in **WP3** will be transferred to single sensor elements in the vector array to increase the sensitivity of single elements in different directions. Finally, packaging of 2D sensor arrays will be used to obtain 3D vector sensitivity.

With a second array approach, we pursue the reduction of the LOD in the low frequency regime (1 Hz - 1 kHz) by averaging over many sensor elements operating in parallel. Here, the requirements of resonator reproducibility and automatic adjustment of the sensor electronics is of tremendous importance to sort out non-working devices and excite each sensing element at an optimum frequency. To avoid the mechanical coupling of sensor elements, low clamping loss structures developed in **WP3** will be used. Although the MEMS area theoretically allows for many thousands of sensors, the maximum number is expected to be limited by the sensor electronics. Different grouping and readout strategies from **WP4** will be used for the sensor electronics to increase the number of parallelized elements. Due to the complexity of interleaved mechanics, electronics, and magnetism, the optimization process will be based on the electric and magnetic modelling of the sensor arrays. As a final step, we will apply noise cancelling methods and multi-mode operation as investigated previously for operating the sensor arrays in non-shielded environments in cooperation with **B2**.

Prospects

By the end of the second funding period, we expect to have reached a level of maturity with respect to technological readiness that allows us to continue as a transfer project with one or more industrial partners. In addition to the new applications that have emerged already in the current funding period, we plan to address new biomedical but also other applications by taking advantage of the robustness of the sensor, its extraordinary bandwidth and dynamics, and its vector characteristics. Even more potential is seen in sensor arrays. In this connection, different application specific approaches for integration of the MEMS sensor and sensor arrays together with the electronics in one chip will be investigated.

3.5 Role within the Collaborative Research Centre

Collaborations are discussed in the individual work packages and listed below:

- A1: magnetic characterization and layer deposition
- A5: sensor electronics
- A6: structural analysis of magnetic component
- A10: magnetic noise modelling and analysis
- B1: noise measurements and reduction
- B2: dual-mode operation and signal processing
- B7: application of ΔE sensors and arrays for cell localization
- Z1: design and manufacturing of established single ΔE sensors for applications in the CRC

A4 is mainly involved in the following focus groups: "Concepts based on ΔE -effect", "Comparison of sensor concepts", "Modelling", and "Magnetic layers".

3.6 Differentiation from other funded projects

No other projects related to ME materials are currently investigated by the applicants outside the SFB126.

3.6.1 Previous funding

Funding within the CRC started in 07/2016. A PhD student, Patrick Wiegand, has been supported with a grant from the CRC 1261 since November 2018. He has been active in data collection during the preliminary studies.

3.6.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/2	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral re-researcher, 100%	2	68.4	2	136.8	2	136.8	2	136.8	2	68.4
Total		68.4		136.8		136.8		136.8		68.4
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables	8.5		7.4		7.4		9.2		4.0	
Others	8.5		17.0		13.0		12.5		8.5	
Total	17.0		24.4		20.4		21.7		12.5	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
<category>										
Total	0		0		0		0		0	
Grand total	85.4		161.2		157.2		158.5		80.9	

(All figures in k€)

3.6.3 Requested funding for staff for the new funding period

	Se- quen- tial no.	Name, aca- demic degree, position	Field of re- search	Department of uni- versity or non-uni- versity institution	Project com- mit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	F. Faupel, Dr. rer. Nat., Pro- fessor	Material Science	Institute for Mate- rial Science	4		
	2.	R. Rieger, Dr., Professor	Electronic design	Institute of Electri- cal Engineering and Information Technology	4		
Non-research staff	3.	Rehders, Stefan, Dipl.- Ing. (FH), Lab Engineer		Institute for Mate- rial Science	4		Core support
	4.	Sommer, Pe- ter, Dipl.-Inf. IT Technician		Institute for Mate- rial Science	2		Core support
Requested staff							
Research staff	5.	Wiegand, Pat- rick, M.Sc., Doctoral Re- searcher	Integrated circuit de- sign	Institute of Electri- cal Engineering and Information Technology		E13	
	6.	N.N., Doctoral researcher	Composite Materials	Institute for Mate- rial Science		E13	
Non-research staff							

Job descriptions of staff for the proposed funding period (supported through existing funds):

1. Prof. Dr. rer. nat. Franz Faupel is principle investigator and responsible for the scientific coordination and management of the WP and supervision of the PhD student.
2. Prof. Dr. Robert Rieger is principle investigator and responsible for the scientific coordination and management of the WP and supervision of the PhD student.
3. Dipl. Ing. (FH) Stefan Rehders will design and construct mechanical parts and carry out mechanical repairs.
4. Dipl.-Inf. Peter Sommer will help with the setup of computers and software implementation.

Job descriptions of staff for the proposed funding period (requested funds):

5. The employment of Mr. Patrick Wiegand is essential for the MEMS and ASIC design and testing proposed in this project. His position is anchored in the Rieger group. His duties include the optimization of electronic circuits described in WP4, the simulation of circuits and their validation, circuit layout and tapeout preparation. He also leads the measurement and characterization of the manufactured ASICs. Also, in WP1 he is involved in the transfer of the optimized MEMS sensor structures into a layout that can be manufactured through Europractice. In WP3 and WP5 he conducts the electronics circuit verification and bench measurements in collaboration with the doctoral researcher in the Faupel group.
6. The doctoral researcher will carry out the work described in the work packages WP 1, 2, 3, and 5 in close cooperation with the other doctoral researcher of the Rieger group. A suitable candidate should have a strong background in magnetic materials, modelling and electronics; it is thus planned that the current doctoral researcher Benjamin Spetzler will continue to work on the project in the first year of the next funding period and prepare a suitable master student who will then continue work for the next three years on the project.

3.6.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/2
Institute of Electrical Engineering and Information Technology: existing funds	1.5	1.8	1.8	1.8	1.5
IMS: existing funds from core support	1.5	3.0	3.0	3.0	1.5
Sum of existing funds	3.0	4.8	4.8	4.8	3.0
Sum of requested funds	8.5	17.0	13.0	12.5	8.5

(All figures in k€)

Equipment up to k€ 10, software, consumables for 2020/2

Targets and consumables (gaskets, substrate holders, etc.) for magnetic layers	k€	3.0
Small lithography masks (6) for customized micromachined MEMS ME sensors	k€	2.0
Low-noise digitizing card with 24-bit high resolution and wide dynamic range	k€	3.5

Equipment up to k€ 10, software, consumables for 2021

Targets and consumables (gaskets, substrate holders, etc.) for magnetic layers	k€	4.0
Small lithography masks (6) for customized micromachined MEMS ME sensors	k€	1.8
Small electrical components (amplifier, power supply, circuit components, cables)	k€	1.6

Equipment up to k€ 10, software, consumables for 2022

Targets and consumables (gaskets, substrate holders, etc.) for magnetic layers	k€	4.0
Small electrical components (amplifier, power supply, circuit components, cables)	k€	2.2
Mechanical parts to update the setup for annealing	k€	1.2

Equipment up to k€ 10, software, consumables for 2023

Targets and consumables (gaskets, substrate holders, etc.) for magnetic layers	k€	4.0
Flux concentrator materials (incl. targets)	k€	3.2
Small electrical components (amplifier, power supply, circuit components, cables)	k€	2.0

Equipment up to k€ 10, software, consumables for 2024/1

Small electrical components (amplifier, power supply, circuit components, cables)	k€	1.0
Lithography masks (5) for customized bulk micromachined MEMS ME sensors	k€	3.0

Other costs for financial year 2020/2

1x ASIC production via Europractice and packaging of 10 samples for testing	k€	4.0
1x MEMS production via Europractice PiezoMUMPS	k€	4.5

Other costs for financial year 2021

2x ASIC production via Europractice and packaging of 10 samples for testing	k€	8.0
2x MEMS production via Europractice PiezoMUMPS	k€	9.0

Other costs for financial year 2022

1x ASIC production via Europractice and packaging of 10 samples for testing	k€	4.0
2x MEMS production via Europractice PiezoMUMPS	k€	9.0

Other costs for financial year 2023

2x ASIC production via Europractice and packaging of 10 samples for testing	k€	8.0
1x MEMS production via Europractice PiezoMUMPS	k€	4.5

Other costs for financial year 2024

1x ASIC production via Europractice and packaging of 10 samples for final demonstration	k€	4.0
1x MEMS production via Europractice PiezoMUMPS	k€	4.5

3.6.5 Requested funding for instrumentation for the new funding period

None

3.1 General information about Project A5

3.1.1 Project Title: Piezotronic magnetoelectric composites

3.1.2 Research areas

406-02 Synthesis and Properties of Functional Materials

408-01 Electronic Semiconductors, Components, Circuits, Systems

3.1.3 Project leaders

Adelung Rainer, Prof. Dr. rer. nat.
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Do any of the abovementioned persons hold fixed-term positions? no

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

Biomagnetic sensors that are resistant to noise and have a high signal-to-noise ratio are desired for the envisaged applications within the CRC. One strategy to reduce noise is to place the pre-amplification as close as possible to the sensor. The aim of the proposed project is the investigation of current-based ME sensing devices relying on the piezotronic effect, which provides a pre-amplification directly in the piezomaterial. Furthermore, ZnO and GaN needle-shaped sensors permit a very compact design; therefore, an envisioned biomedical application is a catheter-mounted sensor, for example, for intracardiac magnetic field detection as an alternative to the currently used tunnel magneto resistance (TMR) and giant magneto resistance (GMR) sensors. For comparison, more conventional miniaturized AlN piezotronic sensors will be explored as well. To understand the lower detection limit, transition metal chalcogenides (TMDs) will be employed in piezotronics that currently show the highest potential for miniaturization as they consist of monolayer thicknesses, but are most challenging in terms of sample handling and electrical contact establishment. Consequently, in this funding period it is proposed to examine and understand miniaturized piezotronic devices; in the next funding period, the biomaterial applications with the most successful piezotronic sensors are envisioned. The high resonance frequencies of the small needles require driving the sensors in ΔE mode. In order to apply the piezotronic concept in biomagnetic analytics, the advantages of piezotronic ME sensors, such as the small size and integrated pre-amplification, suggest them for the biomagnetic application of intracardiac probes. The intracardiac application is less challenging in terms of limit of detection (LOD), because the ME sensors in the body are much closer to the natural magnetic sources such as the heart and the field is 100 - 400 times stronger due to the proximity. The pre-amplification inside the piezotronic space charge region makes it robust

for the long way out of the body, if they are used as catheter probes. Broadband low field detection will be enabled by a ΔE -effect sensor design that allows low field readout with high frequencies.

3.3 Research rationale

3.3.1 Current state of understanding and preliminary work

In a biomedical investigation, both electrical and magnetic fields can be measured to obtain information about biological activity. Whereas electrical signals are strongly influenced by the surrounding tissue and the respective dielectric properties between source and sensor, magnetic signals suffer no such influences since the permeability of tissue is almost the same as in free space [Ba18]. Accordingly, the distance between source and sensor defines the magnitude of the detectable magnetic field. A close distance between source and sensor was already realized for small SQUIDS [Ma06], atomic magnetometers [Sa12], or wound coils [Ro85]. Models for 10 000 neurons revealed a magnetic field strength of 50 fT at a distance of 6 cm and a field strength of 126 pT at 1 mm [Ca17]. This indicates that already relatively high LODs allow the measurements when the source-to-sensor distance is short. The requirements for such a sensor in order to minimize tissue damage are a needle-like shape which permits easy insertion via a catheter and, accordingly, a small size. Figure A5-1a shows a magnetic sensor containing two giant magneto resistance (GMR) elements realized on a needle-shaped silicon substrate which was used to detect magnetic fields below 1 nT [Ca17].

Piezoelectric ZnO, compare [A5-9], which frequently occurs in the shapes of micro-needles, compare Figure A5-1b, was already used in the current funding period to realize magnetic field sensors with a LOD of 380 pT/Hz^{1/2} at resonance using the piezotronic effect [A5-10]. The utilization of a piezotronic ZnO sensor has various advantages with regard to integration and noise characteristics. The concept of an internal amplifier in a piezotronic device does not require an additional external signal amplification which makes it simple and compact when miniaturizing a device. Considering the noise of a piezotronic device, the developed theory shows an efficient noise filtering which can help to improve the sensors signal-to-noise ratio.

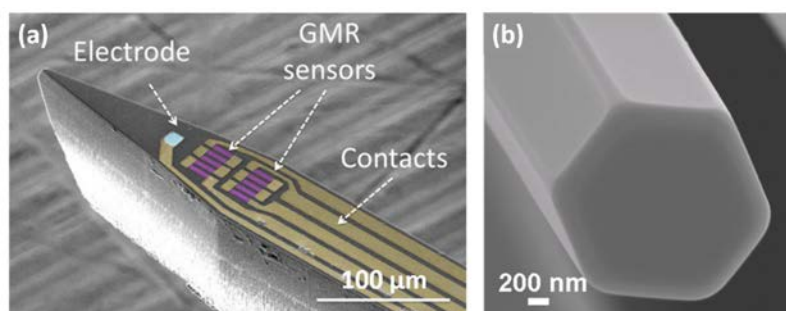


Figure A5-1: SEM image of a) a needle-shaped magnetic field sensor consisting of two GMR sensors on silicon [Ca17] and b) a needle-shaped piezoelectric ZnO crystal, which was used as the basis to realize magnetic field sensors [A5-4].

Z.L. Wang introduced the term piezotronics, which is based on a current, analogous to piezoresistivity, that is increasing or decreasing dependent on the strain in the material [Ga07]. But in contrast to piezoresistivity, piezotronics has the potential of a much higher amplification because the rectifying behavior of a semiconductor space charge zone is utilized. In the present proposal, it is important to discriminate between sensors based on piezotronics and those based on piezoresistivity and piezoelectricity. State-of-the-art ME sensors, as developed in the framework of the CRC, measure in a piezoelectric manner the electric potential (voltage) of the piezoelectric material which builds up under strain and is thus affected by a deformation of a magnetostrictive material in the magnetic field. An alternative measurement of strain in semiconductors is the application of the piezoresistive effect which causes a change in resistivity under strain, only in electrical resistance here but not in electric potential changes.

Piezotronic effects occur in semiconductors with a non-centrosymmetric crystal structure like ZnO or GaN and are based on the change of charge carrier transport behavior in space charge regions (typically at the contacts) driven by piezoelectric potentials. The piezotronic effect as illustrated by Wang is shown in Fig. A5-2 [Zh11] for clarity. The simple schematic diagrams show the space charge region and energy band of a metal-semiconductor (n-type) Schottky contact. Additional piezoelectric charges are caused by a piezoelectric potential at the metal-semiconductor interface which results in band bending and thus a change of the height and width of the Schottky barrier. The charge carrier transport across the metal-semiconductor contact is

therefore strongly dependent on the piezoelectric potential resulting from the piezo-charges which are regulated by the magnitude and sign of the applied strain.

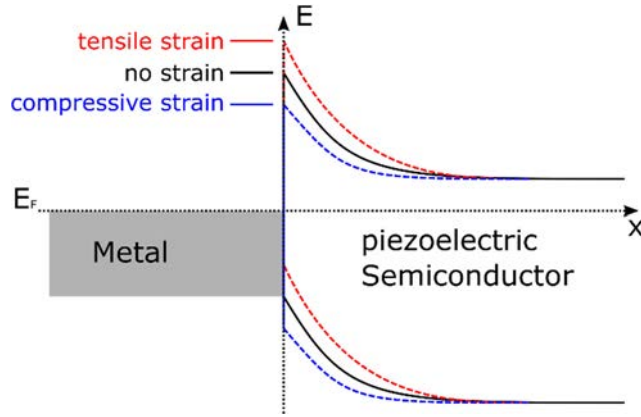


Figure A5- 2: Schematic illustration of the piezotronic effect in a metal-semiconductor contact (Schottky contact) as described by Zhang et al. [Zh11]. The Schottky contact forms at the contact area between the metal (left) and the n-type semiconductor (right). The energy band diagram shows a Schottky barrier for a non-strained semiconductor (black line). The height of the Schottky increases under strain (red line) and decreases under compression (blue line).

AlN based piezotronic devices

The ME sensors used in the present funding period for the piezotronic measurements are state-of-the-art sensors with AlN as the piezoelectric material and were produced by Z1. The only modification to the standard layer configuration is the introduction of an Al/Cr electrode which allows the establishment of an ohmic contact to the AlN. Following the experience with piezotronics based on ZnO, only one Schottky barrier is required whereas a second Schottky barrier lowers the effect [A5-10]. The thickness of the AlN was varied and reduced as far as possible. The columnar growth of the AlN limited the minimum layer thickness and allowed only layer thicknesses starting at 500 nm. The standard characterization of the sensors showed the expected behavior for a piezoelectric measurement and an almost identical behavior for the piezotronic read out, see Figure A5-4. This has already been a great success because it shows that the piezotronic readout is as good as the conventional readout without using an additional external amplification. Accordingly, the internal amplification in the Schottky barrier is working. Even the sensors with the thinnest AlN layers had series resistances which exceeded 1 TΩ. Accordingly, no impedance spectroscopy measurements were performed since the requirement for a successful measurement is a series resistance of 10 GΩ.

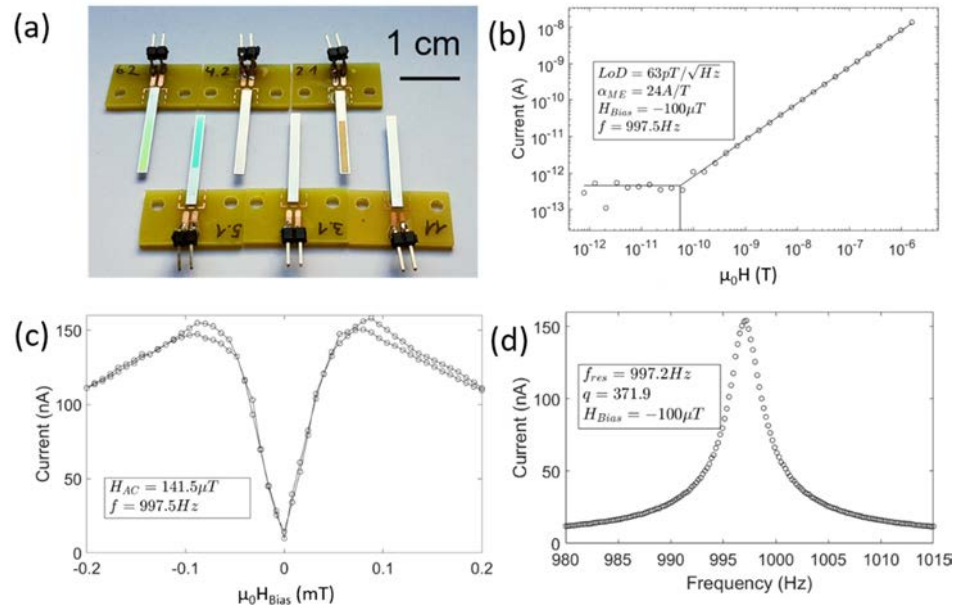


Figure A5-3: AlN sensors measured piezotronically: a) photographic image of the sensors with different AlN layer thicknesses visible by different color of AlN film, b) piezotronic linearity measurement and LOD determination, c) magnetic bias field measurement, and d) resonance curve from piezotronic measurement.

Piezotronic sensors

An ideal piezotronic device in the absence of defects and noise (noise will be discussed in detail below) can be described using an equivalent circuit as shown in *Figure A5-4*. The working point U_{wp} of the Schottky contact defines the amplification factor $1/R_p$ as:

$$\frac{1}{R_p} = \frac{dI}{dU} = I_{0,int} \frac{q}{nkT} \exp\left(\frac{qU_{wp}}{nkT}\right) \quad (A5-1)$$

with intrinsic current $I_{0,int}$, electric charge q , ideality factor n , Boltzmann constant k , and temperature T . The frequency dependent small signal linear response of the Schottky contact depends on the capacitance C_p and diode resistance R_p of the space charge region. The series resistance R_s represents the ohmic contacts to a current/voltage measurement device, compare *Figure A5-4b*. $U_p(t)$ is the sum of the piezoelectrically induced potential in the bulk and in the space charge region. This voltage signal $U_p(t)$ will be translated into an amplified current signal $I(t)$ with the amplification factor $1/R_p$.

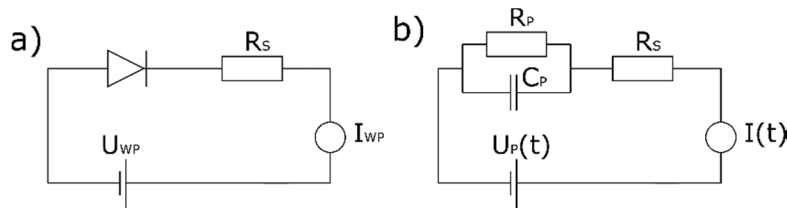


Figure A5-4: Equivalent circuits of an ideal piezotronic sensor for a) large signals with a bias voltage U_{wp} and the series resistance R_p , and b) linearized small signal using piezoelectric potential $U_p(t)$, diode resistance and capacitor representing the space charge region R_p and C_p originating from the diode at working point U_{wp} .

The amplification of the device was investigated using ZnO-based piezotronic devices. ZnO turned out to be a suitable model system for piezo-effects, compare [A5-9], like piezotronics as it permits tuning many degrees of freedom in terms of defects acting as dopant sites, in particular, the crystal dimensions, band structure, and surface properties. Crystals with diameters of 1 - 3 μm were grown using the flame transport synthesis, which was further developed in the framework of this project for piezotronic materials, as partially described in [A5-2] and [A5-5]. With the help of a setup using a nanomanipulator inside of a SEM, the basic piezoresistive and piezotronic properties could be examined at Berkeley University [A5-8] and revealed negligible shear losses and a strain that is occurring homogeneously over the crystal which leads to relatively large piezotronic effects.

A tuning of the surface conductivity and space charge region for the piezotronic states could be achieved in various manners. One example is the modification of the ZnO by introducing Fe, Cu, or Al to form hybrid oxides. These modify the electronic structure as indicated by a modified surface chemistry as described in [A5-7]. Another possibility is to change the surface conductivity by adding conductive material on the ZnO like CNTs and forming hybrid structures as demonstrated in [A5-6]. Partial short circuit on the ZnO by conductive CNT could improve the piezotronic response if this shortcut is separated from the space charge region. In order to elucidate the challenging concept of a partial coating of the ZnO by CNTs, different weight percent of CNTs from 0.8 - 4.0% were realized [A5-6]. For the piezotronics, a compromise between insulation properties that allow the piezo material to build up a high voltage and a certain leakage by conductivity that allows a sufficient current flow must be found, as shown in *Figure A5-5a*. A ME sensor using ZnO combined with magnetostrictive FeCoSiB film was used to detect the response to a magnetic ac field over time. The ZnO was illuminated using UV light before starting the experiment (affecting oxygen vacancies that act as dopants on the surface) and kept in a dark environment during the measurement (affecting a slow decrease in oxygen vacancies concentration). The change in conductivity of the ZnO needle is depicted in the inset of *Figure A5-5a*. A high conductivity causes a breakdown in piezoelectric potential and leads to a non-working ME sensor. A lower conductivity will lead to a working device with a large piezotronic current, whereas an even lower conductivity will reduce the piezotronic current. This effect was further investigated by using Fast Fourier Transformed Impedance Spectroscopy (FFT-IS, compare [Ge14]), measurements and modelled with an equivalent circuit as depicted in *Figure A5-4b*. A single, representative fit is depicted in *Figure A5-5b* and shows excellent agreement with the recorded data. From these fits R_s , R_p , C_p could be determined when switching UV light on and off as shown in *Figure A5-5c*. It can be seen that there is an instant and drastic change in all components when switching on UV light. Both resistances drop by several orders of magnitude. This effect can be attributed to the increased concentration of free charge carriers due to illumination. When switching off the UV light, the response is much slower. This is due to the well-described effect of photo-induced holes

which react with chemisorbed oxygen species and lead to molecular O_2 that desorbs from the ZnO surface. The process leaves an excess of electrons in the conduction band and diminishes the energy of the depletion layer, thus decreasing the ZnO film resistivity [Fa10]. This effect becomes visible when reducing the free charge carrier concentration and restores slowly to a high resistive state. From the model used, it can be assumed that the series resistance R_s represents the space charge region, which has only a minor influence on the piezotronic device. The parallel resistance R_p represents the conductive channel inside the ZnO crystal. A low R_p leads to a short circuit of the piezoelectric potential and no measurable piezotronic effect. An R_p that is too high leads to a working device but shifts the working point to very low potentials, since most of the applied potential drops over R_p and not the space charge region. Since R_p should scale directly with the geometry of the piezoelectric material, short devices with a large area are preferred for high quality piezotronic devices.

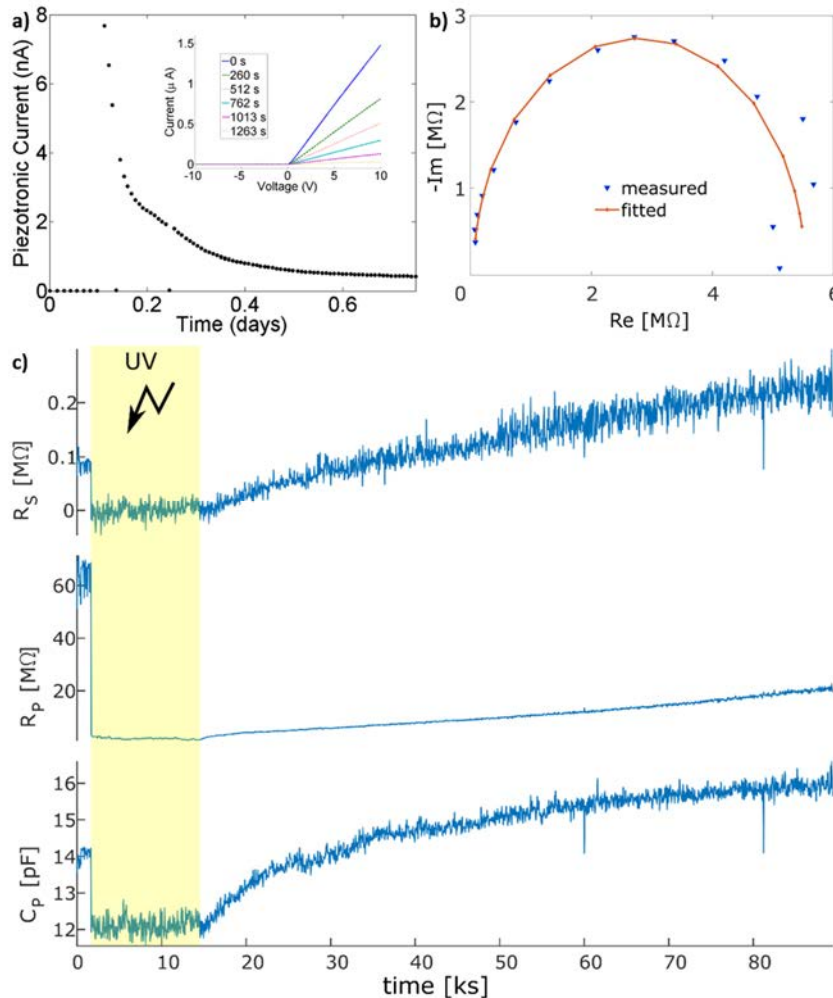


Figure A5-3: a) Piezotronic measurement using ZnO with a variable conductivity as shown in the inset. A high conductivity at the beginning causes a breakdown in the piezoelectric potential, and no piezotronic current can be detected. Lower resistances lead to a working device with piezotronic output. b) Single fitted dataset of FFT-IS measurement using the equivalent circuit as shown in c) Fitted data for the three components described in

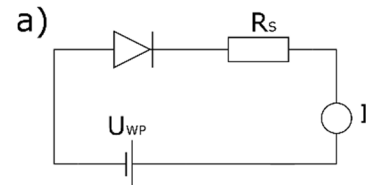


Figure A5-4b. for a single crystalline ZnO needle with and without UV illumination (365 nm). When switching on UV light there is a fast response in all components. Both R_p and R_s drop several orders of magnitude. When

Besides the amplification using suitable piezotronic components, the magnitude of the piezotronic current was also increased by using mechanical undamping of the sensor. In cooperation with **A2**, a mechanism was developed which allows direct integration into the sensor. Instead of using electronic concepts, the restoring force of the oscillator was tuned by introducing external forces which act on the sensor. An electret material as used for sensor readout in **A2** was positioned opposing the oscillator. The non-linear electrostatic interaction between electret and resonator leads to an increased oscillation amplitude and simultaneously a lower resonance with larger bandwidth. The effect was observed in measurements and successfully modelled by numerical simulations using standard harmonic oscillator theory which was expanded by an anharmonic part describing the interaction with the electret. A further detailed description of the phenomenon can be found in **A2** [A5-3].

Integrated piezotronic devices

Understanding sources of noise is important for the design of sensors in order to improve the signal-to-noise ratio (SNR). Conventional lock-in measurements with long integration times of typically 1 s and low pass filtering do not allow time-resolved analysis of the data, e.g. to identify single noise events. For white noise, the calculated LODs of a sensor should differ if normalized to $\text{Hz}^{1/2}$. Measurement with different integration times ranging from 1 s to 1 ms for a sensor at a resonance frequency of $f = 1 \text{ kHz}$ were performed using both piezoelectric and piezotronic readout as depicted in Figure A5-6a. The normalized LODs show a reduction of the LOD for short integration times up to a factor of 3 for the piezoelectric and the piezotronic measurements. A possible explanation for this totally unexpected behavior are noise events which occur on a timescale smaller than 1 s and larger than 1 ms. Thus, a short integration time allows a measurement between two noise events.

A modification of the setup was done to permit the parallel measurement of both the classical lock-in data and the live, time-resolved data. To investigate the quality of the live data measurement, a digital lock-in was post-processed on the data using Matlab routines. The result was that the measured lock-in and the calculated lock-in match very well. Figure A5-6b shows a measurement of the lock-in data compared to calculated lock-in data for 1 ms.

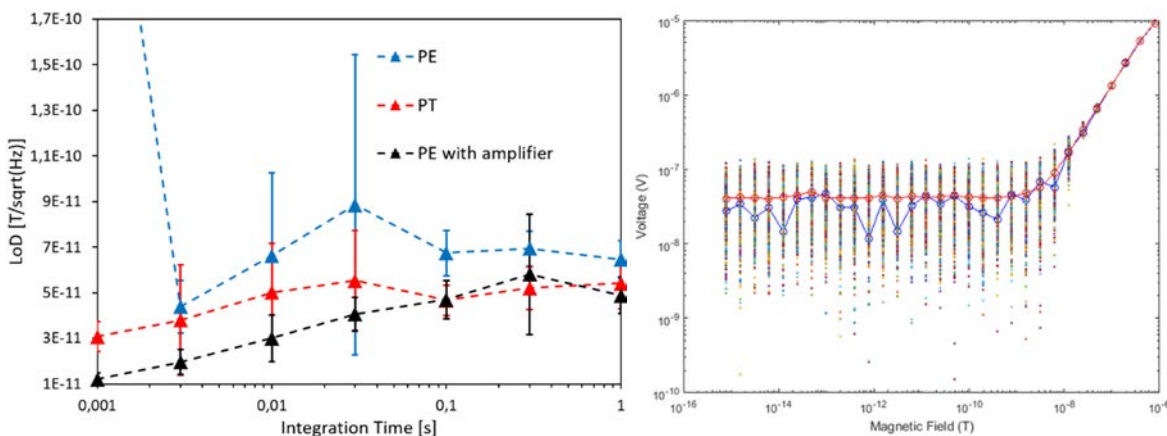


Figure A5-6:a) Piezoelectric read out (with and without amplifier) compared to piezotronic read out for different integration times using standard lock-in. b) Lock-in measurement (blue) together with 1000 calculated digital lock-in data points for each field strength and their average value (red).

Comparing the different AlN layer thicknesses, an improvement of the sensors was observed when using short integration times and thin AlN layers. Figure A5-7 shows the change in LOD when comparing thin AlN layers of 500 nm and thick AlN layers of $2 \mu\text{m}$. The measurements were performed using both piezoelectric and piezotronic measurements. The LODs were increasing when using piezoelectric measurements for short integration times of 1 ms as well as for long integration times. A possible explanation for this observation is the existence of burst noise on a timescale well above 1 ms but below 1 s. Such noise events are always present in long measurements of 1 s, but the chance of measuring between two burst events is high when choosing a small integration time of 1 ms. Shorter integration times are not desirable since the integration should not be less than a single oscillation period of the sensor. With piezotronic readout, the LODs were unchanged for long integration times and showed lower LODs for integration times of 3 ms and 1 ms. This result shows that thin layers and short integration times are desired when using piezotronic readout. However, the columnar growth of AlN used here is not suitable for very thin layers of electronic quality. This requires the usage of other materials, e.g. single crystalline GaN, that show stable and ultra-thin sheets, see e.g. [A5-2].

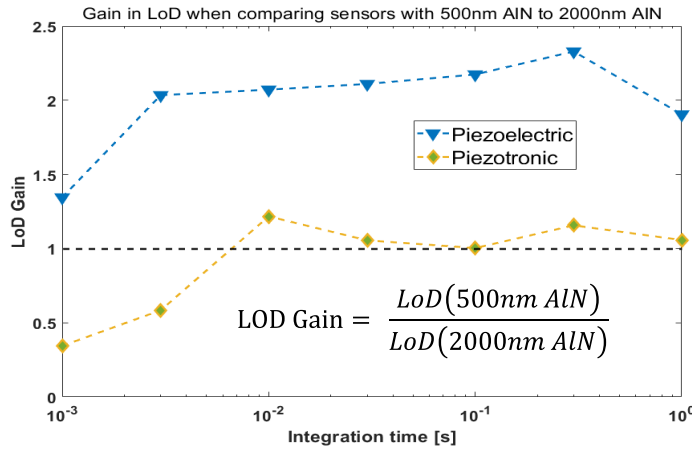


Figure A5-4: Gain of the LOD when comparing sensors with 500 μm to 2 μm AlN. Positive values are a higher LOD whereas negative values are an improved, lower LOD. The piezoelectric measurement shows in this case higher LODs for all integration times. The piezotronic measurement shows almost identical LODs when using long integration times and a lower LOD for short integration times.

GaN as piezotronic material

Investigations on the suitability of GaN for piezotronic sensor were performed and are currently under evaluation [A5-2]. In contrast to AlN, GaN with quite a similar structure (similar lattice constant, same crystal structure) has a pronounced stability, which make GaN the second most important semiconductor after silicon. But in contrast to ZnO, GaN with a low defect density is much more difficult to synthesize. In the framework of this proposal, we utilized ZnO as an epitaxial template for the piezoelectric GaN, which has almost the same lattice constant. In collaboration with Ion Tiginyanu from the TUM in Moldova, an epitaxial CVD coating was carried out, and in collaboration with **A6** it was elucidated that the GaN that is surrounding the ZnO is single crystalline as well and follows the c-axis orientation of the ZnO. Furthermore, it was possible to form hollow tubes by removing the ZnO and to form in such a way hollow piezocrystals with thin film wall thickness, as shown in Figure A5-8 [A5-2]. These free standing and rolled up thin films are free from clamping effects. Other than the conventional thin films, these can be contacted relatively simply on the (0001) facet.

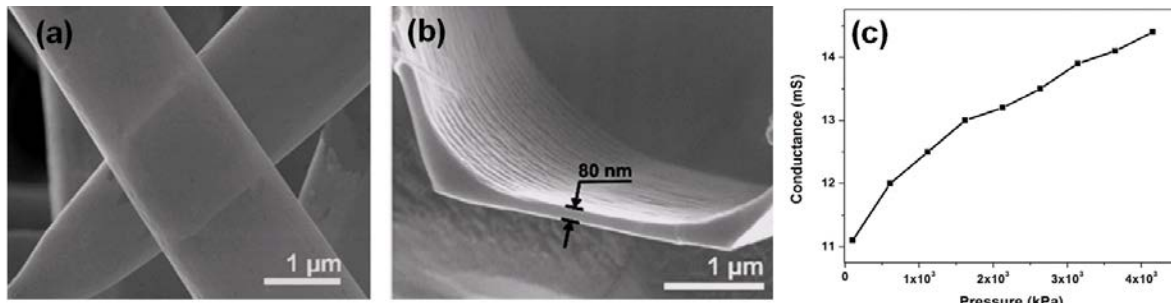


Figure A5-8: Piezoelectric hollow and oriented GaN single crystals. a) Two GaN single crystal tubes (tube axis (0001) direction) with very low wall thickness ~ 20 nm. Please note that they are already electron transparent inside the SEM. b) View inside a thicker tube in cross section with thicker 80 nm walls. c) The crystals are already utilized as a pressure sensor and show piezotronic/piezoresistive current dependence over 40 atm; the exact mechanism is under investigation, see [A5-1].

Besides, GaN offers higher quality in terms of electronic structure and will help to lower the noise of the sensor. This can be mainly attributed to the lower concentration of defect states in the bandgap, which act as noise sources for thermally excited electron-hole pair generation. On the other hand, the high series resistance may be compensated by using a third ohmic contact to control the current flow through the Schottky barrier.

Noise sources and noise reduction in piezotronic devices

As we will show below in our piezotronic case, space charge regions in general reduce the shot noise. By limiting the current, the space charge region low pass filters the random arrivals of the carriers. This results in less shot noise by reduced variation in the carrier distribution [Te43]. Following the theory for an ideal piezotronic current, see equation A5-1, the total current of a piezotronic device can be defined using a modification of the standard diode equation [Ca03] to accommodate the piezoelectric potential U_p and noise:

$$I(t) = [I_{0,int} + I_{N,int}(t) + I_{0,def} + I_{N,def}(t)] \exp\left(\frac{q[U_{wp} + U_p(t) + U_N(t)]}{nkT}\right) \quad (\text{A5-2})$$

with intrinsic current $I_{0,int}$, intrinsic noise current $I_{N,int}$, defect generated current $I_{0,def}$, defect generated current noise $I_{N,def}$, electric charge q , external working point voltage U_{wp} , voltage noise U_N , ideality factor n , Boltzmann constant k , and temperature T . The intrinsic current $I_{0,int}$ describes the generation current in the bulk of the semiconductor (scaling with n_i^2 and typically showing an ideality factor $n = 1$) and within the space charge region (scaling with n_i and typically showing a non-ideality factor $n = 2$) with n_i being the charge density. In wide band gap materials, only the non-ideal diode is relevant since n_i^2 is negligibly small in comparison to n_i . High quality Schottky diodes are therefore typically designed using wide band gap materials since they intrinsically show extremely small leakage currents [Ge93]. Accordingly, the intrinsic noise current $I_{N,int}$ is reduced when using large band gaps.

A second current $I_{0,def}$ is coupled to the defect assisted generation rate in the interfaces around and within the space charge region. Defects often create electronic states close to band edges, which induce large leakage currents due to the easy thermal generation of free charges and simultaneously imply large non-linearity factors n (3 to 10). By being thermally generated, such currents exhibit Poisson distributed noise $I_{N,def}$ in a wide frequency range.

Besides the current, also the voltage contains noise U_N which may be addressed to thermo-mechanical excitation of the material. In total, there are three noise sources in a piezotronic device which can disturb the measurement. Using the equivalent circuit model, as described in Figure A5-4b a filtering of the noise occurs. First, the filtering of the voltage noise U_N is discussed. The large capacitance of a space charge region short circuits high frequency signals thus inducing a well-known low pass behavior ($1/(1 + i\omega R_p C_p + R_s/R_p)$). If the series resistance can be neglected, we find a $1/f$ noise starting often at very small frequencies around 100 Hz [LE11]. The filtering of the total current noise $I_{N,tot} = I_{N,def} + I_{N,int}$ is described by the filter function ($1/(1 + i\omega R_s C_p + R_s/R_p)$), which as well serves as a first order low pass filter with a time constant $R_s C_p$.

In summary, a piezotronic device improves the signal-to-noise ratio by internal amplification, generating a low ohmic output signal of the device that can be measured with a post-amplifier without the typical additional noise sources of a high ohmic device (Schottky noise, inductively induced noise into the wiring), and by acting as an intrinsic low pass that filters out many sources of noise in the transformation chain from magnetic field to piezo-voltage. Two main sources limit the amplification of the piezotronic device and in addition produce extra noise: a large defect-induced leakage current $I_{0,def}$ with an extra thermally induced noise and a large series resistance R_s with extra Schottky noise. The reason for relevant large series resistances is not the wiring of the ohmic contacts but intrinsic ohmic losses, e.g. within the insulating piezoelectric material, if the device design needs a current flow.

References

- [Ba03] X. D. Bai, P. X. Gao, Z. L. Wang, E. G. Wang, Dual-mode mechanical resonance of individual ZnO nanobelts. *Appl. Phys. Lett.* **82**, 4806–4808 (2003).
- [Ba18] F. S. Barnes, B. Greenebaum, *Biological and medical aspects of electromagnetic fields* (CRC press, 2018).
- [Ca03] J. Carstensen, G. Popkirov, J. Bahr, H. Föll, CELLO: an advanced LBIC measurement technique for solar cell local characterization. *Solar Energy Materials and Solar Cells.* **76**, 599–611 (2003).
- [Ca17] L. Caruso, T. Wunderle, C. M. Lewis, J. Valadeiro, V. Trauchessec, J. Trejo Rosillo, J. P. Amaral, J. Ni, P. Jendritza, C. Fermon, S. Cardoso, P. P. Freitas, P. Fries, M. Pannetier-Lecoeur, In Vivo Magnetic Recording of Neuronal Activity. *Neuron.* **95**, 1283-1291.e4 (2017).
- [EI11] J. K. Ellis, M. J. Lucero, G. E. Scuseria, The indirect to direct band gap transition in multilayered MoS₂ as predicted by screened hybrid density functional theory. *Appl. Phys. Lett.* **99**, 261908 (2011).
- [Fa10] S.-W. Fan, A. K. Srivastava, V. P. Dravid, Nanopatterned polycrystalline ZnO for room temperature gas sensing. *Sensors and Actuators B: Chemical.* **144**, 159–163 (2010).
- [Ga07] Y. Gao, Z. L. Wang, Electrostatic potential in a bent piezoelectric nanowire. The fundamental theory of nanogenerator and nanopiezotronics. *Nano letters.* **7**, 2499–2505 (2007).
- [Ge93] M. W. Geis, N. N. Efremow, J. A. von Windheim, High-conductance, low-leakage diamond Schottky diodes. *Appl. Phys. Lett.* **63**, 952–954 (1993).
- [Ge14] M.-D. Gerngross, J. Carstensen, H. Föll, Electrochemical growth of Co nanowires in ultra-high aspect ratio InP membranes: FFT-impedance spectroscopy of the growth process and magnetic properties. *Nanoscale research letters.* **9**, 316 (2014).
- [Hs70] S. T. Hsu, R. J. Whittier, C. A. Mead, Physical model for burst noise in semiconductor devices. *Solid-State Electronics.* **13**, 1055–1071 (1970).

- [Hu06] Y. Huang, X. Bai, Y. Zhang, In situ mechanical properties of individual ZnO nanowires and the mass measurement of nanoparticles. *J. Phys.: Condens. Matter*. **18**, L179-L184 (2006).
- [LE11] F. A. LEVINZON, L. K. J. VANDAMME, Comparison of 1/f Noise in JFETs and MOSFETs with several Figures of Merit. *Fluct. Noise Lett.* **10**, 447–465 (2011).
- [Ma06] P. Magnelind, *High-T c SQUIDS for magnetophysiology-development of a magnetometer system and measurements of evoked fields from hippocampal neurons in vitro* (Chalmers University of Technology, 2006).
- [Ro85] B. J. Roth, J. P. Wikswo, The magnetic field of a single axon. A comparison of theory and experiment. *Biophysical Journal*. **48**, 93–109 (1985).
- [Sa12] T. H. Sander, J. Preusser, R. Mhaskar, J. Kitching, L. Trahms, S. Knappe, Magnetoencephalography with a chip-scale atomic magnetometer. *Biomedical optics express*. **3**, 981–990 (2012).
- [Te43] F. E. Terman, Radio engineers' handbook (1943).
- [Zh11] Y. Zhang, Y. Liu, Z. L. Wang, Fundamental theory of piezotronics. *Advanced Materials (Deerfield Beach, Fla.)*. **23**, 3004–3013 (2011).

Project-related publications by participating researchers

a) Articles published by outlets with scientific quality assurance

- [A5-1] M. Dragoman, V. Ciobanu, S. Shree, D. Dragoman, T. Braniste, S. Raevschi, A. Dinescu, A. Sarua, Y. K. Mishra, N. Pugno, R. Adelung, I. Tiginyanu, Sensing up to 40 atm Using Pressure-Sensitive Aero-GaN. *Phys. Status Solidi RRL*. **13**, 1900012 (2019).
- [A5-2] I. Tiginyanu, T. Braniste, D. Smazna, M. Deng, F. Schütt, A. Schuchardt, M. A. Stevens-Kalceff, S. Raevschi, U. Schürmann, L. Kienle, N. M. Pugno, Y. K. Mishra, R. Adelung, Self-organized and self-propelled aero-GaN with dual hydrophilic-hydrophobic behaviour. *Nano Energy*. **56**, 759–769 (2019).
- [A5-3] M. Mintken, M. Schweichel, S. Schröder, S. Kaps, J. Carstensen, Y. K. Mishra, T. Strunskus, F. Faupel, R. Adelung, Nanogenerator and piezotronic inspired concepts for energy efficient magnetic field sensors. *Nano Energy*. **56**, 420–425 (2019).
- [A5-4] Y. K. Mishra, R. Adelung, ZnO tetrapod materials for functional applications. *Materials Today*. **21**, 631–651 (2018).
- [A5-5] T. Frömling, R. Yu, M. Mintken, R. Adelung, J. Rödel, Piezotronic sensors. *MRS Bulletin*. **43**, 941–945 (2018).
- [A5-6] F. Schütt, V. Postica, R. Adelung, O. Lupan, Single and Networked ZnO-CNT Hybrid Tetrapods for Selective Room-Temperature High-Performance Ammonia Sensors. *ACS Applied Materials & Interfaces*. **9**, 23107–23118 (2017).
- [A5-7] O. Lupan, V. Postica, J. Gröttrup, A. K. Mishra, N. H. de Leeuw, J. F. C. Carreira, J. Rodrigues, N. Ben Sedrine, M. R. Correia, T. Monteiro, V. Cretu, I. Tiginyanu, D. Smazna, Y. K. Mishra, R. Adelung, Hybridization of Zinc Oxide Tetrapods for Selective Gas Sensing Applications. *ACS Applied Materials & Interfaces*. **9**, 4084–4099 (2017).
- [A5-8] S. Kaps, S. Bhowmick, J. Gröttrup, V. Hrkac, D. Stauffer, H. Guo, O. L. Warren, J. Adam, L. Kienle, A. M. Minor, R. Adelung, Y. K. Mishra, Piezoresistive Response of Quasi-One-Dimensional ZnO Nanowires Using an in Situ Electromechanical Device. *ACS Omega*. **2**, 2985–2993 (2017).
- [A5-9] N. Faraji, R. Adelung, Y. K. Mishra, J. Seidel, Nanoscale electromechanical and electronic properties of free-standing ZnO nano- and microstructured platelets. *Nanotechnology*. **28**, 405701 (2017).
- [A5-10] J. Gröttrup, S. Kaps, J. Carstensen, D. Smazna, Y. K. Mishra, A. Piorra, C. Kirchhof, E. Quandt, R. Adelung, Piezotronic-based magnetoelectric sensor. *Phys. Status Solidi A*. **213**, 2208–2215 (2016).

3.4 Project plan

Objectives

The aim of the proposed project is the investigation of current-based ME sensing devices relying on the piezotronic effect. The needle-shaped sensors with the integrated piezotronic pre-amplification allow very compact design, and therefore an envisioned biomedical application is a catheter-mounted sensor, for example, for intracardiac magnetic field detection as an alternative to the currently used TMR sensors. For comparison, more conventional miniaturized AlN piezotronic sensors will be explored as well. To understand the size limitations, transition metal dichalcogenides (TMDs) will be employed in piezotronics that show currently the highest potential for miniaturization, as they consist of monolayer thicknesses, but are nonetheless the most challenging. Consequently, in the second funding period, it is proposed to examine and understand miniaturized piezotronic devices. In the third funding period, the biomaterial applications with the most successful piezotronic sensors are envisioned. High resonance frequencies of the small needles are required to drive the sensors in ΔE mode (see **A4**). The findings of the ongoing funding period raise the following working hypotheses:

- The current noise inside the space charge region is much less compared to the noise in the rest of the piezoelectric material. Thus for a piezotronic sensor, a thickness reduction of the piezoelectric material is desirable so as to have a length in the same order of magnitude as the space charge region. This should drastically reduce the total current noise of the device. The series resistance of the device limits the overall current flow and thus the sensitivity of the device. The series resistance can be reduced by decreasing the distance between the electrodes of a device.
- A large bandgap and a low defect concentration in the piezoelectric material reduce the thermal generation of free charges and will reduce the noise level of the device. AlN has a large bandgap of more than 6 eV. GaN has a lower but still large enough bandgap of 3.2-3.4 eV and is available in very high quality with low defect concentrations by epitaxial growth. Due to this low defect concentration, GaN-based devices will be more suitable for the proposed low noise ME sensors since they promise an improved SNR.
- The doping and resulting increase of conductivity due to an increase of free charge carriers is not aspired to, since the doping will increase the thermally activated charge carriers and accordingly increase the noise of the device and decrease the piezoelectric effect.
- The width of the space charge region is defined by the height of the Schottky barrier, defect (dopant) concentration, and applied bias voltage. Considering thermal noise and series resistances, the space charge region should be as large as possible compared to the distance between the electric contacts. Whereas the maximum bias voltage is limited by the breakdown voltage, the defect concentration or intrinsic doping concentration is mainly defined by choice of the piezoelectric material. In these terms, GaN is the best material since it is available with very low defect and intrinsic dopant concentrations. The choice of the electrode material is limited to only a few technically relevant materials, those being Au, Pt and Al, which can be deposited without formation of thick oxide layers.
- Time-resolved measurements already lead to the same detection limits as lock-in measurements. The advantage of time-resolved measurements is the easier correlation of (noise-) signals and test stimulus, which can help to improve the separation of signal and burst noise or disturbances and reduce the detection limit. Part of the noise may be signal induced, which would be detectable as a characteristic noise footprint in the time domain. By choice of a suitable algorithm, the time-resolved data can be filtered to reduce the uncorrelated noise.
- The design of piezotronic sensors using only two wires, which are needed for powering the sensor, can as well be used for an amplified sensor readout. Here the Schottky barrier acts as a built-in amplifier. This approach is unique among the ME sensors in the CRC. The combination of the piezotronic readout with a small sensor device as manufactured in **Z1** offers the application as an intracardiac catheter.

Proposed research methods

(1) Processing

The fabrication of the thin film-based sensor device will center on state-of-the-art ME sensors as produced in **Z1**. Post processing will be carried out using electron beam lithography and focused ion beam techniques in the Kieler Nanolabor and electrochemical etching in already existing setups using custom built galvanostat/potentiostat devices. For the free standing, needle-like sensors, the ZnO fabrication is an established method within the group and will be carried out in various furnaces allowing different sizes of single crystalline ZnO needles. Epitaxial GaN synthesis will be carried out in cooperation with Prof. Ion Tiginyanu from the TUM in Moldova. The TMD sensor materials will be delivered by Prof. David .C. Johnson from University of Oregon in collaboration with **A6**.

(2) Functional and Structural Characterization

Magnetic measurements will be performed in a custom setup available in the group which offers acoustic, electric, and magnetic shielding and the generation of well-defined, homogeneous magnetic ac and dc fields in a volume of several 10 cm³. Low noise Keithley instrument devices (sourcemeter 2400 & current source 6221) are used for the generation of the magnetic fields. Measurement devices for the sensor response contain Stanford research lock-in amplifier SR830 and dual channel low pass filter SR640 to avoid anti-aliasing. The time-resolved data is recorded using a 16bit adc with a maximum sampling rate of 1 MHz, Measurement Computing USB-2537, controlled using National Instruments Labview software. Impedance spectroscopy is carried out using a custom built device which allows synchronous recording of 4 channels using Measurements Computing USB-1604HS and signal generation using Measurement Computing USB-2537. The data processing will be carried out using Matlab. The structural characterization will be performed in close

cooperation with **A6** using TEM as well as high resolution X-Ray methods at the world's most modern synchrotron facilities.

Work plan

Following the general objective and the corresponding working hypotheses, the work program is structured into five work packages, which are summarized together with the work schedule in Tab. A5-1:

Table A5-1: Work schedule

		2020		2021				2022				2023				2024	
		3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2
WP1	Multiterminal Piezotronics																
WP 2	Needle-shaped Sensors																
WP 3	Large Bandgap Materials																
WP 4	Characterization (TMDs)																
WP 5	Miniaturization																

WP1: Multiterminal Piezotronics

The piezotronic signal of AlN-based sensors can be further improved by introducing a third electrical terminal to the device. This additional contact should have an ohmic characteristic and will be used to apply an additional bias voltage to the AlN. The concept of the three terminal device is depicted in Figure A5-9. Whereas conventional two terminal devices contain a space charge region which is small in size compared to the distance between the electrodes, a third top contact with only a short distance to the existing contact will allow a space charge region which is relatively large compared to the distance between the top contacts and, thus, minimizes series resistance effects. The application of a bias voltage between the top contacts allows tailoring of the space charge region to extend it to the same size as the distance between the top contacts. This should lead to a strong increase of the piezotronic current, because the series resistance of the non-active piezoelectric material is drastically reduced. In addition, low current noise in the space charge region will cause an overall reduction of noise if its width is large compared to the non-active regions of the piezoelectric material, compare equation (A5-2).

The assembly of the 3 terminal devices will be carried out as a post processing step for existing sensor designs. Electron beam lithography as well as focused ion beam will be utilized to partially remove the top electrode and deposit a new additional top electrode.

The proposed sensor design offers advantages due to the accessible piezoelectric material within the space charge region (SCR). The tailoring of the space charge region will be carried out to identify piezotronic current limiting factors and noise sources of the device. This can be achieved by exposing the space charge region to different stimuli such as light, gas atmosphere, or ion bombardment and study the effect on the piezotronic current signal. The surface will be altered by electrochemical etching which will result in a decrease of surface defects and a correspondingly higher electrical quality of the piezoelectric material. Cooperation with **A6** is planned to investigate properties inside the SCR.

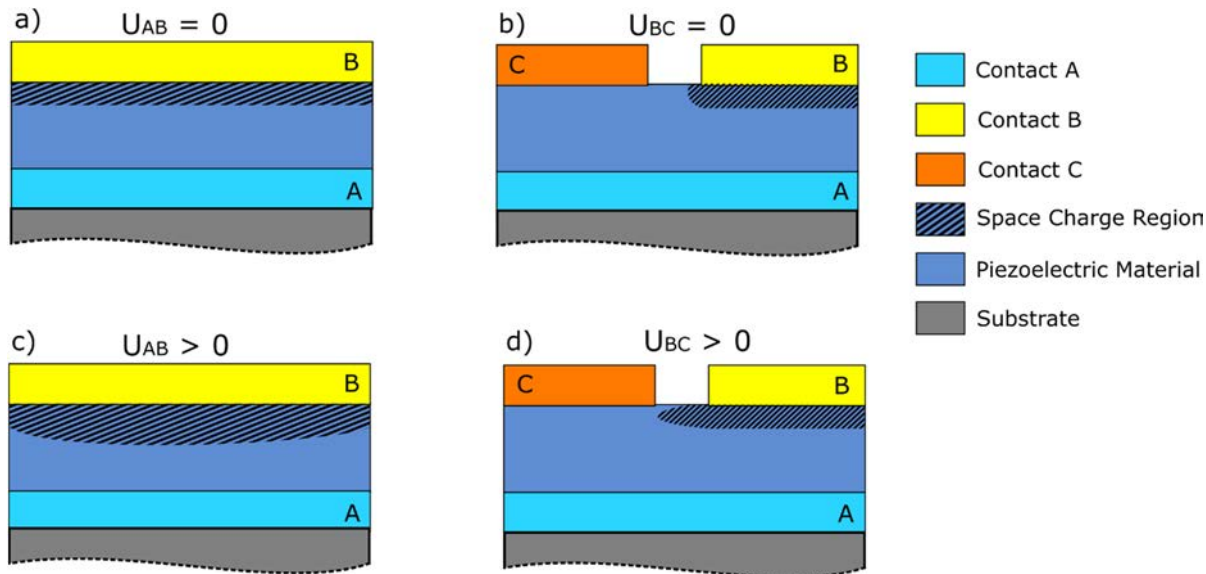


Figure A5-9: Conventional 2 terminal device (shown in a) & c)) compared to the new concept of three terminal devices (shown in b) and d)). a) For existing piezoelectric sensors, the space charge region in the piezoelectric material is typically small compared to the distance between the electrical contacts A and B. b) When using a third contact C with only a short distance to the contact B, the space charge region becomes relatively large compared to the distance between contacts B and C. c) In 2 terminal devices, the application of an external bias voltage can only slightly increase the size of the space charge region. d) In 3 terminal devices, the application of a bias voltage between contacts B and C allows a precise tuning of the space charge region to extend it to the same size as the distance between the contacts B and C.

WP2: Needle-shaped Sensors

The synthesis of piezoelectric ZnO is well established within the proponents group [A5-9]. High quality single crystalline ZnO wires will be grown and, for first studies of the piezotronic properties, attached to a state-of-the-art magnetostrictive cantilever as used in other projects of the CRC. This will allow the construction of an ME sensor with high q-factor and permit a direct comparison to AlN-based sensors using the same geometry. Comparisons of AlN- and ZnO-based sensors are important to verify the abovementioned working hypotheses and to develop a theoretical description of such piezotronic ME sensors. The effect of Schottky barrier height on both signal and noise of the sensor will be investigated by changing the work function of ZnO or using different electrode materials like Ag (4.26-4.74 eV), Au (5.10-5.47 eV), or Pt (5.12-5.93 eV). Investigations in **A6** showed an alteration of the work function of ZnO, as displayed in Figure A5-10. It was observed that a strain in the ZnO which was induced by a coupling to a magnetostrictive material changes the work function of ZnO drastically. Thus, close cooperation with **A6** is planned in this work package. Furthermore, a modification of the ZnO in the area of the space charge region will be performed. This will be achieved by electrochemical etching of ZnO to reduce the density of surface defects consequently increasing the width of the space charge region. The best results are expected when the space charge region reaches a length which is close to the distance of the electrodes. Miniaturization of the sensor will be done in WP5.

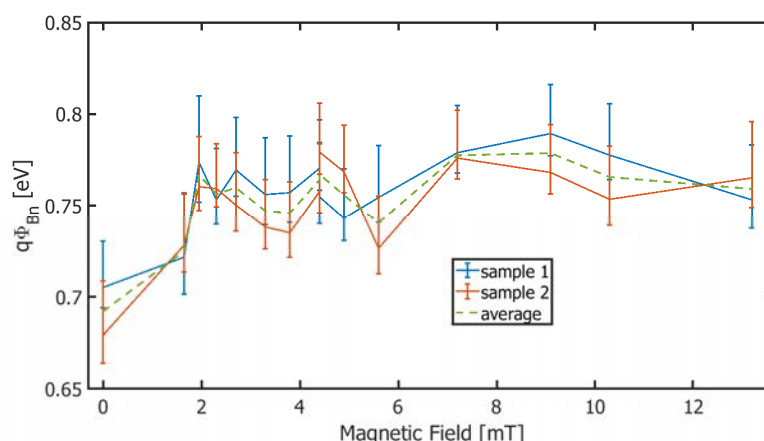


Figure A5-10: Change in work function of ZnO when applying strain by coupling ZnO to the magnetostrictive material FeCoSiB. It can be clearly seen that the work function of ZnO is increased by 10% upon application of the external magnetic field. The measurement was performed in **A6**.

WP3: Large Bandgap Materials

A requirement for piezotronic devices is the presence of high quality contacts. Following the production of ZnO-based sensors, the ZnO will be used as a template for the growth of GaN as demonstrated in Figure A5-8. Again, the sensor device will allow direct comparison to other piezotronic sensors using AlN or ZnO. Due to the high electronic quality and large bandgap of GaN, these sensors are the most promising candidates for high performance in terms of best signal-to-noise ratio piezotronic sensors. In parallel, GaN-based sensors will be realized by utilizing high quality GaN as commonly used for high power devices in the well-established collaboration with Prof. Ion Tiginyanu. For comparison, state-of-the-art GaN thin film crystals will be purchased as well.

When realizing sensors based on GaN, the results of the devices using AlN and ZnO will be included to obtain the highest possible signal-to-noise ratio. This includes electrochemical etching as well as three terminal devices to allow the expansion of the space charge region. Interfaces, bulk GaN, and especially the space charge region will be studied in detail in cooperation with **A6** and the information will be used to develop a more detailed theoretical description of the piezotronic effect in ME sensors.

WP4: Characterization

The fabrication of sensors developed in WP1 - WP3 will be accompanied by measurements to investigate the response to a magnetic field. Conventional measurements using dc bias fields to set the working point and the ac field to be detected will be performed using lock-in techniques. As already shown, time-resolved data can be recorded to perform a lock-in analysis or different mathematical routines, e.g. robust fitting. The established lock-in analysis will be used as a figure of merit to rate the quality of the results of other analytical concepts. FFT-IS will be used to study the response of the sensors for various frequencies and to analyze the homogeneity of the contacts. The results will be used to develop and fit an electrical equivalent circuit, which describes the individual components of the sensors: space charge region, contacts, and bulk material.

In addition to the sensors developed in WP1-WP3, transition metal dichalcogenides (TMDs) will be used in piezotronic devices. The TMDs will be provided by **A6** and assembled using the techniques which are established for the other piezotronic ME sensors. TMDs offer the possibility to study the bandgap-dependent characteristics (noise and sensitivity) since the size of the bandgap can be altered by choosing different amounts of layers [E111]. The investigations will be accompanied by in operando studies using X-Ray and TEM techniques in **A6**.

The noise sources of the piezotronic sensors will be investigated relying on the noise model presented. For ZnO-based piezotronic sensors, a second slope was observed in the double logarithmic plot which corresponds to a sensor response proportional to the square root of the signal. This second slope occurred always for small magnetic fields just above the noise level and implies a reduced noise amplitude in this regime. The origin and the resulting noise characteristics of this second slope will be studied. Heating of the sensors will be used to separate noise sources which are expected to have different temperature profiles.

Burst noise [Hs70] contained in the measurement signals can be uncorrelated or correlated to the measurement signal. An uncorrelated burst noise can principally be eliminated from the signal by a lock-in analysis, whereas correlated, i.e. phase coupled, burst noise is difficult to eliminate. Both types of burst noise will be addressed in the analysis and separated from the signal. Besides sine waves, artificial biomedical signals will be generated and investigated using time-resolved analysis. Especially signals which are relevant for intracardiac analysis will be studied. Different noise sources may have characteristic fingerprints in the time-resolved data, which can allow an identification of individual noise sources and an exclusion from the signal.

WP5: Miniaturization

A piezotronic ME sensor based on a single ZnO micro needles offers great potential for the integration in a miniature sensing device for in vivo measurements, e.g. in a cardiac catheter. The high aspect ratio of the needles does not require additional preparation techniques to modify the geometry as for Si-based devices, compare Figure A5-1. The needle will be coated with multiple functional layers using sputter deposition under permanent rotation to allow for a homogeneous film thickness. A possible sensor design is shown in Figure A5- 11. A ZnO single crystal will be coated by an insulating layer, e.g. SiO₂ followed by deposition of a layer of magnetostrictive FeCoSiB. When using a masking on the tip of the ZnO needle, the magnetostrictive layer can act as the top contact, whereas the substrate is the bottom contact. Since no external signal amplification is required for a piezotronic ME sensor, the complete sensor will be very compact. The sensor could be positioned very close to a biomagnetic source, which will improve the localization of a source and does not require LODs below 100pT. The very high resonance frequencies of individual ZnO needles are well above 100 kHz [Ba03], [Hu06] which is suitable for a readout using ΔE techniques and will be carried out in close collaboration with **A4**.

The size of piezotronic AlN-based sensors will be reduced in collaboration with **Z1**. The effect of the sensor size will be studied and the higher resonance frequencies will be used to realize a ΔE readout in collaboration with **A4**. To investigate a possible application in a catheter, the effect of different a surrounding media on the resonance and sensor response will be studied.

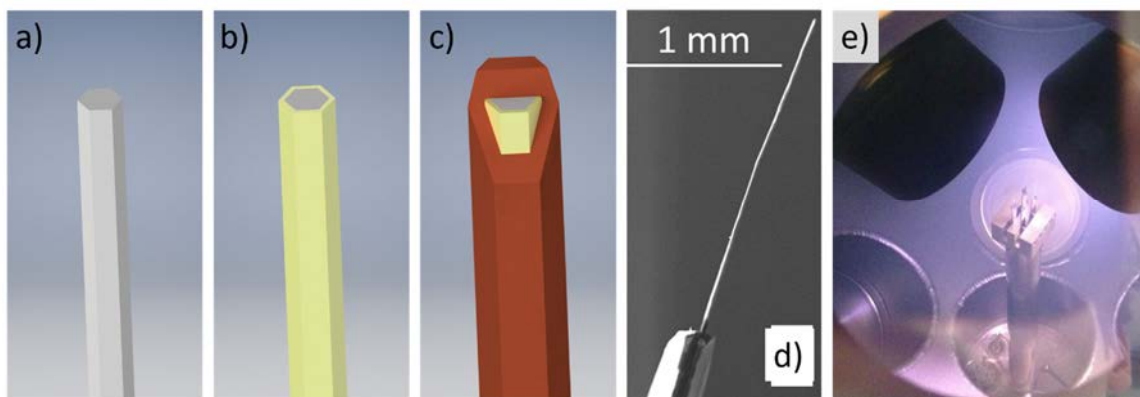


Figure A5- 11: Single needle ZnO-based ME sensor. a) A single crystalline ZnO needle will be coated by an b) insulating layer of SiO₂ followed by c) a coating of a relatively thick layer of FeCoSiB. d) SEM image of a ZnO needle mounted on a glass substrate. e) Sputter deposition of ZnO needles using a two- source geometry under permanent rotation.

3.5 Role within the Collaborative Research Centre

A2	Sensor undamping
A4	ΔE sensor readout
A6	TEM
A8	Modelling of the sensors
Z1	Sensor fabrication
Z2	Sensor characterization

A5 is mainly involved in the following focus groups: “Comparison of sensor concepts”, “Concepts based on ΔE effect” and “Biomedical Applications”.

3.6 Differentiation from other funded projects

There are no other funded projects investigating either piezotronic devices or magnetic sensors.

3.7 Project funding

3.7.1 Previous funding

This project has been funded within the Collaborative Research Centre since 7/2016.

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum
Doctoral researcher, 100 %	1	34.200	1	68.400	1	68.400	1	68.400	1	34.200
Total		34.200		68.400		68.400		68.400		34.200

Direct costs	Sum	Sum	Sum	Sum	Sum
Equipment up to k€ 10, software, consumables	5.0	10.0	10.0	10.0	5.0
Total	5.0	10.0	10.0	10.0	5.0

(All figures in k€)

3.7.3 Requested funding for staff for the new funding period

	Se- quen- tial no.	Name, academic degree, position	Field of research	Department of university or non- university institution	Project commit- ment in hours per week	Cate- gory	Fund- ing source
Existing staff							
Research staff	1	Adelung, Rainer Prof. Dr., Professor	Nano Materials	IMS	4		Core support
	2	Carstensen, Jürgen, Dr., Senior Researcher	Nano Materials	IMS	3		Core support
	3	Kaps, Sören, Dr., Senior Researcher	Nano Materials	IMS	3		Core support
Non-research staff	4	Bahr, Jörg, Dipl.-Ing. (FH), Technician		IMS	4		Core support
Requested staff							
Research staff	5	Martha Gerhardt Doctoral Researcher		IMS			

Job description of staff (supported through available funds):

1. Prof. Dr. Rainer Adelung is planning and coordinating the experiments and collaborations within the Collaborative Research Centre. He advises the scientific staff in the execution of the work within the project and in the interpretation of the obtained results.
2. Dr. Jürgen Carstensen is an expert in the field of semiconductors and will help to understand the mechanisms for noise generation and provide help when etching the surface of the piezoelectric materials.
3. Dr. Sören Kaps is an experienced scientist and will be advising the experimental work in the lab, especially the synthesis of ZnO, sensor assembly, and characterization of ME sensors.
4. Dipl.-Ing. (FH) Jörg Bahr will support the students and doctoral researchers in the project in all areas regarding the mechanical construction of experimental setups. He is responsible for the maintenance of different scientific devices.

Job description of staff (requested):

5. Martha Gerhardt will perform the scientific experiments for the proposed project as described in the work plan. Synthesis of ZnO, deposition of electrical contacts, and assembly of ME sensors will be part of the experiments. Using both existing setup for characterization of the devices as well as the further improvement of the used methods will be done parallel to theoretical considerations and lead to improved understanding of piezotronics.

3.7.4 Direct costs

(All figures in k€)	2020/2	2021	2022	2023	2024/1
Funds available	1.5	3.0	3.0	3.0	1.5
Funds requested	5.0	10.0	10.0	10.0	5.0

Equipment up to k€ 10, software, consumables for 2020/2

Precursor material	k€	2.5
Electronic consumables (for read-out and characterization setups)	k€	2.5

Equipment up to k€ 10, software, consumables for 2021

Cleanroom costs (FIB preparation)	k€	6.0
Precursor material	k€	1.0
Sputter Deposition Targets (1x SiO ₂ , 1x FeCoSiB)	k€	2.0
Electronic consumables (for read-out and characterization setups)	k€	1.0

Equipment up to k€ 10, software, consumables for 2022

Cleanroom costs (FIB preparation)	k€	7.0
Substrate materials (single crystals)	k€	2.0
Electronic consumables (for read-out and characterization setups)	k€	1.0

Equipment up to k€ 10, software, consumables for 2023

Cleanroom costs	k€	3.0
High Quality Materials, e.g. GaN	k€	5.0
Electronic consumables (for read-out and characterization setups)	k€	2.0

Equipment up to k€ 10, software, consumables for 2024/1

Cleanroom costs	k€	2.0
High Quality Materials, e.g. GaN	k€	3.0

3.1 General information about Project A6

3.1.1 Project title: Microstructure and structural change of ME and piezotronic sensors

3.1.2 Research area(s):

307-01 Experimental Condensed Matter Physics
406-02 Synthesis and Properties of Functional Materials

3.1.3 Project leader(s)

Murphy, Bridget, PD Dr. rer. nat.
15.06.1969

Kienle, Lorenz, Prof. Dr. rer. nat.
09.04.1967

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Do any of the above mentioned persons hold fixed-term positions? no

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

Magnetoelectric (ME) sensors for ultralow magnetic fields display complex phenomena due to their magnetic and crystallographic structure that determine their function as components of novel sensor systems with a focus on magnetic multilayer, piezotronic and surface acoustic wave (SAW) sensors. Diverse materials systems are targeted for the development of advanced analytical methods in order to elucidate these properties on multiscales and with excellent resolution and precision. **A6** focuses on the complementary characterization techniques of transmission electron microscopy (TEM) and synchrotron-based X-ray scattering techniques (XRD) to meet these requirements. Using both methods, we can target our studies to investigate the structure and strain in one or in both components of ME sensors from fabrication to operation. Previously, we have focused on crystalline components. In this funding period, we intend to establish a novel methodological combination for amorphous magnetostrictive (multi)layers linking synchrotron-based pair distribution analyses with complementary electron diffraction and X-ray spectroscopy (EDX) techniques in close cooperation with the project partners from **A1**. Thus, in addition to crystalline information crucial for designing best quality ME sensors, atomic and magnetic structure and composition can also be interrelated for the amorphous components delivering valuable input to **A10** for a model-based structure-property description of the sensors. Moreover, the impact of heat treatment as the essential processing parameter on short-range ordering and magnetic properties will be analyzed via combined *in situ* XRD and TEM. Together with **A5** and **A9** crystalline piezomaterials (e.g. AlScN, GaN, ZnO) as components of novel SAW- and ΔE sensors for piezotronic readout are examined for understanding the strain behavior on multiscales and in 3D, e.g. by coherent X-ray diffraction imaging (CXDI). Particularly challenging are the envisaged combined methodolog-

ical developments for new experiments of *in situ* electron microscopy and *in operando* X-ray scattering, like X-ray ptychography and atomic resolution TEM imaging techniques. These experiments require the development of novel devices for *in situ* straining and *operando* measurement in magnetic field (nano-XRD). Few- and single layer transition metal dichalcogenides (TMD) and TMD-based heterostructures (**A5** and external cooperation with D.C. Johnson from University Oregon) will be probed for their mechanoelectrical properties *in situ* and their application as piezotronic components of novel sensors. The ultimate goal of our research is to identify real-structure property relations and by that rules for the synthesis and design of tailor-made materials for highly sensitive and low noise ME sensors.

3.3 Project progress to date

3.3.1 Report and current state of research

In the steady pursuit of pushing the limit of detection (LOD) of magnetic-field sensors, it is the aim of **A6** to contribute with in-depth structural characterization *in situ*, *ex situ* and *in operando*. We demonstrated that synchrotron based methods combined with electron microscopy offer unique capabilities in elucidating the essential real-structure property relations of sensor materials thus enabling knowledge-based improvement. The additional value of such a combined approach has rarely been demonstrated with both methods utilized to their full capabilities [Fa15, Ga04, Ch15]. Moreover, the combined approach allows fundamental studies of the crystallographic structure and strain contributions from the micro- to the nanoscale, providing additional value for the development of nanoanalytical science in general. Together with cooperating projects, we contributed with specific results to all work packages of the first-period proposal as briefly summarized in the following.

Complex microstructure of piezoelectric and magnetostrictive sensor components and composites

In order to develop our understanding of the fabrication process, FeCoSiB-based exchange-bias multilayer films were analyzed concerning the effect of field annealing and the resulting structural and magnetic properties by *in situ* and *ex situ* HRTEM and XRD experiments. Up to 250 °C, the FeCoSiB remains in the amorphous structure, and complementary magnetic studies reveal a defined exchange bias. At higher temperatures a slight decrease of the total anisotropy field was observed although partial crystallization was evidenced via the formation of crystalline filaments (<6 nm) [Hr14]. The relatively low temperature stability of amorphous FeCoSiB used as magnetostrictive phase is crucial for process engineering and sensor packaging. As an alternative, the high temperature stability of FeCo/TiN multilayer thin films with individual layer thicknesses down to one nm has been motivation for us (**A1**, and KIT Karlsruhe) to study the microstructure and strain contributions before and after annealing. The structural integrity of the multilayers was confirmed by atomically resolved STEM EDX, cf. Figure A6-1a. The experimental electron diffraction pattern agrees well with simulations based on a columnar supercell model of fcc TiN and bct FeCo. Defects in the microstructure have been discovered, quantitatively characterized and related to failure during the sputtering process. The unexpected low magnetostrictive response and high saturation fields were linked to their structural origin of atomic scale strain variations in the FeCo lattice (Fig. A6-1b). The intrinsic strain variation from bottom to top of these films has been determined by nano-XRD to gradually change (Fig. A6-1c) and strain relaxation could be evidenced by tracing the (002) reflection of as-deposited and annealed samples.

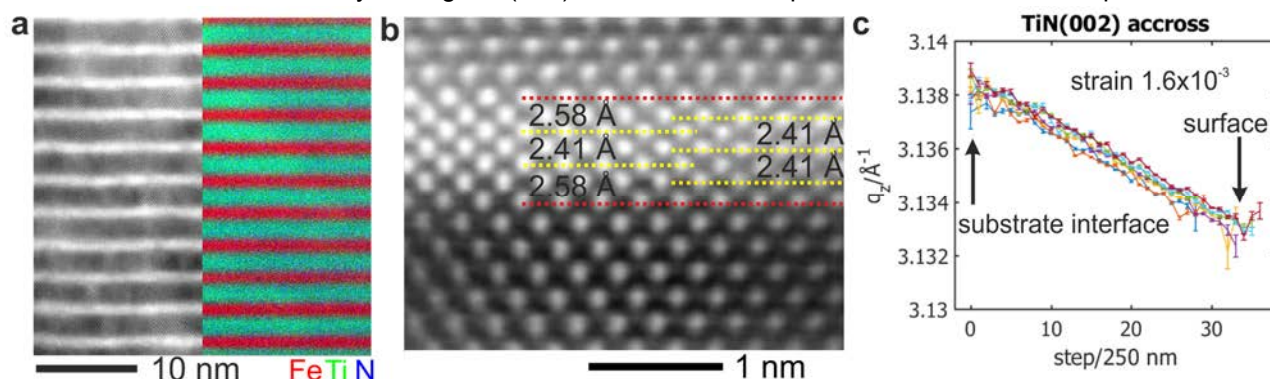


Figure A6-1: a) STEM image and elemental map of a FeCo/TiN multilayer film. b) HRSTEM image showing pseudo-epitaxial relationship between the constituent lattices and anisotropic lattice distortions of the FeCo unit cells (value for isotropic behaviour: 2.93 Å). c) Measurement of film strain by nano-XRD monitoring the position change of the (002) reflection while scanning from the substrate interface to the film surface.

Novel piezoelectric materials and composites were prepared and analyzed by the combined approach of HRTEM and XRD. First, the piezoelectricity of AlN was enhanced to improve the performance of MEMS (**Z1**)

by substitution to form $\text{Al}_{1-x}\text{Sc}_x\text{N}$ [A6-8]. Moreover, ferroelectric switching was unambiguously demonstrated for the first time [Fi19], making this material an interesting component of future SAW sensors (A9). The appearance of ferroelectricity in AlScN can be related to the continuous distortion of the original wurtzite-type crystal structure towards a layered-hexagonal structure with increasing Sc content. Approaches to successfully establish exclusive *c*-axis orientation of the material up to $x \sim 0.43$ were revealed, with electrode pre-treatment and cathode-substrate distance found to exert significant influence. Second, lead-free thin films of $(\text{Ba}_{0.85}\text{Ca}_{0.15})(\text{Ti}_{0.9}\text{Zr}_{0.1})\text{O}_3$ were deposited by pulsed laser deposition as (111) textured thin films which exhibit a clamped piezoelectric response $d_{33,f}$ of up to 190 pm/V and a dielectric coefficient of $\epsilon_r = 2000$ at room temperature. The columnar microstructure of this relaxor material exhibits a high density of twin- and anti-phase boundaries as rationalized by modeling. The exact symmetry of the columnar domains has been determined using convergent beam electron diffraction. The major structural component is described as a tetragonal distorted variant of the cubic perovskite-type. Additionally, coherently intergrown nanodomains were observed with a 7-layer modulation along the growth direction of the films [A6-4]. Third, the elastic coupling in ME composites plays an essential role for their properties. The electrically induced strain at the epitaxial interface of a ME composite $0.72\text{Pb}(\text{Mn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - 0.28PbTiO_3 - CoFe_2O_4 has been characterized by *in operando* X-ray scattering experiments and HRTEM. *In operando* X-ray scattering experiments during an applied electric field show that all strain induced lattice changes are reversible ruling out plastic deformation. The non-perfect elastic coupling of $87\% \pm 7\%$ in this epitaxial system can be explained by the presence of planar defects in the CFO as confirmed by HRTEM [A6-1]. Furthermore, the underlying microscopic mechanisms of magnetostriction in the case of CoFe_2O_4 were investigated. It was shown that magnetostriction in these materials originates from the switching of crystallographic domains, similar to ferroelastic or ferroelectric domain switching [A6-10].

Piezotronic model systems: Material aspects and *in situ* deformation

Typically, the piezotronic effect is exploited in nanoelectronic devices over a Schottky barrier which potential height is modified by the strain-related piezopotential and therefore induces a current change in an externally biased electric circle. With respect to the piezotronic relevant piezoelectric materials ZnO and GaN, the details of structure, the modification of intrinsic electric properties and their strain induced changes have been investigated in close cooperation with A5. For instance, *in situ* nano-XRD experiments (see Figure A6-2) were performed to analyze both the intrinsic (coating-induced) and the extrinsic (magnetic-field-induced) strain at the coupled interface of piezoelectric ZnO microrods coated with FeCoSiB (Fig. A6-2a). While the intrinsic strain is in the range of 10^{-4} , the extrinsic strain is one order of magnitude smaller (Fig. A6-2b). Additionally, the strain relaxation distance of around $5 \mu\text{m}$ for both kinds of strain superimposes, indicating a correlation. The value of both intrinsic and extrinsic strain can be adjusted by controlling the diameter of the rod like composite as the nano-XRD and finite element (FEM) simulation show (Figs. A6-2c). To summarize, the intrinsic interface strain within the ZnO increases exponentially by decreasing the rod diameter while the extrinsic strain increases linearly within the given range. This study shows that miniaturizing the crystal morphology has a huge impact on ME composite properties, resulting in a strongly enhanced strain field and magnetic response [A6-6].

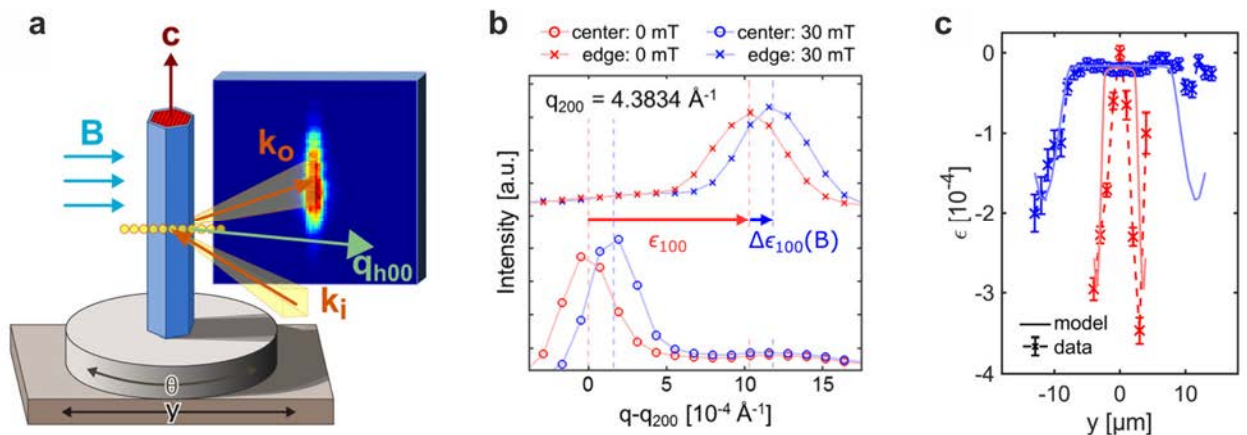


Figure A6-2: Nano-XRD investigation of a ZnO rod coated with FeCoSiB. The ZnO (200) Bragg reflection was measured across the rod with sub micrometer resolution. a) Nanodiffraction setup and measurement geometry. b) Movement of Bragg reflections at the edge (x) and center (o) of a $9 \mu\text{m}$ rod without (red) and with (blue) an external magnetic field applied. c) Comparison of the strain distribution in a hexagonal ZnO pyramid with a $1 \mu\text{m}$ FeCoSiB layer: FEM simulation (solid lines) and the measurement data. [A6-6]

ZnO nanowires were mounted on an electrical push-to-pull device, which enables the application of tensile strain and measurement of *in situ* electrical properties. The results from ZnO nanowires revealed a periodic

variation in stress with respect to the applied periodic potential, which has been discussed in terms of defect relaxation [A6-9]. In a second approach the shape memory alloy NiTi was applied for fabrication of miniaturized traction engines (functional grids) as alternative of expensive commercial *in situ* holders. Due to the shape memory effect pre-strained functional grids can be used for straining inside TEM by use of customary heating holders. The grids can be produced in tailored designs to fit for varied straining applications. For instance, micro tensile tests were performed and the results were compared with finite element simulations to estimate the applied forces on the sample and to predict the functionality of different grid designs. As first example, we showed the impact of the straining on a ZnO network [A6-7]. Push-pull devices employed for similar studies with nano-XRD highlighted sample bending to be a problem, in future functional grids will be adapted for X-ray scattering experiments to compare results on multiscales in WP4.

The 3D examination of defects in ZnO-nanostructures is complicated by their anisotropic nature, e.g. in case of nanospikes where buried defects are producing hardly interpretable superposition contrast in HRTEM. Adding the cross-section of the nanospikes to the plan-view analyses enables to reconstruct the full 3D characteristics with excellent resolution. To do so, a shadow focused ion beam technique was established to prepare multiple electron-beam transparent cross-section specimens of ZnO nanospikes. The combination of plane view and cross-section perspective provides the complete description of a multiply twinned microstructure. Two twin laws were identified with different twin-interface energies, namely the most pronounced orientation $[2\bar{1}\bar{1}0]^W/(01\bar{1}1)$ (low energy) and $[2\bar{1}\bar{1}0]^W/(01\bar{1}3)$ (high energy) [A6-2].

The tailored modification of the electrical characteristics by surface functionalization or doping of piezoelectric ZnO microstructures has been achieved by a variety of pure metal or metal oxide particles. In this respect, the surface functionalization by ZnAl_2O_4 nanocrystals [Ho18] and surface structure modification by Ga_2O_3 was demonstrated to significantly increase the conductivity of ZnO. HRTEM in combination with chemical analyses (EDX) confirmed that the gallium oxide nanoparticles (β - γ - Ga_2O_3 phases) form embedded nanoinclusions at the hybridized ZnO surface and may effect a doping of ZnO in such a way [Sm17].

In case of the piezotronic sensor systems envisioned by **A5** the materials focus is increasingly shifted to GaN as alternative piezotronic material. In **A6**, we investigated GaN in various morphologies ranging from bulk single crystalline wafers presented in Figure A6-3 to hollow and nano-architected structures [Ti19]. Single crystalline n-GaN wafers grown by hydride vapor phase epitaxy (HVPE) were examined by a combination of TEM and XRD. For these wafers, self-organized three-dimensional structured architectures with spatially modulated electrical conductivity are revealed by photo-electrochemical etching (Fig. A6-3a). Detailed structure analyses give striking evidence for inelastic strain manifesting in distortions of the wurtzite-type structure. The deviation from hexagonal symmetry by angular distortions of the β angle between the basal plane and c-axis is found to be of around 1° by ED (Fig. A6-3b,c) and high-resolution XRD (Fig. A6-3d). It is concluded that the lattice distortions are generated by the misfit strains originating during crystal growth, which are slightly relaxed upon photoelectrochemical etching [A6-3].

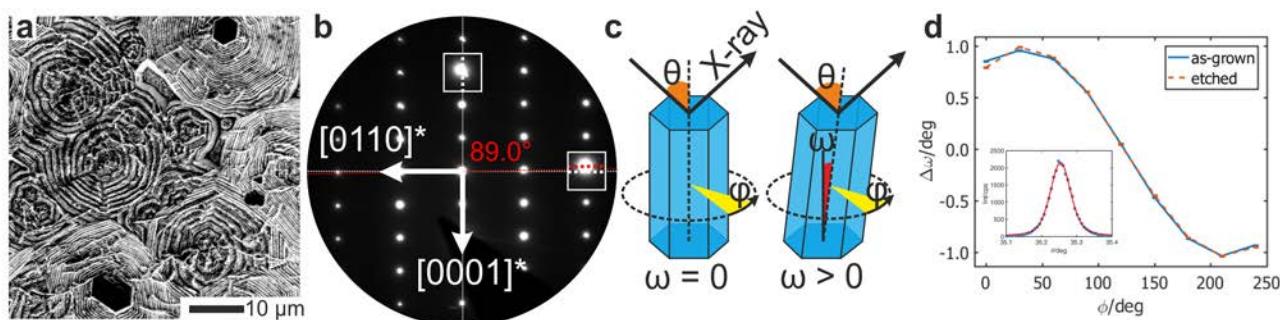


Figure A6-3: a) SEM image of HVPE grown GaN surface with electric property modulation revealed after photoelectrochemical etching. b) ED pattern of a bulk GaN cross-section showing a deviation from rectangularity with $\beta = 89^\circ$ ($\omega \sim 1^\circ$). c) Geometry for HRXRD experiments with (left) and without (right, $\omega > 0$) triclinic lattice distortions measured in dependence of the sample horizontal rotation angle ϕ in a 2θ geometry. d) Variation of the deviation parameter $\Delta\omega$ in dependence of ϕ from HRXRD indicating a strain induced triclinic lattice distortion (inset: XRD rocking curve demonstrating a single crystalline structure) [A6-3].

To investigate the interrelation of strain and piezotronic effect, ZnO microrods were selected as model systems for detailed analyses. The goal of our examinations was to quantify the change of the structure upon application of an external force and simultaneously to monitor the changes in electrical conductivity, see Figure A6-4a for the schematic experimental setup. The external force leads to a change in the piezo potential of ZnO, which leads to a different Schottky barrier height at the ZnO/Au interface and by this to a change in the conductivity. First task was to build a dedicated setup to investigate the piezotronic properties and the crystal structure simultaneously, together with the possibility to apply a mechanical stress along [0001] of

ZnO. The experimental results show that the overall strain increases and the rod is deformed in the sample holder (Fig. A6-4b). Strain in the gold coated Schottky contact area of the rod and in pure ZnO were compared for multiple mechanical stresses from 0 MPa to 300 MPa, see Figure A6-4c. In pure ZnO virtually no increase of the strain is visible; the strain in the Schottky contact area on the other hand is increasing until it saturates around 100 MPa. The change of the barrier height (see Fig. A6-4d) showed a complementary behaviour, i.e., the current decreases with applied mechanical stress highlighting a proportional behaviour between strain and Schottky barrier height due to the piezotronic effect.

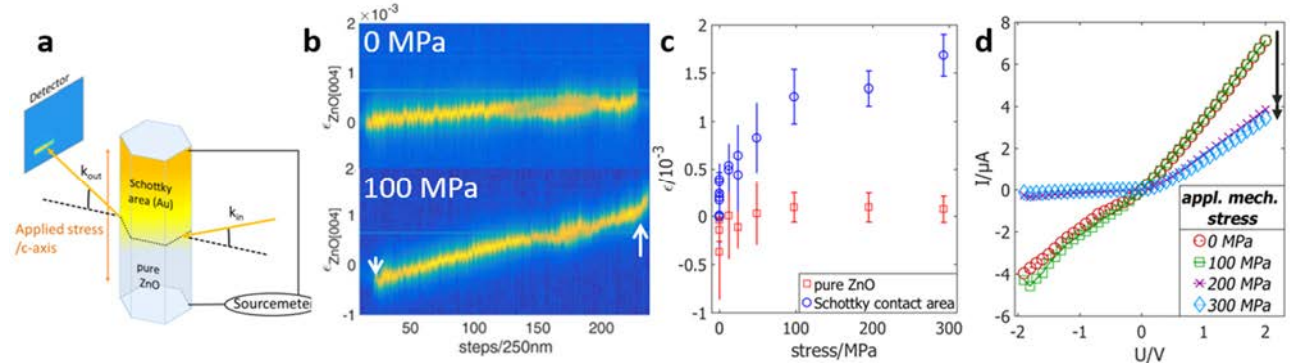


Figure A6-4: a) Experimental setup for nano-XRD investigations. The Au coated ZnO rod was scanned in 250 nm steps to measure the (0002) reflection. b) (0002) Bragg intensities from the Schottky contact area show the strain across the rod as mechanical stress is applied to the rod from 0 to 100 MPa. The rod is bent in the sample holder visualised by compressive strain on the left side and relaxation on the right. Additionally, the mean strain increases from 2.4×10^{-4} to 4.8×10^{-4} , respectively. c) The strain for different mechanical stress in the Schottky contact area (blue circles) and in pure ZnO (red squares). In the pure ZnO area the strain increases only within the experimental error while in the Schottky contact area the strain increases rapidly, saturating after 100 MPa. d) Separately, the current voltage behaviour was investigated for increasing applied mechanical stress from relaxed state to 300 MPa, see inset of the figure. The Schottky contact diode like behaviour is visible with a piezotronic change of the current flow (arrows), while the stress is increasing.

The local strain distribution in ZnO model systems was investigated by combining CXDI (Coherent X-ray Diffraction Imaging) and GPA (Geometrical Phase Analysis in TEM). CXDI provides a unique possibility to image the strain within an entire rod section via high resolution rocking curves which were collected for the ZnO (100) Bragg peak for a rod cross-section entirely illuminated by coherent X-rays. The ZnO rod was coated with 100 nm of gold. The rocking curves can be merged together yielding a 3D representation of the Bragg reflection. In Figure A6-5a, a slice through this 3D Bragg reflection is shown. From this measured data it is possible to reconstruct the amplitude and phase of the scattered beam and hence the 3D strain distribution, see Figure 6-5b. Here, highlighted areas at the Au/ZnO interface show both compressive strain up to 1.1×10^{-3} and relaxation strain up to -1.4×10^{-3} . These "strain centers" are spatially confined to areas smaller than 100 nm. In complementary HRTEM studies, GPA maps (Fig. A6-5c) show local strain hot spots at the interface with values up to 6×10^{-2} and $\sim 1 \times 10^{-2}$ on average. These results interrelate large scale investigations to strongly confined strain analysis on the nanoscale.

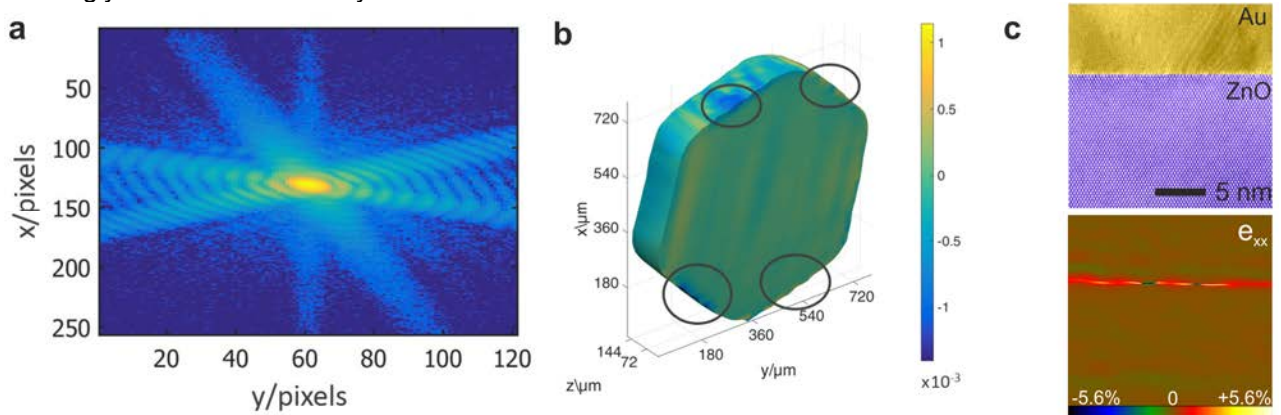


Figure A6-5: CXDI experiment on a gold coated ZnO rod: a) Slice of the ZnO (10-10) Bragg reflection. b) Real space reconstruction showing the strain distribution with an isosurface of 0.1. Strain centers are marked with circles. c) Investigation of interfacial strain by HRTEM and GPA of in-plane (e_{xx}) strain at the Au/ZnO interface.

In collaboration with partners from the University Oregon (Prof. D.C. Johnson) preliminary work on transition metal dichalcogenides (TMD) which are representing novel piezotronic model systems for the actual applica-

tion were performed [Wu14]. Particularly, the combined approach of Scanning TEM (STEM) and X-ray techniques prove valuable for the determination of real-structure property relations of few layer MoSe₂ [A6-5]. It was shown that the material exhibits unexpected nanoscale 1D ordering which enhances the anisotropic character of the structure. The fruitful collaboration was also extended to TMD-based heterostructures which show interesting structural transformations upon heating. In case of the system (VSe)-(LaSe), layers of V₃Se₄ and not the van-der-Waals layer type of VSe₂ were demonstrated to be part of a strongly disordered heterostructure. This kind of heterostructure lacking the van der Waals gap structure was firstly demonstrated, substantially broadening the simple picture of TMD heterostructures [Da16].

References

- [Ch15] C. Chluba, W. Ge, R. L. de Miranda, J. Strobel, L. Kienle, E. Quandt, M. Wuttig, Ultralow-fatigue shape memory alloy films. *Science*. **348**, 1004–1007 (2015).
- [Da16] T. Dankwort, A.-L. Hansen, M. Winkler, U. Schürmann, J. D. Koenig, D. C. Johnson, N. F. Hinsche, P. Zahn, I. Mertig, W. Bensch, L. Kienle, Nanostructure, thermoelectric properties, and transport theory of V₂VI₃ and V₂VI₃/IV–VI based superlattices and nanomaterials. *Phys. Status Solidi A*. **213**, 662–671, (2016).
- [Fa15] F. Fahrnbauer, T. Rosenthal, T. Schmutzler, G. Wagner, G. B. M. Vaughan, J. P. Wright, O. Oeckler, Entdeckung und Strukturbestimmung eines ungewöhnlichen Sulfidtellurids mithilfe einer effektiven Kombination von TEM und Synchrotron-Mikrodiffraction. *Angewandte Chemie*. **127**, 10158–10161 (2015).
- [Fi19] S. Fichtner, N. Wolff, F. Lofink, L. Kienle, B. Wagner, AlScN: A III-V semiconductor based ferroelectric. *Journal of Applied Physics*. **125**, 114103 (2019).
- [Ga04] S. García-Martín, M. A. Alario-Franco, H. Ehrenberg, J. Rodríguez-Carvajal, U. Amador, Crystal Structure and Microstructure of Some La_{2/3-x}Li_{3x}TiO₃ Oxides: An Example of the Complementary Use of Electron Diffraction and Microscopy and Synchrotron X-ray Diffraction To Study Complex Materials. *J. Am. Chem. Soc.* **126**, 3587–3596 (2004).
- [Ga10] K. J. Ganesh, M. Kawasaki, J. P. Zhou, P. J. Ferreira, D-STEM: A Parallel Electron Diffraction Technique Applied to Nanomaterials. *Microscopy and Microanalysis*. **16**, 614–621 (2010).
- [Ha92] V. G. Harris, K. D. Aylesworth, B. N. Das, W. T. Elam, N. C. Koon, Structural origins of magnetic anisotropy in sputtered amorphous Tb-Fe films. *Phys. Rev. Lett.* **69**, 1939–1942 (1992).
- [He92] F. Hellman, E. M. Gyorgy, Growth-induced magnetic anisotropy in amorphous Tb-Fe. *Phys. Rev. Lett.* **68**, 1391–1394 (1992).
- [Hi11] A. T. Hindmarch, A. W. Rushforth, R. P. Campion, C. H. Marrows, B. L. Gallagher, Origin of in-plane uniaxial magnetic anisotropy in CoFeB amorphous ferromagnetic thin films. *Phys. Rev. B*. **83**, 212404 (2011).
- [Ho17] M. Holler, M. Guizar-Sicairos, E. H. Tsai, R. Dinapoli, E. Müller, O. Bunk, J. Raabe, G. Aeppli, High-resolution non-destructive three-dimensional imaging of integrated circuits. *Nature*. **543**, 402–406 (2017).
- [Ho18] M. Hoppe, O. Lupan, V. Postica, N. Wolff, V. Duppel, L. Kienle, I. Tiginyanu, R. Adelung, ZnAl₂O₄-Functionalized Zinc Oxide Microstructures for Highly Selective Hydrogen Gas Sensing Applications. *physica status solidi (a)*. **215**, 1700772 (2018).
- [Hr14] V. Hrkac, E. Lage, G. Köppel, J. Strobel, J. McCord, E. Quandt, D. Meyners, L. Kienle, Amorphous FeCoSiB for exchange bias coupled and decoupled magnetoelectric multilayer systems: Real-structure and magnetic properties. *Journal of Applied Physics*. **116**, 134302 (2014).
- [Mu16] X. Mu, D. Wang, T. Feng, C. Kübel, Radial distribution function imaging by STEM diffraction: Phase mapping and analysis of heterogeneous nanostructured glasses. *Ultramicroscopy*. **168**, 1–6 (2016).
- [Pf18] F. Pfeiffer, X-ray ptycography. *Nature Photonics*. **12**, 9–17 (2018)
- [Pr97] T. Proffen, R. B. Neder, DISCUS, a program for diffuse scattering and defect structure simulations. *J. Appl. Cryst.* **30**, 171–175 (1997)
- [Ro04] J. M. Rodenburg, H. M. Faulkner, A phase retrieval algorithm for shifting illumination. *Applied physics letters*. **85**, 4795–4797 (2004).
- [Sc18] E. M. Schmidt, R. B. Neder, Analysis of chemical short-range order using single-crystal diffuse scattering. *Acta Cryst.* **A74**, 317–318 (2018)
- [Sm17] D. Smazna, N. Wolff, S. Shree, F. Schütt, Y. K. Mishra, L. Kienle, R. Adelung, Enhancing the Conductivity of ZnO Micro- and Nanowire Networks with Gallium Oxide. *Proceedings of the 2017 IEEE 7th International Conference Nanomaterials*, Art.No. UNSP 01FNC07 (2017).
- [Ti19] I. Tiginyanu, T. Braniste, D. Smazna, M. Deng, F. Schütt, A. Schuchardt, M. A. Stevens-Kalceff, S. Raevschi, U. Schürmann, L. Kienle, N. M. Pugno, Y. K. Mishra, R. Adelung, Self-organized and self-propelled aero-GaN with dual hydrophilic-hydrophobic behaviour. *Nano Energy*. **56**, 759–769 (2019).

- [Wu14] W. Wu, L. Wang, Y. Li, F. Zhang, L. Lin, S. Niu, D. Chenet, X. Zhang, Y. Hao, T. F. Heinz, J. Hone, Z. L. Wang. Piezoelectricity of single-atomic-layer MoS₂ for energy conversion and piezotronics. *Nature*. **514**, 470–474 (2014).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [A6-1] C. T. Koops, **S. B. Hrkac**, M. Abes, **P. Jordt**, J. Stettner, A. Petraru, H. Kohlstedt, V. Hrkac, **N. Wolff**, **L. Kienle**, O. H. Seeck, G. Nisbet, O. M. Magnussen, **B. M. Murphy**, Elastic Coupling at Epitaxial Multiferroic Interfaces: in situ X-ray Studies of Electric Field Induced Strain. *Proceedings ICNBE 2019, IFMBE Proceedings* **77**, 187–191 (2019)
- [A6-2] **N. Wolff**, V. Hrkac, J. J. Ditto, V. Duppel, Y. K. Mishra, D.C. Johnson, R. Adelung, **L. Kienle**, Crystallography at the nanoscale: planar defects in ZnO nanospikes, *J. Appl. Cryst.* **52**, (2019)
- [A6-3] **N. Wolff**, **P. Jordt**, T. Braniste, V. Popa, E. Monaico, V. Ursaki, A. Petraru, R. Adelung, **B. M. Murphy**, **L. Kienle**, I. Tiginyanu, Modulation of Electrical Conductivity and Lattice Distortions in Bulk HVPE-Grown GaN. *ECS J. Solid State Sci. Technol.* **8**, 141–146 (2019).
- [A6-4] A. Piorra, V. Hrkac, **N. Wolff**, C. Zamponi, V. Duppel, J. Hadermann, **L. Kienle**, E. Quandt, (Ba_{0.85}Ca_{0.15})(Ti_{0.9}Zr_{0.1})O₃ thin films prepared by PLD: Relaxor properties and complex microstructure. *Journal of Applied Physics*. **125**, 244103 (2019).
- [A6-5] E. C. Hadland, H. Jang, **N. Wolff**, R. Fischer, A. C. Lygo, G. Mitcheson, D. Li, **L. Kienle**, D. G. Cahill, D. C. Johnson. Ultralow thermal conductivity of turbostratically disordered MoSe₂ ultra-thin films and implications for heterostructures. *Nanotechnology*. **30**, 285401 (2019).
- [A6-6] **S. B. Hrkac**, C. T. Koops, M. Abes, C. Krywka, M. Müller, M. Burghammer, M. Sztucki, T. Dane, S. Kaps, Y. K. Mishra, R. Adelung, J. Schmalz, M. Gerken, E. Lage, C. Kirchhof, E. Quandt, O. M. Magnussen, **B. M. Murphy**, Tunable Strain in Magnetoelectric ZnO Microrod Composite Interfaces. *ACS Appl. Mater. Interfaces*. **9**, 25571–25577 (2017).
- [A6-7] U. Schürmann, C. Chluba, **N. Wolff**, D. Smazna, R. Lima de Miranda, P. Junker, R. Adelung, E. Quandt, **L. Kienle**, Functional NiTi grids for in situ straining in the TEM. *Ultramicroscopy*. **182**, 10–16 (2017).
- [A6-8] S. Fichtner, **N. Wolff**, G. Krishnamurthy, A. Petraru, S. Bohse, F. Lofink, S. Chemnitz, H. Kohlstedt, **L. Kienle**, B. Wagner, Identifying and overcoming the interface originating c-axis instability in highly Sc enhanced AlN for piezoelectric micro-electromechanical systems. *Journal of Applied Physics*. **122**, 035301 (2017).
- [A6-9] S. Kaps, S. Bhowmick, J. Gröttrup, V. Hrkac, D. Stauffer, H. Guo, O. L. Warren, J. Adam, **L. Kienle**, A. M. Minor, R. Adelung, Y. K. Mishra, Piezoresistive Response of Quasi-One-Dimensional ZnO Nanowires Using an in Situ Electromechanical Device. *ACS Omega*. **2**, 2985–2993 (2017).
- [A6-10] M. Abes, C. T. Koops, **S. B. Hrkac**, J. McCord, N. O. Urs, **N. Wolff**, **L. Kienle**, W. J. Ren, L. Bouchenoire, **B. M. Murphy**, and O. M. Magnussen, Domain structure and reorientation in CoFe₂O₄, *Phys. Rev. B*. **93**, 195427 (2016)

3.4 Project plan

Objectives

The main objective of **A6** is to provide the real structure property relations for diverse sensor designs, like ME and piezotronic sensors. In this regard, the state of the art has to be extended by the development and application of novel methods. Moreover, the synergistic approach of synchrotron-based techniques and TEM is required to enable multiscale analyzes from the atomic scale up to practically relevant micron size. *In situ* and *in operando* examinations shed new light on the functional mechanisms of the sensors, their performance and potential fatigue. The main objective is associated with the following working hypotheses:

- The amorphous structure of magnetostrictive layers as essential component of mostly all sensor designs strongly impacts the functional properties. It is expected that fluctuations of the structure exist, particularly on the nanoscale and at interfaces of multilayer materials. The examinations will focus on the interrelation of preparation, structure and property of these materials. A major goal would be to find identifiers in the amorphous structure indicating specific magnetic / magnetostrictive properties.
- The strain in piezo- and ferroelectric components is not uniform, but local variations are relevant, e.g. at the Schottky barrier of piezotronic devices, which have to be analyzed for their intrinsic nature by in-depth structural characterization *in situ*, *ex situ* and *in operando*. Moreover, the strain examinations have to be extended three-dimensionally by CXDI and linked to the nanostructural data as obtained by state-of-the-art TEM.

- The true role of strain in ME sensor materials and its impact on device function can be understood by combinations of novel techniques with the main focus on *in operando* imaging. A key objective in this period is to image a sensor in operation.
- In combination with modelling and nanoanalytics a prediction of the strain behavior at interfaces in ME sensors is possible. Using this knowledge we intend to derive and suggest structural models for sensors with enhanced performance.

Proposed research methods

The ambitious goals of **A6** require the best available experimental setups and cutting-edge technology. In order to enhance the experimental capacity of the two existing TEMs, a probe corrected scanning electron microscope (STEM with atomic resolution) will be installed in 2020 at the Faculty of Engineering. The relevant funds for the STEM were granted on 09.07.2019 by the DFG (INST 257/620 FUGG). The instrument will be equipped with a cold field emitter for high resolution EELS, an atomically resolving wide-angle EDX detector and diverse image detectors providing not just Z-contrast but also enhanced contrast for light-element imaging. Dedicated simulation techniques including crystallographic computation and supercell approaches will be applied for advanced data interpretation. The PDF measurements and corresponding data calculation for amorphous magnetic materials will be conducted with our external collaboration partners from KNMF (Dr. Kübel). TMD as novel model systems for piezotronic devices will be prepared via the MER (modulated element reactants) approach in the labs of our external collaboration partners at University Oregon (Prof. D.C. Johnson). *In situ* high resolution XRD methods as outlined in preliminary work will be used for *in situ* and *in operando* investigations at the most brilliant third generation X-ray synchrotron sources worldwide. In particular, we plan detailed *in situ* X-ray reflectivity and Grazing Incidence X-ray Diffraction (GID) with the LISA diffractometer at the P08 beamline at PETRA III [A6-6, A6-1] optimized for such studies. B. Murphy and her team built the diffractometer, therefore have extensive experience with its operation and development. Furthermore, the P03 beamline at PETRA III is ideal for microdiffraction experiments and ID13 at European Synchrotron Radiation Source (ESRF) for nanodiffraction experiments. In addition, we plan to continue to use the 34-ID-C XOR/UNI beamline at the Advanced Photon Source (APS) for *in situ* coherent XRD imaging investigations of strain in microstructure. Beamlines P010 at PETRA III and ID1 at ESRF may also be considered.

Work plan

The objectives of this project will be addressed in six work packages. In the following, the key tasks, challenges and approaches will be described including the collaboration within the project and within the CRC.

Table 1: Work schedule (red = PhD TEM, blue = PhD XRD)

No.	Work package	2020		2021				2022				2023				2024	
		3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2
1	Real structure property relations for (amorphous) magnetic (multi)layers																
2	<i>In situ</i> examination of the structural evolution in amorphous magnetic (multi)layers																
3	3D and nanoscale strain distribution in piezotronics																
4	<i>In situ</i> mechanoelectrical examination																
5	<i>In operando</i> strain imaging																
6	Synergy of TEM & XRD																

WP1: Real structure property relations for (amorphous) magnetic (multi)layers

Detailed knowledge on the amorphous structure of amorphous metallic glasses, including local variations, and therefore potential sources of stress is of vital importance for the entire CRC in order to explain macroscopic magnetic property variations and hence sensor output characteristics. Having a strong collaboration with **A1** and **Z1**, we will exploit a novel methodological combination using X-ray and electron diffraction tech-

niques capable of resolving the structural and chemical environment with respect to atomic correlation functions of short-range ordered materials. It is known, that the uniaxial magnetic anisotropy linked to the structural anisotropy can be varied for example by process parameters [He92] and interface effects [Hi11]. Consequently, the in-depth analysis of the amorphous structure with respect to local variations is of great interest as the adatom configuration is known to determine the magnetic anisotropy [Ha92]. In this respect, the analysis of the Pair Distribution Function (PDF) via synchrotron data provides results with excellent precision; however, the spatial resolution is limited by the lateral dimensions of the synchrotron micro-/nanoprobe. These spatially more averaged investigations will be complemented by 4D-STEM radial distribution function (RDF) analyses mapping out minute differences in the structural environment with a spatial resolution of ~ 1 nm [Ga10, Mu16]. This technique has been demonstrated valuable for the characterization of amorphous metallic films and will be applied to the amorphous FeCoSiB sensor components in close collaboration with Dr. C. Kübel through beam time application at the Karlsruhe Nano Micro Facility (KNMF). In case of unforeseen problem with experimental external capacity, data can also be recorded through proposals within the ESTEEM3 project or the method could be transferred to Kiel in perspective. In a recent proof-of-principle experiment on a FeCoSiB film we demonstrated the interrelation of chemical composition, local structure and magnetic properties, cf. Figure A6-6. A columnar segregation into Fe/Co rich and deficient regions was evidenced for the amorphous FeCoSiB film as observed with Z-contrast imaging and high-resolution chemical analyses (Fig. A6-6a,b). These differences in the local chemical environment could be directly linked to perturbations in the RDF calculated for positions within the film (Fig. A6-6c-e) and at the Ta/FeCoSiB interfaces (Fig. A6-6f). Such information is highly relevant for e.g. exchange-biased FeCoSiB/Ta/Cu/MnIr/Ta films produced in **A1** and **Z1**. Two reference RDFs for FeCoSiB correlated to regions of high and low Z contrast intensity indicate a complementary spatial distribution (see circled area in Fig. A6-6c,d). Further, we will investigate the strength of such novel interface effects in various systems produced by our collaboration partners from **A1** and **A9**, e.g., exchange of Ta/Cu seed-layer by Ru interlayers in exchange coupled systems, FeCoSiB coupled permalloy MnIr/NiFe bi-layers for exchange spring systems and SAW ME sensors. Of particular interest for the temperature stability of these amorphous magnetostrictive films is also the distribution of Boron which will be retrieved by mapping of the B-K-edge of spatially resolved and energy filtered electron energy-loss spectroscopy data. Consequently, we expect to uncover the structural and chemical reasons for magnetic property variations of the amorphous films enabling knowledge-based improvement of deposition parameters and post-processing procedures, as well as providing substantial input for the theoretical description of the sensor systems (**A10**).

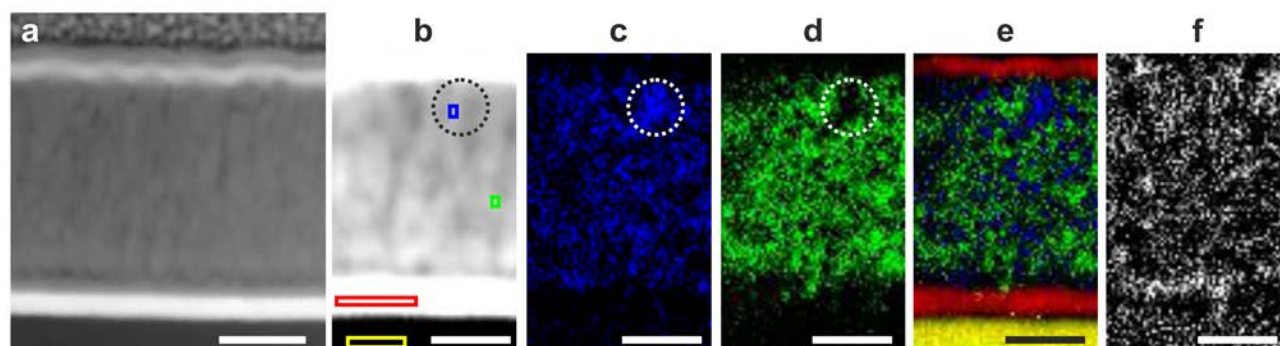


Figure A6-6: a) Z-contrast image of a FeCoSiB layer with variation in stoichiometry. b) (Virtual) HAADF image calculated from the STEM measurement. Results from MLLS fitting using two RDF references found in the FeCoSiB layer, Ta and SiO₂: Image for the fitting coefficients for c) the first FeCoSiB reference RDF and d) the second FeCoSiB reference RDF. e) Superposition image of RDF distributions extracted from the coloured boxes in (b). f) Residual error function displaying some misfit of the local RDF to the chosen reference RDFs showing clear deviation at the bottom Ta/FeCoSiB interface (scalebar a-f:20 nm).

WP2: *In situ* examination of the structural evolution in amorphous magnetic (multi)layers

This work package will focus on effects of external stimuli on magnetic (multi)layers and transition metal dichalcogenides (TMD) which will be investigated *in situ* and *ex situ* using the X-ray scattering and TEM methods in close synergy. First, the impact of moderate annealing below the crystallization temperature on the short-range order and hence on the local RDFs will be analyzed up to the early stages of crystallization, e.g. providing information about a potential interrelation of crystallization and chemical segregation at interfaces in FeCoSiB-based multilayers. In a previous work, we could demonstrate the structural differences between FeCoSiB multilayers which were heated *in situ* and *ex situ* shown in Figure A6-7a-c. In case of TMD, amorphous precursors can be obtained which crystallize gradually upon heating. Further, it is expected that heating supports the gradual release of chalcogene atoms under rearrangement of the layered TMD structure. The TEM experiments will be performed using advanced MEMS-based heating holders in

order to overcome sample-drift and thus achieve ultimate resolution. The magnetic microstructure, e.g. microdomains in multilayers can be efficiently probed using Lorentz microscopy by Fresnel mode observation (magnetic domain walls), and Foucault mode (magnetic domains) in TEM. In case of high resolution XRD heat as well as magnetic fields can be applied for examining structural changes of the amorphous components and to monitor interrelated changes in structure (Figure A6-7d) and strain. Thus, a crucial step of processing can be analyzed, namely, the adjustment of specific magnetic anisotropies by field annealing. Overall, these experiments should provide a model for the structural and chemical evolution of the materials targeted which can be used in collaboration with **A1**, **A10** and **Z1** to rationalize functional changes of the materials upon thermal processing.

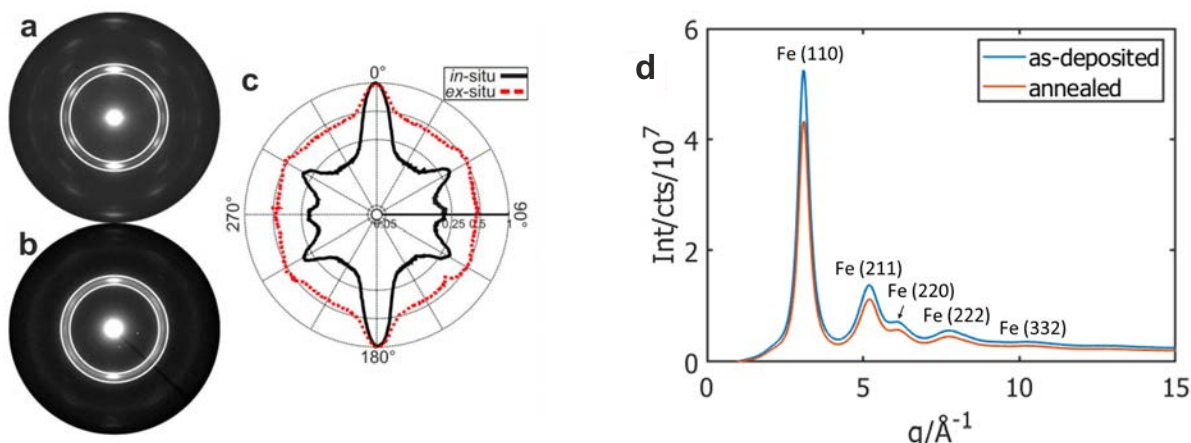


Figure A6-7: SAED patterns recorded after the annealing of the exchanged coupled systems at 350 °C: (a) *in situ* and (b) *ex situ* annealing at 350 °C. (c) Normalized radial intensity distribution for the marked regions in the SAED pattern. [Hr14] (d) Powder diffraction pattern of FeCoSiB as deposited and after annealing, where a decrease in intensity is observed upon annealing. Fits show that with annealing, the position shifts to higher values and the FWHM decreases indicating a lattice parameter contraction accompanied by an increase of the crystalline domain size.

WP3: 3D and nanoscale strain distribution in piezotronics

Strain distribution in 3D, in particular on the nanoscale, are of great interest and importance for the further understanding and enhancement of sensor applications, especially in the field of piezotronic sensors developed by **A5**. The proposed scheme for synergistic multiscale investigation of structure and interrelated strain response of the sensors can increase the performance and improve the fabrication process. To achieve this goal we will combine results from the structure analysis with results from functional investigations from sensors produced by **Z1**, but especially from **A5**. We will put our focus principally on piezotronic model sensors containing (aero)ZnO, (aero)GaN and AlN improved for piezotronic readout. Here, we will probe the mechanical stress and the induced piezo potential which is utilized to control the Schottky barrier height at metal / semiconductor interfaces and by this the electric properties of the sample in dependence of the metal contact and layer thickness on samples from **A5**.

Additionally, TMD few-layer and heterostructure materials will be investigated as a new 2D material class with promising properties and internal stresses (see Fig. A6-8a). The number of TMD layers has to be adjusted since it must be odd, in order to break centro-symmetry and achieve piezotronic behavior [Wu14]. Alternatively disorder and by that local symmetry breaking may be probed as trigger to overcome the property restriction on layer-number. The group of D. C. Johnson, University of Oregon, will provide the well-tailored TMD samples by the modulated element reactant (MER) approach; FeCoSiB/TMD model systems will be introduced into simple ME sensor devices and their field or strain dependent characteristics will be measured in cooperation with **A5**. The (aero)ZnO and (aero)GaN samples will be provided by **A5** and in cooperation with Prof. Tiginyanu (Technical University Moldova). In collaboration with **A9** AlScN used in SAW sensors will be investigated with X-rays to determine ferroelectric domain size in combination with interfacial strain.

The interfacial strain and 3D strain distribution in the numerate samples will be investigated by modern and highly excellent techniques on the micro- and nanoscale, namely, nano-XRD, coherent X-ray diffraction imaging (CXDI) and X-ray ptychography in combination with atomically resolved STEM, nanobeam electron diffraction (NBED) and geometric phase analysis (GPA) known capable of strain mapping. CXDI and ptychography (Figure A6-8b) make use of coherent scattering of X-rays from structures providing an over-determined system to reconstruct the amplitude and phase of the scattered beam by advanced algorithms to resolve e.g. shape and 3D strain distribution of the specimen. The main advantage of CXDI over nano-XRD

is the higher spatial resolution down to 10 nm and the capability to resolve the strain distribution in all three dimensions in the investigated area. Whereas for CDXI is that the sample diameter is limited by the coherence length of the beam, for modern synchrotrons this is around 1 μm , ptychography overcomes size restrictions by superposition of scanned patterns. Since both, the experimental and processing challenges are immense; ptychography will be approached following initial nano-XRD and CXDI studies.

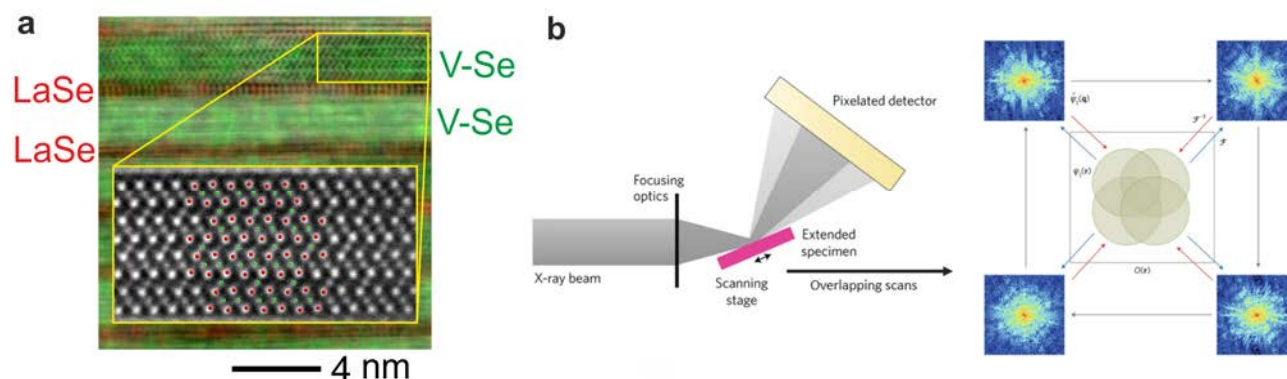


Figure A6-8: a) Nanoscale chemical and structure analysis of a TMD LaSe/V-Se heterostructure. The structural motif of V_3Se_4 is compressively strained. b) Setup for X-ray ptychography based on coherent scattering. For the measurement the X-ray beam is guided across the specimen to sample a larger area with overlapping points. In the pictures on the right, the speckle of the diffracted beam in different overlapping positions is shown. From these data the amplitude and phase of the structure factor can be reconstructed to obtain the electron density of the specimen. (Image extracted from [Pf18]).

Together, this methodic combination will give novel insight into the microscopic strain distribution with an advanced spatial resolution of 10 nm compared to classical X-ray scattering experiments which currently deliver a resolution of 200 nm but usually in only one direction [Ro04, Ho17]. Ptychography especially gives the opportunity to investigate larger samples. TEM with its extremely high spatial resolution down to the atomic scale combined with a moderate strain resolution will be important to clarify local structural changes in the samples. Together with the X-ray studies, this enables a complete understanding of the samples on all relevant length scales.

WP4: *In situ* mechanoelectrical examination

In this WP the main goal is the *in situ* investigation of strain distribution in mechanically stressed or bent samples using complementary XRD and TEM/SEM methods. The samples of choice are piezotronic devices, for example (aero)GaN (A5) and TMD with metal contacts and magnetic structures, for example FeCoSiB (multi)layer structures provided by A1. For the *in situ* monitoring of elastic or irreversible structural changes, it will be necessary to design and test two novel experimental setups that are enabling the application of a mechanical stress to the samples with high spatial precision and are capable of performing simultaneous measurements, for example electrical measurements. The requirements of both the TEM/SEM and CXDI experiments must be met. In terms of sample dimensions and available space, the requirements are different for both techniques. Hence, there is need for two experimental setups to allow comparison between both experiments. For scanning nano-XRD investigations a dedicated ME setup was designed in the last funding period, but was found to be insufficient for the more exacting CXDI experiments demanding the development of a new setup. The samples will be probed for magnetic structure variations under deformation stresses using the Lorentz TEM technique. Here, the preliminary works on the functional grid platform during the first funding period will be extended to alternate deformation modes, like torsion. This development will be beneficial for the understanding of the strain distribution in WP3 and will give new insight into the structure of magnetic samples under mechanical load. This WP will also lead to the development of novel *in situ* stressing devices for SEM (Figure A6-9) with respect to subtle bending of TMD materials and electrical probing. In case of SEM the STEM detector of our Zeiss SEM is available in order to detect changes in the defect structure upon deformation by characteristic diffraction contrast. In this case, the dimensions of the thin structures to be deformed are comparable to those of the advanced XRD and in specific for CXDI mechanical stress experiments.

Figure A6-9: Schematic of an *in situ* straining device with electrical contacting via micromanipulators in the SEM. The TMD materials are contacted onto a flexible membrane which can be strained to probe the electrical characteristics.

WP5: *In operando* strain imaging

Bringing the strain investigations on the sensor components closer to the biomagnetic sensing applications is the goal of this WP and is central to the CRC objective. This will be achieved by investigating the *operando* behavior by means of nano-XRD, CXDI, ptychography and *ex situ* TEM investigations. The composites we plan to investigate are piezotronic driven sensors with (aero-)GaN and aero-ZnO being the piezo material. These novel materials were already topic of preliminary TEM examination, cf. Figure A6-10a [Ti19] for aero-GaN. In contrast to WP3, where the strain distribution in nanoscale samples is the main research topic, in this WP we want to investigate the magnetic field dependent behavior of the samples. For this challenging approach we will map the strain distribution and its variation under magnetic stimulus. Our preliminary *in operando* investigations using the CXDI technique on ZnO microcrystals coated with a ferromagnetic layer are presented in Figure A6-10b, showing minute variations in the magnetic field induced strain distribution. To benefit from the better understanding of the strain distribution obtained in WP3, we will expand our investigations of the samples to *in operando* measurements. The samples will be produced in Kiel and then brought to the finest synchrotron sources in the world (e.g. PETRA III, ESRF, APS) to perform the *in operando* studies. In a first step the novel composites of aero materials (A5) will be studied at high resolution in their pristine state with TEM for morphology, chemical integrity, defects and strain distribution at the interfaces of the components. Particular focus is on the internal interfaces of FeCoSiB coated aero materials and the magnetic structure of FeCoSiB in contact with aero-GaN or aero-ZnO. Next, Nano-XRD will be applied offering great design flexibility of the samples and yielding good average information on the samples response in magnetic fields with a great strain resolution and a spatial resolution that is defined only by the beam size of the beamline. Preliminary electrical investigations in Kiel (Figure A6-10c) show a dramatic change in the current-voltage plot for an applied magnetic field so a considerable strain response is expected. This will be beneficial for the understanding of the strain behavior. From the first funding period of this CRC we gained great experience in handling microscopic samples and gathered experimental routine with nano-XRD and CXDI analysis. The ptychography technique will enable investigations to another scale. Overall, these *in operando* investigations will give further insight into the *operando* response of local strain behavior, and so, enable a deeper understanding of the strain behavior and by this improve the performance of the sensors that is hugely depending on the mechanical properties and dynamics of the sensors.

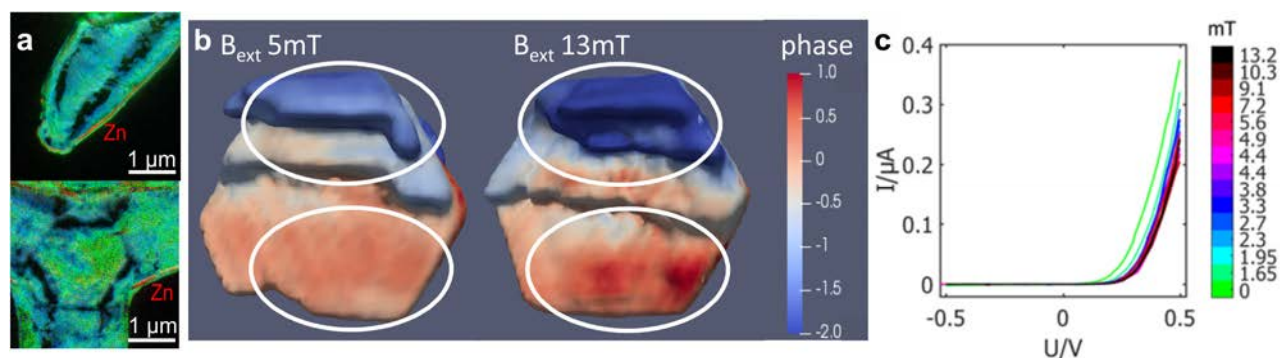


Figure A6-10: a) Energy filtered TEM images of aero-GaN tetrapods showing the interface stabilization of residual ZnO with GaN surviving extreme hydrothermal conditions. b) Reconstructed phase images of CXDI measurements of strain fields in ZnO crystals using the (0002) Bragg reflection, partially coated with magnetostrictive FeCoSiB on the bottom edge to induce a bending with applied magnet field. For probing an external magnetic field of 5 mT and 12 mT was applied. In cross-section, the delineation into negative and positive phase output is visible on opposite faces of the ZnO crystal which increase in total value with respect to the applied magnetic field strength. The induced magnetostrictive strain in the FeCoSiB is transferred into the ZnO crystal resulting in an anisotropic bending describing compressive and tensile strain along the crystal. c) Piezotronic response of rod described in b. The I-V response is shown as a function of increasing magnetic field.

WP6: Synergy of TEM & XRD

The synergy of TEM and XRD is well suited for multiscale analyses; however, to boost the field of nanoanalytics in general a strategy has to be developed for merging the different experimental data. In a first step cross-over data has to be identified which enables to overcome the barrier in-between atomic scale (TEM) and micronscale (XRD) examination. For example diffuse (X-ray or electron) scattering may provide cross-over data in the case of low-dimensionally ordered (e.g. TMD) crystals. In order to derive structural models

for diffuse scattering data the examinations may start at the atomic scale (TEM) to provide a first atomistic model of disorder. This model can be extended to larger scales by crystallographic simulation [Pr97, Sc18] or supercell approaches, thus, enabling further scaling for simulation of the relevant spectroscopic and/or X-ray data. Consequently a prediction of the large-scale experimental results from nanoscale analytics would be accessible. Complementarily it will be also possible as indicated in Figure A6-11, to go the other way around, i.e., starting from large scale information, like data from Raman spectroscopy, to determine simulation-assisted models of defects and their density. These models are refined according to suitable cross-over data to find coincidence in between simulated and experimental data obtained from very differently sized samples.

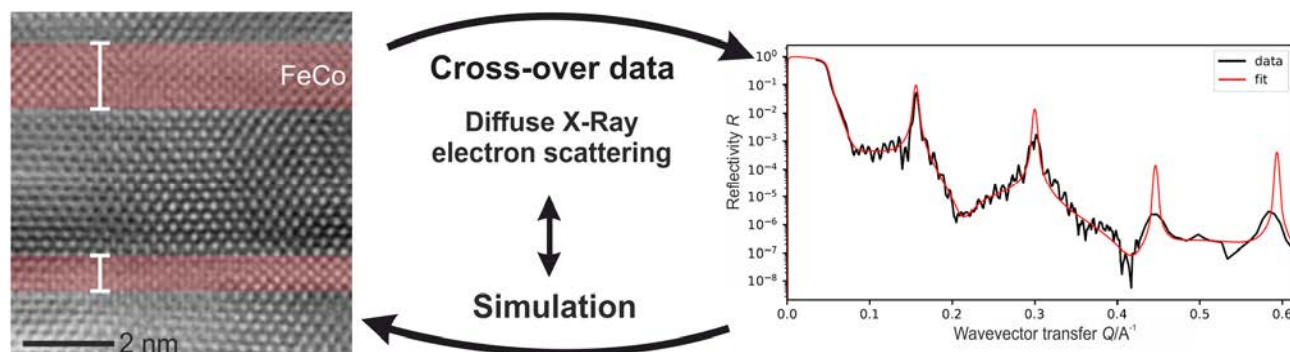


Figure A6-11: Scheme for the synergetic combination of TEM and X-ray methods providing multiscale information. Left: Imaging of defect structure in multilayers FeCo/TiN by STEM, right: reflection-broadening in XRR data with simulated data.

Prospects

A6 represents the competence center for advanced structural and chemical studies. Novel methods and synergistic combinations will be applied for detailing real structure property relations. Thus, a fundamental understanding of sensor function on atomistic level can be provided and the knowledge-based improvement of diverse sensor designs is made available. As a vision we intend to broaden and upgrade our synergistic approach by including modern atomistic simulations, like DFT which have to be linked to the specific cutting-edge experiments (e.g. EELS). Moreover we intend to establish novel imaging techniques for electron microscopy, like Phytography, which require hardware presently unavailable in Kiel. Combining modern XRD and PDF methods along with TEM and 4D-STEM RDF we will be able to characterize all components crystalline and amorphous, of ME sensors providing a holistic view of the structure and strain in fabrication and operation. Developing these methods within this project will further the understanding of the function of ME devices and contribute to knowledge based improvements in ME sensors.

3.5 Role within the Collaborative Research Centre

The unique combination of synchrotron based techniques and atomically resolved electron microscopy enables us to analyze the piezotronic devices (**A5**) as well as the multilayer materials from **A1** on all relevant length scales, *ex situ*, *in situ* and *operando*. **A6** develops new and advanced examination methods in close collaboration with these projects. Moreover, **A6** establishes the competence center for advanced nanoanalytical research within the CRC. In order to identify new scientifically demanding tasks which cannot be foreseen at the present date, **A6** also provides preliminary examinations for several other projects, particularly **A2**, **A7**, **A9**, **A10** and **Z1**. Additional characterization of samples that is not part of the work packages will be performed by permanent staff, e.g. of the TEM center (Dr. Schürmann). Scheduled tasks are at the moment:

- A1:** Investigation of nanoscale structure properties of various multilayer systems
- A2:** Nanoscale analysis of sensor components
- A5:** Strain and structure in piezotronic devices
- A7/9:** Structural characterization of piezoacoustic and magnetostrictive components, e.g. AlScN, FeCoSiB
- A10:** Input of morphological parameters for description of suitable submodels
- Z1:** Advanced characterization of sensor materials to improve fabrication technology

The major goal of these experiments is to understand the role that structure and stress play in sensor performance from the atomic scale to grain size to microscopic sample size. By understanding these key parameters via XRD and TEM studies, we can work towards knowledge-based sensor design. In addition, we

aim to develop micro and nanostructure analysis by achieving a united approach of these powerful structural determination methods.

Project **A6** will participate in the focused research groups “Magnetic Layers” and “Magnetoelectric Sensors”.

3.6 Differentiation from other funded projects

None of the currently funded projects of the applicants is related to the present scope of magnetoelectric sensing.

3.7 Project funding

3.7.1 Previous funding

Funding of this project within the Collaborative Research Centre 1261 started in July 2016.

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/2	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Postdoctoral re-researcher, 100 %	1	36	1	72	1	72	1	72	1	36
Doctoral re-researcher, 75 %	1	24.90	1	49.80	1	49.80	1	49.80	1	24.90
Total		60.90		121.80		121.80		121.80		60.90
Direct costs	Sum		Sum		Sum		Sum		Sum	
Consumables	6.50		13.00		13.00		13.00		6.50	
Specific travel costs	2.60		3.10		3.10		3.10		0.50	
Total	9.10		16.10		16.10		16.10		7.00	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Total	-		-		-		-		-	
Grand total	70.00		137.90		137.90		137.90		67.90	

(All figures in k€)

3.7.3 Requested funding for staff for the new funding period

	Sequen- tial no.	Name, aca- demic de- gree, posi- tion	Field of research	Department of university or non-university institution	Project commitment in hours per week	Category	Funding source
Existing staff							
Research staff	1	Kienle, Lo- renz, Prof. Dr., Profes- sor	TEM	IMS	4		Core support
	2	Murphy, Bridget, PD Dr., Group Leader	XRD	IEAP	4		Core support
	3	Schürmann, Ulrich, Dr., Senior Re- searcher	TEM	IMS	4		Core support

Non-research staff	4	Stettner, Jochim, Dr., Senior Researcher	Solid State Physics	IEAP	2		Core support
	5	Giri, Rajandera, Dr. Post doc. Researcher	XRD	IEAP	2		Core support
	6	Szillus, Christin, Technician		IMS	4		Core support
	7	Greve, Matthias Dipl. Ing., Technician		IEAP	2		Core support
Requested staff							
Research staff	8	Niklas Wolff, Postdoctoral Researcher	TEM	IMS		E14	
	9	N.N. Doctoral Researcher	XRD	IEAP		E13 75 %	

Job description of staff (supported through available funds):

- 1., 2. Prof. Kienle and Dr. Murphy will design the joint TEM and XRD experiments with particular emphasis on the methodologically challenging *in situ* observation tasks. Both will represent the project internally and externally.
1. Prof. Kienle will participate in data evaluation and TEM experiments. He is the supervisor of the Postdoc working on the TEM subproject as well as the accompanying bachelor's and master's theses.
2. Dr. Murphy will apply for X-ray beamtime at external research facilities and will participate in these experiments personally. She is the supervisor of the PhD candidate working on the XRD subproject as well as the accompanying bachelor's and master's theses.
3. Dr. Schürmann is the coordinator of the TEM center Kiel. He will perform preliminary examinations and service for the project as specified in section 1.5.
4. Dr. Stettner: Development and support of the X-ray diffractometer laboratory source.
5. Dr. Giri: Participation in the data collection at the synchrotron beamlines.
6. Mrs. Christin Szillus is responsible for the maintenance of the TEM preparation labs. She will introduce and support in advanced TEM preparation techniques, particularly FIB.
7. M. Greve: Technical support for development and construction of sample environment, for the laboratory X-ray source and for the LISA diffractometer at PETRA III.

Job descriptions of staff for the proposed funding period (requested funds):

8. An experienced postdoctoral researcher with detailed knowledge about state-of-the-art electron microscopy and data evaluation is required. Niklas Wolff is presently in the final stage of his doctoral project; the disputation is scheduled for May 2020. Besides experimental work in Kiel, he will apply with Prof. Kienle for TEM beamtime at external research facilities and will conduct these experiments. He will prepare the results for publication in scientific journals and will present them on international conferences. The ambitious project goals require detailed knowledge and experience about the material systems and methods, and, the project plan provides the chance for further qualification, e.g. in terms of habilitation.
9. The Ph.D. researcher will design and build the *in situ* X-ray piezotronic apparatus and will carry out experiments on nanocomposites and model sensor systems in the laboratory and at the synchrotron, analyze data, and will prepare the results for publication in scientific journals.

3.7.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/2
Funds available*	3.00	6.00	6.00	6.00	3.00
Funds requested	9.10	16.10	16.10	16.10	7.00

(All figures in k€)

Project-specific travel costs (per year)	2020/2	2021	2022	2023	2024/1
4 trips for 2 people to DESY, Hamburg (8 days) For the experiments at PETRA III beamline P02/P03/P10 funding is required as it is not covered by DESY (per person 450 € for housing, 50 € for traveling)	0.50	1.00	1.00	1.00	0.50
2 trips for 2 people to APS USA (6 days) we plan one run each year at the APS (per person 1000 € for housing, flight 1100 €)	2.10	2.10	2.10	2.10	0

(All figures in k€)

The experiments at third-generation hard X-ray synchrotron sources are central to this project. Experiments require 24 h shift operation and the presence of at least 2 researchers at the experiment at any time, because of the complexity of the studies (parallel operation of diffractometer, 2D detectors, piezotronic measurements). Previous experiences show that a minimum of 4 researchers with experience in the procedures are necessary for these studies. These will be the Ph.D. student and three other scientists of the Murphy group. Typically, 2 to 4 experimental runs consisting of 1 day of experimental preparation and 3 days of SXRD studies are planned per project year.

TEM beamtime at the TEM center of the Faculty of Engineering, CAU: the TEM center is listed within the RIsources (RI = Research Infrastructure) portal operated by the German Research Foundation, cf. http://risources.dfg.de/detail/RI_00354_de.html. Calculated costs for the beamtime (including TEM preparation via FIB, consumables like chemicals for TEM preparation, TEM grids etc.) are based on the statutes of the TEM center (Tecnai F30, cf. <http://srs.matwis.tf.uni-kiel.de/temzentrum/satzung>):

(80 hours à 85 € = 6.8 k€) in total and per year = 6.8 k€

Chemicals, substrates (additional to those provided by Z1, A1 and A5)	2 k€
Evaporation materials and targets	0.7 k€
Sample supports for X-ray experiments, including grids for cross section samples, capillaries for nanowires, disposable stretching cells	3 k€
Lab consumables and tools for sample preparation and mounting (silver glue, forceps, vacuum spare parts, etc.)	0.5 k€

Total 6.2 k€

Equipment up to k€ 10, software, consumables for 2020/2

TEM beamtime, FIB preparation and consumables	k€	3.4
Samples, sample holders, materials and tools for X-ray experiments	k€	3.1

Equipment up to k€ 10, software, consumables for 2021

TEM beamtime, FIB preparation and consumables	k€	6.8
Samples, sample holders, materials and tools for X-ray experiments	k€	6.2

Equipment up to k€ 10, software, consumables for 2022

TEM beamtime, FIB preparation and consumables	k€	6.8
Samples, sample holders, materials and tools for X-ray experiments	k€	6.2

Equipment up to k€ 10, software, consumables for 2023

TEM beamtime, FIB preparation and consumables	k€	6.8
Samples, sample holders, materials and tools for X-ray experiments	k€	6.2

Equipment up to k€ 10, software, consumables for 2024/1

TEM beamtime, FIB preparation and consumables	k€	3.4
Samples, sample holders, materials and tools for X-ray experiments	k€	3.1

3.7.5 Requested funding for instrumentation for the new funding period

None

3.1 General information about research project A7

3.1.1 Project Title: Electrically modulated magnetoelectric sensors

3.1.2 Research areas:

3.1.3 Principal investigator(s)

Quandt, Eckhard, Prof. Dr.-Ing.
05.04.1960

Inorganic Functional Materials
Institute for Materials Science
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Do the above mentioned persons hold fixed-term positions? No

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no

3.2 Summary

Research of the first funding period has shown that electrically modulated mesoscopic ME composites, targeting especially high frequency mechanical resonances, far higher than flexural modes, lead to dramatically enhanced converse ME effect. This is observed by vibrometry as well as in-situ MOKE studies. Exciting high frequency resonances of an ME composite immersed in an inductor while matching the inductive self-resonance to the mechanical resonance provides intrinsic amplification towards the converse ME effect, thus forming an overall resonant circuit. This resonant circuit proves very sensitive to external magnetic fields: 215 pT/Hz^{1/2} are obtained at DC, reaching 73 pT/Hz^{1/2} at 10 Hz. The use of magnetostrictive (MS) materials involving sophisticated exchange bias leads to even lower detection limits of 30 pT/Hz^{1/2} at 10 Hz. As high frequency resonances typically undergo less damping than flexural modes, high mechanical quality factors are readily reached at ambient pressure. The combination of high frequencies and high mechanical quality factors leads to increased available sensing bandwidth on the order of several hundred Hertz, suitable to biomagnetic as well as deep brain stimulation (DBS) application requirements.

The work of the second funding period will be focused on deriving a comprehensive signal-to-noise model of the electrically modulated ME sensor. The work on the model will be performed in close collaboration with modelling and characterization (**A8**, **A10**, and **B1**). More detailed objectives are to investigate the influence of (1) the homogeneity of the resonance mode, (2) the nature of the magnetization reversal processes, (3) the orientation of the easy axis, and (4) the resonance frequency of the U mode on the signal and the noise of these sensors. Finally, the influence of the size of the sensor on its overall performance will be investigated, as many biomagnetic applications require a high spatial resolution.

3.3 Research rationale

3.3.1 Current state of understanding and preliminary work

In project A7 the active electric excitation of magnetoelectric (ME) composites is chosen in contrast to exploitation of the direct ME effect. This direct ME effect, being of completely passive nature, shows severe drawbacks when the composite is subject to magnetic fields out of mechanical resonance, thus suffering from narrow bandwidth and thus limited applicability to real biomagnetic signals. Furthermore, $1/f$ noise limits direct detection when entering the frequency regime of biomagnetic interest.

According to the obtained results, this chapter contains the following sub-chapters:

- 1.) Electric frequency conversion mimicking magnetic frequency conversion (MFC)
- 2.) Exciting high frequency resonances
- 3.) Inductive readout of electrically excited ME sensors
- 4.) Electrically excited ME sensors using exchange bias multilayers

3.3.1.1 Electric frequency conversion mimicking magnetic frequency conversion (MFC)

The motivation for this research was to show whether the successful but energy-consuming and frequency limited magnetic frequency conversion (MFC) (A1) [A7-7] can be miniaturized by electric frequency conversion (EFC). This was achieved by ME composites having two piezoelectric layers: one for the excitation, one for the detection. The results reveal that EFC is possible [A7-10, A7-4] and that mixing occurs in the magnetostrictive layer excited via inverse magnetostriction by the piezoelectrically induced stress. As a consequence, linear piezoelectric materials, e.g. AlN, are usable as the excitation layer. This was demonstrated for the first bending mode, and has shown that even under high excitation amplitudes, only the region close to the clamping of the cantilever contributes to the output signal. This use of two PE phases is patented under [A7-P1]. Characterization was performed with a specifically built optical beam deflection set-up that employs a linear optical system to obtain the time domain data of the cantilever motion under excitation [A7-9]. This was also used to investigate thermal-mechanical noise of cantilevered composites [A7-8]. Signal-to-noise investigations for different orientations of the magnetic easy axis showed the superior behavior of the 90° orientation (with respect to the long cantilever axis) and lead to a strongly reduced noise in the vicinity of the mechanical resonance.

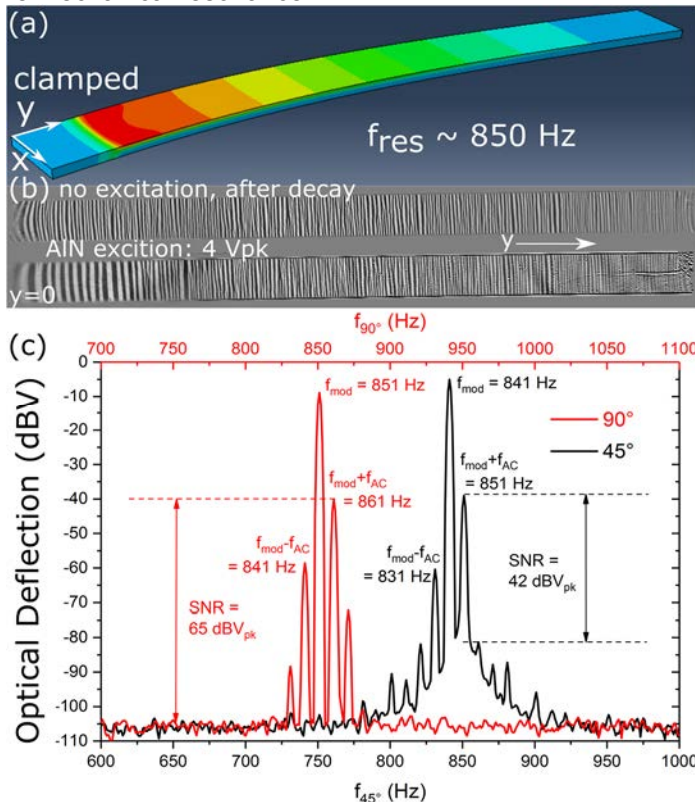


Fig. A7-1: Magnetoelastic behavior of the first flexural mode. (a) FEM simulation indicating stress concentration near the clamping. The stress is very inhomogeneous and leads to a strong peak near the clamping. Red indicates strong stress magnitude. (b) Static MOKE images of unexcited FeCoSiB layer after demagnetization and for resonantly excited cantilever by PE. A significant domain width modulation occurs near the clamping of the cantilever at high excitation voltages. (c) Cantilever tip deflection frequency spectrum obtained by FFT of time data. The two traces stem from cantilever composites having 90° as well as 45° anisotropy orientation to their long axis. Both were excited slightly below their 1st flex. resonance, in order to fulfill the condition of $f_{\text{mod}} + f_{\text{AC}} = f_{\text{res}}$. Sidebands next to the PE-applied driving voltage, termed carrier (f_{mod}), indicate the mixing with the 10 Hz magnetic test signal (f_{AC}). The sidebands at $f_{\text{mod}} + f_{\text{AC}}$ are largest in amplitude because they coincide with the resonance (f_{res}) of the composite. The composite holding 90° magnetic orientation shows far less noise around f_{mod} .

3.3.1.2 Exciting high frequency resonances

As EFC was shown to be possible, the next step was to investigate cantilevers that fulfill the requirements, especially regarding the sensor's bandwidth. Very low frequency DC operation was readily shown to be enabled [A7-5, A7-3]. Depending on the application, the bandwidth should be between at least twenty and a few hundred Hertz, and as an electric modulation scheme is utilized, the use of much higher frequencies becomes attractive. Furthermore, high frequency resonance modes are advantageous as they are less sensitive to acoustic noise and vibrations. Depending on the specific mode shape, they are furthermore less affected by air damping, thus providing higher mechanical quality factors Q . Considering rather high quality factors of around 1000 [A7-5] and a bandwidth defined by the resonance frequency divided by $2Q$, the resonance frequency required for broadband magnetic detection is in the hundreds of kHz regime.

Fig. A7-2 shows a mechanical displacement spectrum between 300 and 700 kHz recorded by a Polytec (UHF-120) vibrometer at the IFW Dresden. In this frequency range, many out-of-plane resonance excitations can be observed, while the so-called U1 and U2 modes show by far the largest amplitudes (log scale). A detailed representation of these two modes is shown in Fig. A7-2a,b. Both show a strong curvature along the short axis of the cantilever, in the U1 mode monotonically increasing towards the free end of the cantilever, while the U2 mode shows maximum curvature at about 30% of the free length and a nodal point at about 70 % of the free length.

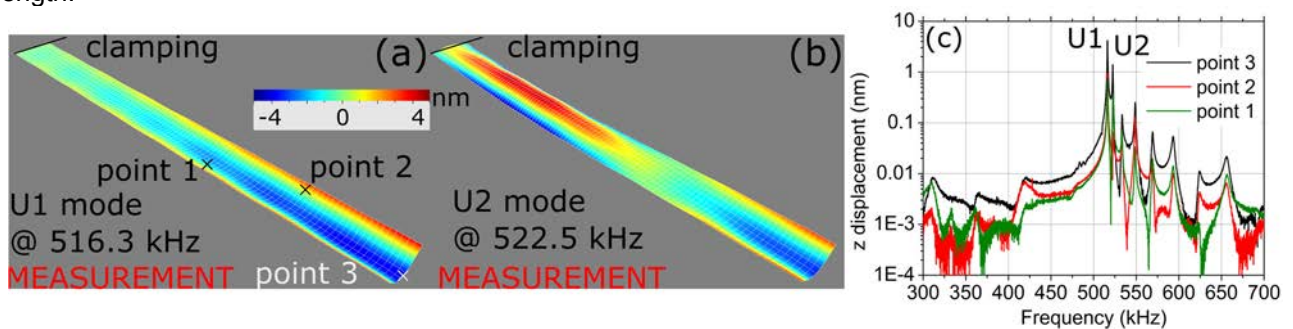


Fig. A7-2: Mechanical U modes, characterized by strong curvature along the short cantilever axis. (a) U1 mode, monotonic curvature of same phase, strongest curvature at the far end of the cantilever. (b) U2 mode, exhibiting a nodal point at about 70% of the free length, strong anti-phase curvature near clamping and at the free end. (c) Mechanical out-of-plane displacement spectra for three different points on the cantilever surface. A variety of peaks corresponding to mechanical activity are present. The strongest mechanical activity by far is present for U1 and U2 modes.

Thin 150 μm borosilicate glass, exhibiting an elastic modulus about 2.5 times lower than that of silicon, offers excitability of all low order flexural modes with a simple full length electrode. The U modes were also successfully excited and exploited under high drive conditions, showing nonlinearities [A7-6]. Furthermore, the U modes were patented for application as magnetic field sensor under [A7-P2].

3.3.1.3 Inductive readout of electrically excited ME sensors

A research stay in the group of Prof. Fetisov in Moscow has led to the application of a pick-up coil to replace the second PE phase for the converse ME readout, as shown in Fig. A7-3. While electrically exciting a linear PE phase, the readout is performed involving a pick-up coil, which monitors magnetic flux (θ) changes of its MS core. This approach is widely adopted within the thick film ME composites community; there the coil is tightly wrapped around the resonator [Wa16], [Fe14] as to make up two of the four ports for either excitation or readout. Very early studies used a similar concept for bulk samples [Me86], [Me92], obtaining values down to 8 pT/Hz^{1/2} at 1 Hz for samples of several centimeters in size. Using thin film composites in conjunction with coils is a rather novel, hybrid approach. In this case, we chose a polymeric bobbin holding the coil that leaves the resonator mechanically unaffected, as it is free to oscillate within the coil.

Pickup coils for the readout have different advantages, such as low noise, the possibility to use the coil self-resonance as an amplifier, and a bandpass filter before A/D conversion. Furthermore, the coil offers advantages in design freedom but disadvantages in terms of integration and miniaturization. The coil advantages are specifically beneficial if used for high frequency flux changes, as the induced voltage scales with frequency by $V_{ind} \propto \frac{d\theta}{dt}$. The intrinsically very low noise essentially only consists of Johnson noise of $\sim 1 \text{ nV/Hz}^{1/2}$ for a DC winding resistance of 50 Ohm. Coils in combination with highly sensitive magnetic field sensors are well known: In parallel fluxgates, which use two coils around a magnetic core to magnetically excite and readout the signal at a harmonic frequency [Pri79]. This, however, typically requires large amounts of energy for periodic saturation of the core by an Oersted field. Search coil magnetometers (SCM), on the contrary, work entirely passive and require only one coil winding with a vast number of turns, as huge

inductance values are required to be sensitive to low frequencies; thus, SCMs are prohibitively bulky [Ro08]. More details can be found in chapter 1.2.3.2.

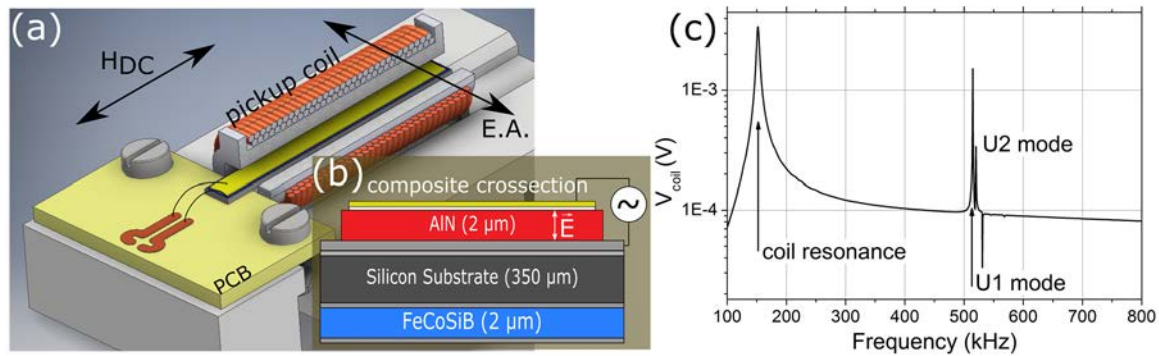


Fig. A7-3: Schematic setup for converse ME readout. (a) The ME cantilever is fixed to a piece of PCB board using cyanoacrylate adhesive, and wire bonding is used to contact top and bottom electrodes. The PCB board is fixed to the holder using polymeric screws. An external magnetic field is applied along the long axis of the assembly (H_{DC}), orthogonal to the induced magnetic easy axis (E.A.). (b) Cross-sectional view of typical composites. The top side of a Si substrate hosts the PE layer, the dielectric in a plate capacitor structure. On the bottom side of the silicon substrate, the MS layer is deposited [A7-5]. (d) Spectrum taken by means of the pickup coil; at about 150 kHz the coil self-resonance, at about 515 kHz and 520 kHz, U1 and U2 modes, respectively.

With the frequency regime 100 kHz...800 kHz covered by exciting the piezoelectric material and using converse ME pickup coil readout, the self-resonance of the pickup coil is visible at about 150 kHz and merely the two distinct U-mode oscillations are present in the coil output spectrum. These findings are compiled in Fig. A7-3c.

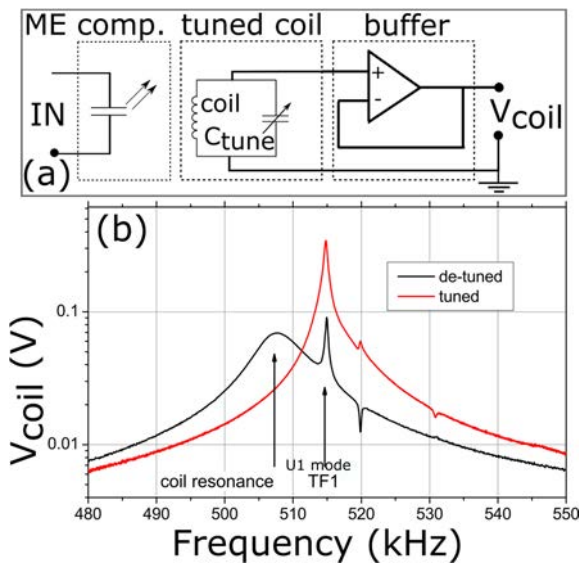


Fig. A7-4 (a) The circuit depicting the ME composite as a radiative capacitor structure. The signal is induced in the resonant coil, and the current is buffered by a low noise unity gain buffer amplifier. C_{tune} is a trimmer capacitor used for matching the coil self-resonance to the mechanical resonance. (b) Frequency response analysis. Pickup coil self-resonance ($Q \sim 150$) and mechanical resonance frequency ($Q \sim 1000$), denoted U1. In the de-tuned and tuned cases in order to maximize voltage output of the sensor.

The coil self-resonance, which is of much lower quality factor, is exploited to amplify the converse ME voltage response of the system. The coil self-resonance frequency f_r is given by $f_r = \frac{1}{\sqrt{LC}}$, L being the inductance and C the parasitic capacitance. By means of a small tuning capacitor (C_{tune}) parallel to the coil, the coil self-resonance can be shifted downwards and thus matched to the mechanical resonances, which leads to large intrinsic amplification of the signal without adding additional magnetic noise. Fig. A7-4a shows the schematic system composed of composite, tuned coil, and its unity gain buffer amplifier. The effect of coil tuning can be seen in Fig. A7-4b, apart from the strongly de-tuned case of Fig. A7-3c where the U modes show up far to the right of the coil resonance. The tuned system proves to be very sensitive towards external AC and DC magnetic fields (H), as a magnetic field sweep in Fig. A7-5a shows. By exciting the PE material in its U1 resonance mode at 80 mV, an external field leads to dramatic modulation of the coil voltage (V_{coil}). At high magnetic fields above about 3 Oe, the material magnetically saturates, and the induced voltage drops to zero. Upon increase of the magnetic field, the induced voltage reaches a maximum at about 0.5 Oe; although this is the point of highest induction, the working point is given by the derivative of the curve, effectively relating voltage to applied field.

Fig. A7-5b shows a zoom-in view of the low field regime around zero. Here the sensitivity is maximum, reaching 40 kV/T, and highly symmetric with direction of saturation [A7-1]. It furthermore illustrates the working principle: as a magnetic field is applied to this transfer curve, the

coil voltage amplitude is raised or lowered depending on the sign of the external field, giving rise to amplitude modulation of the voltage signal. For this, the external magnetic signal should have a frequency much smaller than the carrier. The exact upper corner frequency is determined by the bandwidth of the mechanical resonance.

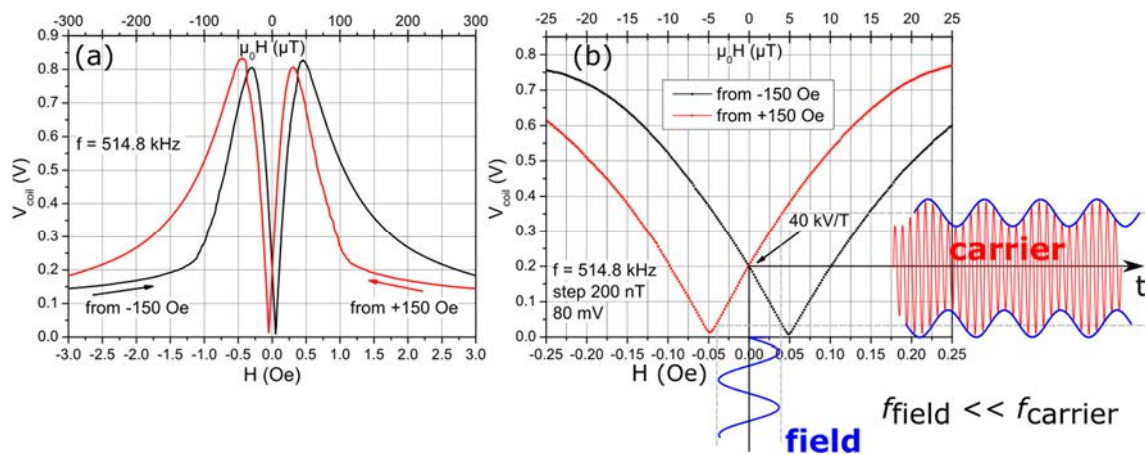


Fig. A7-5: Coil voltage after the buffer amplifier and at resonant driving of U1 mode with an amplitude of 80 mV with respect to an externally applied field H . a) Maximum induced voltage reaches above 800 mV at a field of 45 μT , coming from opposite saturation. At high external fields, the induced voltage drops to near zero. Towards zero field, the induced amplitude decreases dramatically down to zero at coercivity, where a phase reversal occurs at a field of 5 μT . b) Close-up revealing maximum field sensitivity of 40 kV/T at zero bias field, as well as a schematic signal transfer of a low frequency magnetic field signal giving rise to amplitude modulation of the output signal.

Fig. A7-6a relates the magnetic field sensitivity to the applied carrier voltage. The sensitivity scales nearly linearly with increasing carrier amplitude. This behavior is counteracted by a strong noise increase accompanied by increasing carrier amplitudes. Fig. A7-6b reveals that, at a certain amplitude threshold—in this case about 200 mV—the noise in the vicinity of the carrier (below about 20 Hz, see inset) is vastly increased for a composite consisting of 2 μm single layer FeCoSiB.

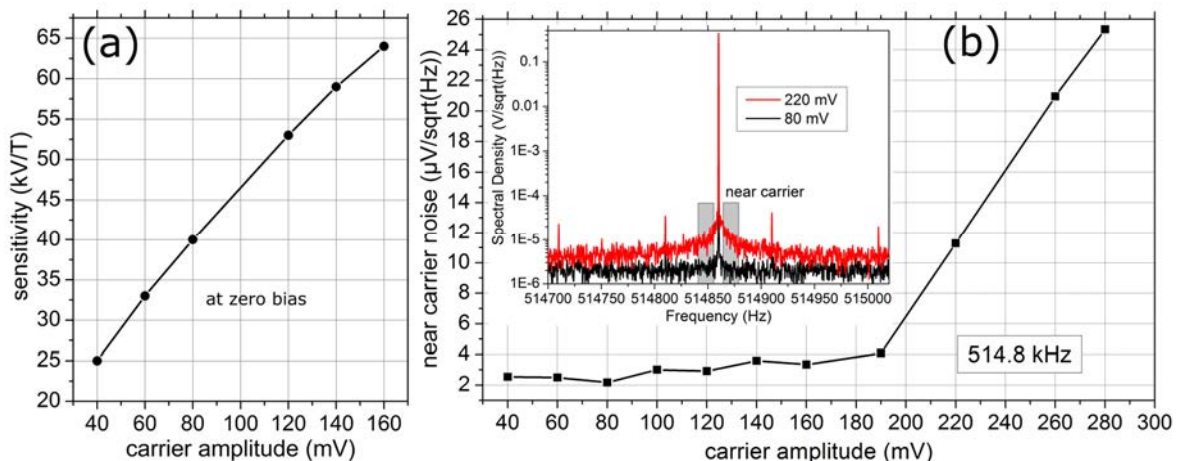


Fig. A7-6: Converse ME Sensitivity and noise behavior of composites employing simple FeCoSiB as MS phase. (a) The sensitivity scales almost linearly with excitation amplitude. (b) Noise in the low frequency regime near the carrier increases step-like at a certain level of excitation, which limits overall performance despite increasing sensitivity. (inset) Near-carrier noise shown for two different carrier amplitudes [A7-1].

However, when choosing a suitable balance of sensitivity and noise and after saturating the sensor composite appropriately, such a composite can reach very low LOD values. This is demonstrated in Fig. A7-7a, where 10 Hz and 23 Hz sinusoidal test signals of 1 nT amplitude are applied to the modulated composite. Visible are the sidebands symmetrical to the carrier peak that stem from the amplitude modulation. Calculating the sensitivity by dividing the sideband amplitude by the known applied magnetic field yields a linear sensitivity of 30.4 kV/T. Subsequent division of the near-carrier noise by the sensitivity yields an LOD of about 75 $\text{pT}/\text{Hz}^{1/2}$

at a frequency of 10 Hz. However, an improved LOD of below $55 \text{ pT/Hz}^{1/2}$ at a frequency of 53 Hz, due to lower noise present at larger offset frequencies, is shown in Fig. A7-7c.

3.3.1.4 Electrically excited ME sensors using exchange bias multilayers

When employing more complex exchange biased multilayer MS material, the near-carrier noise is significantly suppressed even at high excitation amplitudes. When choosing a material with a high exchange bias field (H_{EB}), the noise as well as the sensitivity is lowered. A study using moderately biased MS material, by tuning the FeCoSiB thickness and keeping the biasing layer constant, results in a performance compromise between lowering noise while maintaining high sensitivity.

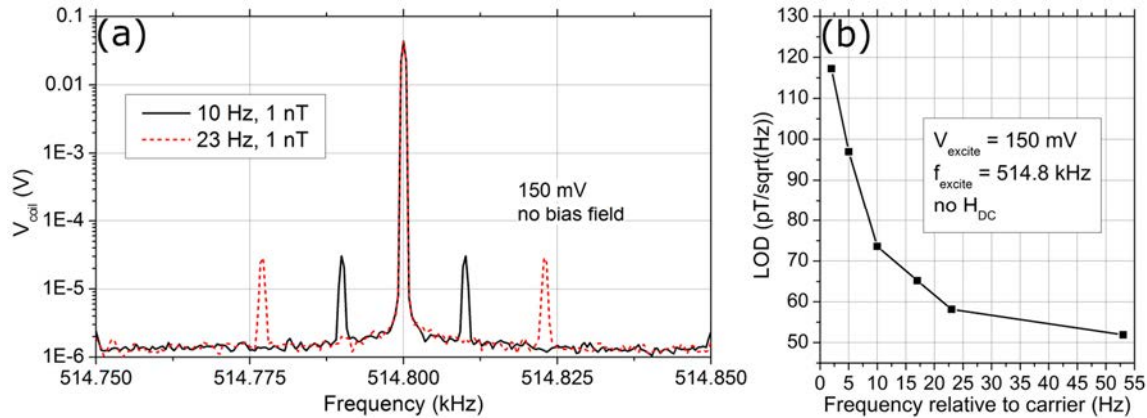


Fig. A7-7: Spectral representation taken from the pickup coil amplifier. (a) Low frequency magnetic signals of 10 Hz and 23 Hz applied with an amplitude of 1 nT. Sidebands around the carrier result from amplitude modulation. (b) Limit of detection (LOD) for different test frequencies. An exponential growth in noise towards the carrier limits the performance.

Fig. A7-8 shows results of such an antiparallel exchange biased (APEB) FeCoSiB stack of $4 \mu\text{m}$ total thickness under the same modulation conditions. This is demonstrated by the sidebands resulting from a 10 Hz as well as a 160 Hz sinusoidal test signal of 2 nT amplitude, indicating a wideband flat LOD of about $30 \text{ pT/Hz}^{1/2}$ at 10 Hz as well as 160 Hz. This advanced EB layer stack and its fabrication have been published [A7-2].

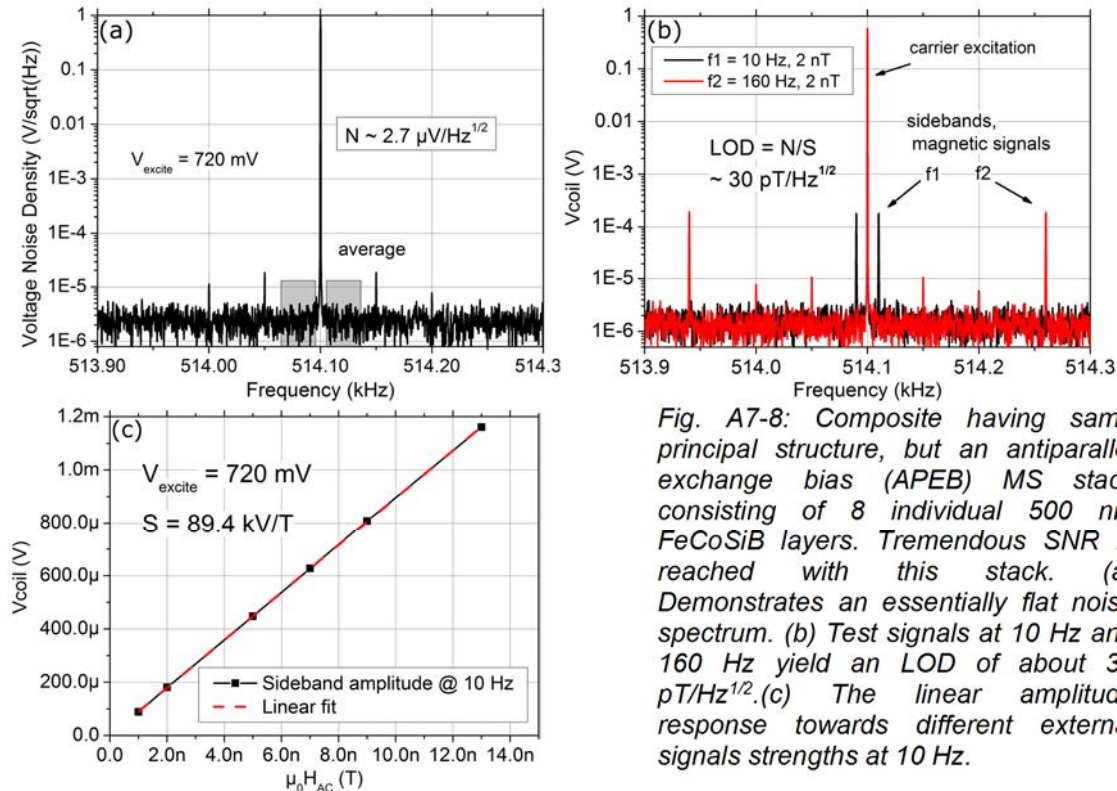


Fig. A7-8: Composite having same principal structure, but an antiparallel exchange bias (APEB) MS stack consisting of 8 individual 500 nm FeCoSiB layers. Tremendous SNR is reached with this stack. (a) Demonstrates an essentially flat noise spectrum. (b) Test signals at 10 Hz and 160 Hz yield an LOD of about $30 \text{ pT/Hz}^{1/2}$. (c) The linear amplitude response towards different external signals strengths at 10 Hz.

Results from this sensor for DC measurements in the time domain is displayed in Fig. A7-9. In this experiment, the applied DC magnetic field was changed stepwise by 2 nT every 5 s. Considering that the signal stepwise change leads to a sensitivity of 50 kV/T, relating the noise density to the sensitivity achieves an LOD of 40 pT/Hz^{1/2}.

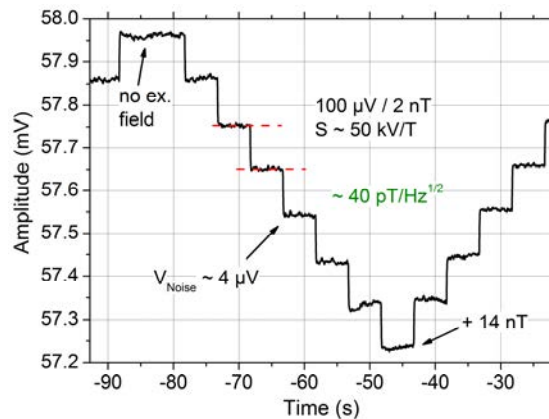


Fig. A7-9: Magnetic staircase signal response, a DC magnetic field step of 2 nT is changed in staircase fashion every 5 seconds. The coil voltage at the modulation frequency changes, giving rise to a DC sensitivity of 50 kV/T. The standard deviation on the steps is about 4 μV; while taking into account the noise equivalent bandwidth of the lock-in amplifier, the noise is estimated to be 2 μV/Hz^{1/2} and results in a LOD of 40 pT/Hz^{1/2}.

References

- [Fe14] Y. K. Fetisov, D. A. Burdin, D. V. Chashin, N. A. Ekonomov, High-Sensitivity Wideband Magnetic Field Sensor Using Nonlinear Resonance Magnetolectric Effect. *IEEE Sensors J.* 14, 2252–2256 (2014), doi:10.1109/JSEN.2014.2309718.
- [Kr10] K. Kratt, V. Badilita, T. Burger, J. G. Korvink, U. Wallrabe, A fully MEMS-compatible process for 3D high aspect ratio micro coils obtained with an automatic wire bonder. *J. Micromech. Microeng.* 20, 15021 (2010), doi:10.1088/0960-1317/20/1/015021.
- [Me86] M. D. Mermelstein, Magnetoelastic amorphous metal fluxgate magnetometer. *Electronics Letters.* 22, 525–526 (1986), doi:10.1049/el:19860358.
- [Me92] M. D. Mermelstein, A magnetoelastic metallic glass low-frequency magnetometer. *IEEE Trans. Magn.* 28, 36–56 (1992), doi:10.1109/20.119814.
- [Pri79] F. Primdahl, The fluxgate magnetometer. *J. Phys. E: Sci. Instrum.* 12, 241, doi:10.1088/0022-3735/12/4/001.
- [Ri10] P. Ripka, M. Janosek, Advances in Magnetic Field Sensors. *IEEE Sensors J.* 10, 1108–1116 (2010), doi:10.1109/JSEN.2010.2043429.
- [Ro08] A. Roux, O. Le Contel, C. Coillot, A. Bouabdellah, B. de la Porte, D. Alison, S. Ruocco, M. C. Vassal, The Search Coil Magnetometer for THEMIS. *Space Sci. Rev.* 141, 265–275 (2008), doi:10.1007/s11214-008-9455-8.
- [Sa59] G. Sauerbrey, Verwendung von Schwingquarzen zur Wägung dünner Schichten und zur Mikrowägung. *Z. Physik.* 155, 206–222 (1959), doi:10.1007/BF01337937.
- [Ta15] A. Tavassolizadeh, P. Hayes, K. Rott, G. Reiss, E. Quandt, D. Meyners, Highly strain-sensitive magnetostrictive tunnel magnetoresistance junctions. *Journal of Magnetism and Magnetic Materials.* 384, 308–313 (2015), doi:10.1016/j.jmmm.2015.01.083.
- [Wa16] J. Wang, *Multiferroic Materials, Properties, Techniques, and Applications* (CRC Press, Milton, 2016).
- [Ya16] E. Yarar, V. Hrkac, C. Zamponi, A. Piorra, L. Kienle, E. Quandt, Low temperature aluminum nitride thin films for sensory applications. *AIP Advances.* 6, 75115 (2016), doi:10.1063/1.4959895.

Project-related publications

a) Articles published by outlets with scientific quality assurance

- [A7-1] P. Hayes, M. Jovičević Klug, S. Toxværd, P. Durdaut, V. Schell, A. Teplyuk, D. Burdin, A. Winkler, R. Weser, Y. Fetisov, M. Höft, R. Knöchel, J. McCord, E. Quandt, Converse Magnetolectric Composite Resonator for Sensing Small Magnetic Fields. *Scientific reports.* 9, 16355 (2019), doi:10.1038/s41598-019-52657-w.
- [A7-2] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. D. Toxværd, M. Höft, R. Knöchel, E. Quandt, D. Meyners, J. McCord, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors. *Appl. Phys. Lett.* 114, 192410 (2019), doi:10.1063/1.5092942.
- [A7-3] C. Tu, Z.-Q. Chu, B. Spetzler, P. Hayes, C.-Z. Dong, X.-F. Liang, H.-H. Chen, Y.-F. He, Y.-Y. Wei, I. Lisenkov, H. Lin, Y.-H. Lin, J. McCord, F. Faupel, E. Quandt, N.-X. Sun, Mechanical-Resonance-Enhanced Thin-Film Magnetolectric Heterostructures for Magnetometers, Mechanical Antennas, Tunable RF Inductors, and Filters. *Materials.* 12 (2019), doi:10.3390/ma12142259.

- [A7-4] D. Viehland, M. Wuttig, J. McCord, E. Quandt, Magnetoelectric magnetic field sensors. *MRS Bull.* 43, 834–840 (2018), doi:10.1557/mrs.2018.261.
- [A7-5] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yarar, A. Piorra, R. Knöchel, Y. K. Fetisov, E. Quandt, Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing. *J. Phys. D: Appl. Phys.* **51**, 354002 (2018), doi:10.1088/1361-6463/aad456.
- [A7-6] Y. K. Fetisov, D. A. Burdin, N. A. Ekonomov, L. Y. Fetisov, A. A. Berzin, P. Hayes, E. Quandt, Bistability in a multiferroic composite resonator. *Applied Physics Letters*. 113, 22903 (2018), doi:10.1063/1.5032182.
- [A7-7] V. Röbisch, S. Salzer, N. O. Urs, J. Reermann, E. Yarar, A. Piorra, C. Kirchhof, E. Lage, M. Höft, G. U. Schmidt, R. Knöchel, J. McCord, E. Quandt, D. Meyners, Pushing the detection limit of thin film magnetoelectric heterostructures. *J. Mater. Res.* 32, 1009–1019 (2017), doi:10.1557/jmr.2017.58.
- [A7-8] P. Durdaut, S. Salzer, J. Reermann, V. Robisch, P. Hayes, A. Piorra, D. Meyners, E. Quandt, G. Schmidt, R. Knochel, M. Hoft, Thermal-Mechanical Noise in Resonant Thin-Film Magnetoelectric Sensors. *IEEE Sensors J.* 17, 2338–2348 (2017), doi:10.1109/JSEN.2017.2671442.
- [A7-9] N. O. Urs, B. Mozooni, P. Mazalski, M. Kustov, P. Hayes, S. Deldar, E. Quandt, J. McCord, Advanced magneto-optical microscopy. *AIP Advances*. **6**, 55605 (2016), doi:10.1063/1.4943760.
- [A7-10] P. Hayes, S. Salzer, J. Reermann, E. Yarar, V. Röbisch, A. Piorra, D. Meyners, M. Höft, R. Knöchel, G. Schmidt, E. Quandt, Electrically modulated magnetoelectric sensors. *Appl. Phys. Lett.* **108**, 182902 (2016), doi:10.1063/1.4948470.
- b) Issued Patents**
- [A7-P1] Hayes, P., Knöchel, R., Piorra A., **Quandt, E.**, Magnetoelktrische Magnetfeldmessung mit Frequenzumsetzung, EP 15 170 985.
- c) Pending Patents**
- [A7-P2] Hayes, P., Toxwaerd, S., Knöchel, R., **Quandt, E.**, Messvorrichtung für schwache, langsam veränderliche Magnetfelder, insbesondere für biomagnetische Felder, DE 10 2019 116 779.5.

3.4 Research Plan

Objectives

The research in the first funding period has revealed that:

- (1) electric frequency conversion, where the sum of the frequency of the electric excitation and the frequency of the magnetic field to be measured (e.g. 10 Hz) matches the resonance frequency of the sensor, is possible and leads to an improvement compared to direct detection out-of-resonance [A7-10];
- (2) the frequency mixing occurs in the magnetic phase, and thus excitation by a linear piezoelectric material (e.g. AlN) is possible [A7-9];
- (3) the sensitivity, the bandwidth, and the LOD can be significantly improved by using higher frequency resonances, especially the so-called U-mode resonances (at about 500 kHz) [A7-5];
- (4) using these higher resonances requires a different read-out scheme, as the bandwidth of this resonance already includes the biomagnetic relevant frequencies (0-100 Hz);
- (5) a pick-up coil readout [A7-1] results in a better LOD than a piezoelectric readout, which is probably a consequence of the high frequency (approx. 500 kHz) of the U-mode resonance;
- (6) internal amplification can be achieved by matching the pick-up coil electrical resonance to the mechanical resonance frequency [A7-4];
- (7) a significant improvement can be obtained by using antiparallel exchange biased multilayers, which were developed in **A1** for magnetic frequency conversion [A7-2]
- (8) for a fixed excitation strength, only part of the sensor contributes to the signal (Fig. A7-14).

Based on these findings, the working hypotheses for the continuation of this sensor approach are as follows:

- (1) A constant stress distribution over the sensor area or at least within the pick-up coil will enhance the effect size and potentially reduce magnetic noise.
- (2) Magnetization changes by pure rotational processes instead of domain wall motion will reduce magnetically induced noise.
- (3) As the U-mode leads to a periodic change from tensile to compressive stress, a tilted magnetic easy axis should lead to rotational changes of the magnetization for both stress states, and thus enhance the effect size.
- (4) Enhancing the resonance frequency should lead – as predicted by Sauerbrey for mass loading [Sa59] – to an enhancement in sensitivity but with unknown consequence on the noise.

As the main objective, the experiments testing these four hypotheses will be used to derive a comprehensive signal-to-noise model of the electrically modulated ME sensor. The work on the model will be performed in close collaboration with modelling and characterization (**A8**, **A10**, and **B1**). More detailed objectives are to investigate the influence of (1) the homogeneity of the resonance mode, (2) the nature of the magnetization reversal processes, (3) the orientation of the easy axis, and (4) the resonance frequency of the U mode on the signal and the noise of these sensors. Finally, the influence of the size of the sensor on its overall performance will be investigated as many biomagnetic applications require a high spatial resolution.

Proposed research methods

Fabrication of ME sensors

The sensors will be fabricated starting from a process flow, which was developed for the preliminary experiments [A7-5], [Fig. A7-10]:

- (1) Double side polished (DSP) Si substrates holding 1500 nm thermal oxide, with a nominal thickness of 350 μm were used as substrates; sputter deposition of 10 nm Ti followed by 100 nm Pt is used for seeding purposes.
- (2) Pulse DC sputter deposition of 2 μm of aluminium nitride (AlN) followed by a deposition of a top electrode formed by sputtered Cr/Au to enable good wire bonding and prevent corrosion.
- (3) Photolithography and subsequent wet chemical etching of Au/Cr by potassium iodine/iodine (KI/I₂) solution, followed by chromium etching by a ceric ammonium nitrate-based solution at room temperature. By electrical continuity tests, the complete removal of conductive chromium residuals is verified. Due to high selectivity of the etchants, no etch stop is required. The AlN etch is performed by using H₃PO₄ at 80 °C for about 20 min.
- (4) To prevent short circuits across the etched sidewalls of the AlN layer, the top electrode is offset by 50 μm in this step; this leads to vastly increased yield. Essentially the same Au/Cr etching from step (3) is done using a narrower mask, keeping the AlN layer.
- (5) Ta/FeCoSiB/Ta is sputter deposited on the smooth backside of the wafer. About 10 nm of tantalum below the FeCoSiB act as an adhesion promoter, and about 5 nm tantalum on top of the FeCoSiB act as oxidation barrier on the top, still permitting magneto-optical investigations of the layer.
- (6) A lithography step of the FeCoSiB using thick, thermally stable resist is necessary; afterwards the layer is etched via Ion Beam Etching (IBE). To ensure the conservation of the amorphous state, cooling pauses are introduced during etching. The endpoint of this etch is detected via a secondary ion mass spectrometry (SIMS) when the Ta and Si signals rise.
- (7) Dicing into cantilever dies is performed by cutting between the layer stacks.

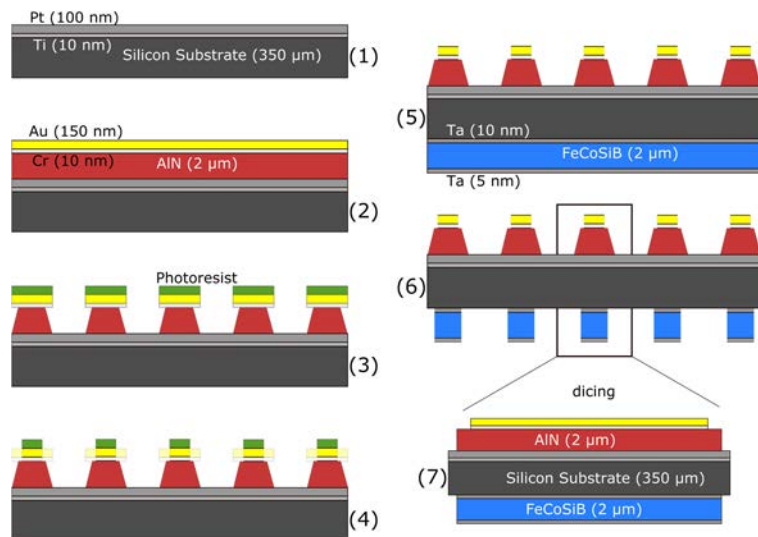


Fig. A7-10: Schematic process flow. (1) DSP Si substrate with oxide, (2) deposition of Ti/Pt/AlN followed by Cr/Au as top electrode on the front. (3) Lithography and wet chemical etching of Cr/Au followed by AlN etch by hot H₃PO₄. (4) Second lithography: narrowing of the AlN layer preventing short circuits, and (5) RF sputter deposition of Ta/FeCoSiB/Ta on the back side. (6) IBE patterning of the FeCoSiB strips. (7) Dicing into individual sensors.

Fabrication of pick-up coil

Coil bobbins are CAD designed and subsequently additively manufactured from polylactide polymer. Subsequent winding with solid enameled or litz copper wire of 100 μm thickness is performed with an automation-assisted winding setup facilitating an integrated winding counter, which was developed in **Z2**.

Functional and structural characterization

The structural characterization of the piezoelectric films will be done by X-ray diffraction (Rigaku SmartLab 9kW), by scanning electron microscopy (Zeiss, Zeiss Ultra Plus), and by transmission electron microscopy using a Tecnai F30 STwin microscope (300 kV, field-emission gun) by **A6**. Compositions will be determined

by energy-dispersive X-ray analysis (EDX). The evaluation of the dielectric and piezoelectric properties at near DC conditions will be carried out by a double beam laser interferometer (aixACCT DBLI).

Dynamic electrical parameters of the ME resonators as well as the pickup coils are determined using an impedance analyser (HP 4395A). For dynamic mechanical measurements, a vibrometry system available at Fraunhofer ISIT will be used. MOKE imaging, static as well as time resolved, is planned in close cooperation with project **A10**. Magnetic hysteresis curves will be recorded by vibrating sample magnetometry (VSM) using a LakeShore model 7300 system. The magnetostrictive properties will be measured in a custom-built cantilever deflection setup, which is also capable of monitoring the time-resolved deflection of the ME cantilever tip. This enables DC magnetostrictive measurements, i.e. cantilever deflection vs. slowly varied magnetic field. Furthermore, the possibility for measurement of the piezomagnetic coefficient is given by adding a small magnetic AC component to the slowly varying DC magnetic field and thus optically probing the slope of the magnetostriction curve. For the measurement of direct magnetoelectric properties, an electromagnet will be used to generate a DC bias field while a pair of Helmholtz coils will generate an AC magnetic field for the measurement.

A lock-in amplifier triggered by the driving-field frequency will be employed to obtain the magnetoelectric response. For the measurement of the noise voltage density spectrum, the output of the sensor will be connected to a battery-powered low noise amplifier in an electrically and magnetically shielded environment. The overall noise from the sensor and the amplifier will be measured with an HF2LI high frequency lock-in amplifier from Zurich Instruments in electrically and magnetically-shielded conditions. The required magnetic test signals are supplied using AC and DC calibrated cylindrical coils connected to low noise precision AC and DC current sources by Keithley, Model 6221. The LOD will be determined at the output of the low noise amplifier by using the high frequency lock-in amplifier, whereas the built-in signal source will be used to apply the carrier signal. These measurements will be performed in collaboration with **B1** and **Z2**.

Work plan

Following the general objective and the related working hypotheses, the work program is structured into six work packages, which are summarized in the work schedule in Tab. A7-1:

Table A7-1: Work schedule

		2020		2021				2022				2023				2024	
		3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2
WP 1	SNR model																
WP 2	Magnetostrictive Material																
WP 3	Resonator design																
WP 4	Pick-up coil																
WP 5	Combination																
WP 6	Miniaturization																

WP1: SNR model of electrically modulated ME sensors

This WP1 reflects the main objective: to derive a comprehensive understanding of the factors determining the signal and the noise of electrically modulated ME sensors. Thus, it will run for the whole second funding period, and on the one hand, will include data from all the other work packages (WP 2 – WP 6), while on the other hand, will guide the individual research focuses of these work packages. WP1 will be performed in close collaboration with **A8** on the resonance modes and the coil design, and with **A10** on modelling and characterization of the magnetic noise. Cooperation is planned with **B1** on phenomenological system noise analysis for all other possible noise sources, including the excitation source noise, preamplifier noise, noise introduced by the pickup coil, acoustic noise, and A/D quantization noise.

An important experimental approach will be to measure the spatially resolved contributions of the sensor to the overall sensor performance by using a coil set-up developed by **Z2** in the first funding period (s. Fig. A7-14). For the important contribution of magnetically induced noise, this spatially resolved data can be compared to local MOKE characterization performed in **A10**. To determine and verify the extent and importance of certain noise sources, a simultaneous magnetic imaging and recording of induced noise is envisioned with either a small single coil or a Helmholtz pickup coil in a collaboration of **A7**, **A10**, and **Z2** including vibrational as well as magnetic characterization. We will primarily employ an optical beam deflection setup suitable for magnetostriction as well as piezomagnetic coefficient measurement which was built in the first period. The electrically modulated ME sensors investigated are characterized at the most appropriate working point in

terms of the electrical modulation amplitude and, if necessary, the magnetic bias field. For this work, the procedure will be used as described in the section “Research methods”.

WP 2: Investigation of the magnetostrictive component

Comparison of single layers and exchange biased multilayers

As in almost all ME sensor concepts, the noise contribution related to magnetic noise of the magnetostrictive phase limits the low frequency LOD of these sensors. According to the working hypothesis, the *in operando* noise of a single layer material with domain wall activity and an APEB multilayer [A7-2] with practically only rotational magnetization changes will be characterized and compared in collaboration with **A1**. This will be complemented by a full functional characterization of the corresponding sensors as described in the section “Proposed research methods”. Especially, it is expected that by identifying the underlying processes which lead to two noise regimes in single layer materials (compare Fig. A7-6b) and by understanding the impact of exchange biasing on the overall performance, deriving the specifications for an adapted MS layer system for the A7 sensor concept will be possible. It is noticeable that various APEB multilayers result in very different sensor performance. Preliminary results in Fig. A7-11 indicate that larger exchange bias fields strongly degrade the sensor sensitivity, and thus a compromise between noise suppression and effect size has to be found. The development and fabrication of these low strength EB films specifically is done in collaboration with **A1**.

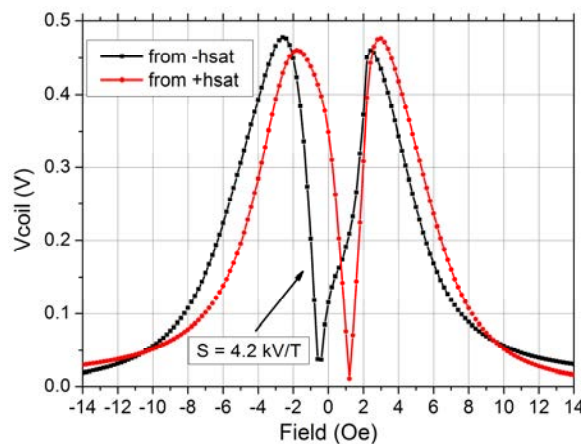


Fig. A7-11: Induced voltage vs external magnetic field for a strongly exchange biased composite. The highest slope is achieved at a working point of -1 Oe, reaching 4.2 kV/T for an excitation voltage of 100 mV. Although the noise floor is very low, at about 1.2 $\mu\text{V}/\sqrt{\text{Hz}}$, the lack of sensitivity outweighs the low noise behavior, leading to an LOD of about 280 pT/Hz^{1/2}. A simple unbiased composite shows about three times more noise, but nearly tenfold sensitivity, compare Fig. A7-5b.

This work package is a cooperation with **A1**. Furthermore, it will include investigations on the overall thickness and thus volume of the MS component. It seems to be straight forward to assume that the effect size will increase with the thickness of the layer, and hence it is important to evaluate the influence of the film thickness on the magnetic noise in collaboration with **A10** (modelling and characterization). Increasing the film thickness may readily lead to a decrease of mechanical Q factor of the resonator as the fraction of the more dissipative magnetic material is increased. This effect needs also to be studied.

Investigation of the orientation of the magnetic easy axis

The U modes periodically change from compressive to tensile stress in the MS film along the cantilever's principal axis (compare Fig. A7-2a,b). Hence, a magnetic easy axis (E.A.) directed along an axis of, e.g., tensile stress would not result in any rotational magnetization change, as the orientation is already optimal. Thus, for example, an orientation of the E.A. with an angle of 45° to the cantilever's short axis would provide an arrangement sensitive to both orthogonal stress directions. A similar concept was successfully applied in previous work on stress-sensitive tunnel magnetoresistive sensors [Ta15] as well as in AMR technology [Ri10]. This work will investigate the performance of fabricated sensors as a function of the E.A. orientation, which is set during thermal field annealing with **A1**, and furthermore will include measurements to determine the directional characteristics of the sensors by applying magnetic fields in a 3D Helmholtz coil setup in collaboration with projects **B1** and **Z2**.

WP 3: Resonator design

(1) Resonator geometry

Simulations on the full sensor structure, including the active layers, will be carried out in cooperation with **A8**. The experimental investigation of the U-mode resonances (compare Fig. A7-2a) reveals that the stress acting on the magnetostrictive film is strongly dependent on the position along the cantilever's long axis. This should lead to an inhomogeneous effect in the pick-up coil. The idea is to improve the overall response by homogenizing the local stress distribution for a given excitation. This can be tailored by the mounting for the resonator but also by the design of the resonator itself. Fig. A7-12 shows as an example a few preliminary

results on simulations for different fixtures of the resonators which show U-mode resonances occurring and exhibiting more homogeneous stress distribution.

This work package will include simulations of different sensor designs, the fabrication of these sensors, and a fully functional characterization of the sensor performance including the experimental verification of the resonance mode. The results will be evaluated with respect to the single-side clamped cantilevers exhibiting the U1-mode, shown in Fig. A7-2a. If possible, altered geometry is locally probed by a tiny pickup-coil such as given in **WP1**.

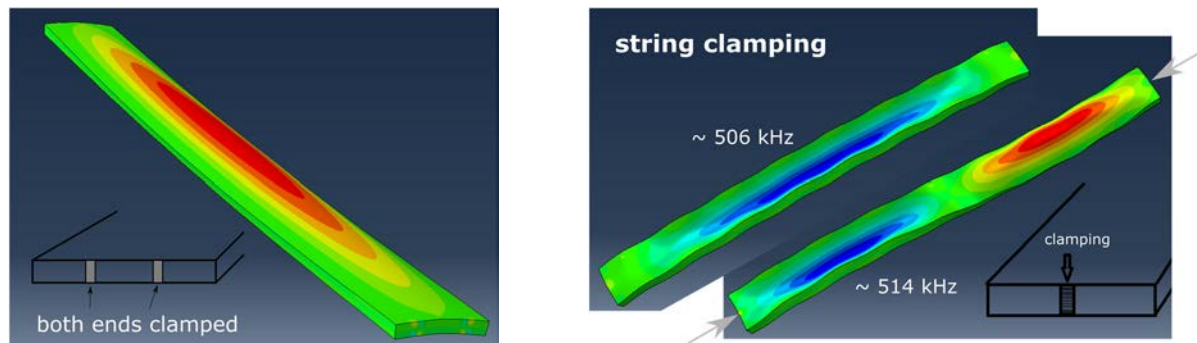


Fig. A7-12: FEM simulations of two mechanical clamping scenarios. Color coded is the stress magnitude, where blue and red are of opposite sign. (left) Cantilever clamped at the nodal points on its ends; a pure U mode with no nodal points is obtained, present at about 500 kHz. (right) Clamping the cantilever like a guitar string on the centers of its ends also leads to the formation of U modes, in-phase for U1 and anti-phase for U2.

(2) Investigation of the electrode design

For resonators with varying mechanical clamping configurations, the influence and efficiency of the piezoelectric excitation has to be evaluated. This is accomplished in the most straightforward manner by varying the top electrode design of the resonator. Practically, one equipotential bottom electrode is most suitable, as it also functions as a seed layer for the c-axis textured AlN growth [Ya16]. By patching the top electrode in an appropriate way suitable for efficient excitation of a specific mechanical mode, several variations are possible. As AlN is a linear piezoelectric material, not requiring electrical poling, push-pull configurations of two top electrode islands are possible in principle. The mode simulated in Fig. A7-12 (right) may require two electrode patches, tiled along the center and excited in an anti-phase manner, and thus specifically promoting this oscillation from an actuation point. Simulations involving such specific functional piezoelectric actuations are performed in collaboration with **A8**.

(3) Influence of the resonance frequency

Preliminary results show that the U modes are able to be excited in a variety of oscillator designs. Fig. A7-13 shows calculations of the frequency trend for varying widths and substrate thicknesses for cantilevered composites. The freestanding length did not show such a drastic influence. It is believed that by employing the modes at even higher frequencies, the sensitivity of the converse effect may even increase. For this purpose, different substrate materials and geometries are investigated in this package.

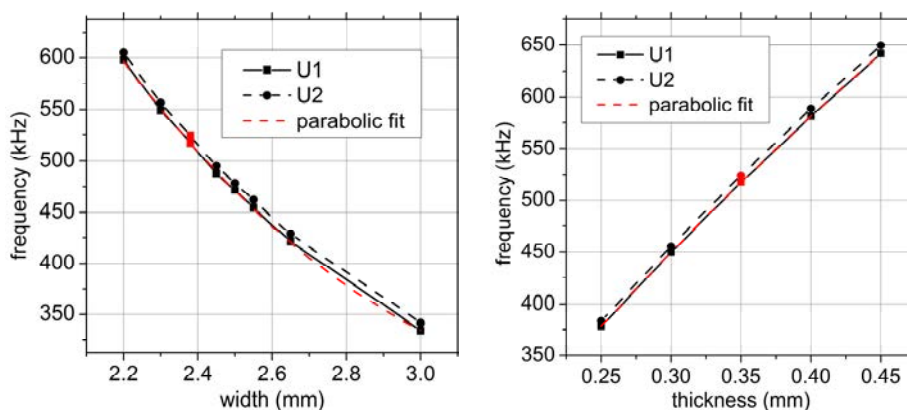


Fig. A7-13: FEM simulations showing the geometrical influences of cantilever width (left) and thickness (right) on U1 and U2 mode resonance frequencies. The red data points indicate experimental data.

As shown, with thick substrates, essentially only the signal amplitude is affected by small magnetic fields; frequency changes are below 0.1%. With thin borosilicate substrates, being mechanically much less compliant than thick silicon leads to strong phase and frequency modulation, as seen in preliminary studies probing for

such effects. The use of thick and narrow cantilever beams theoretically enables U modes up to a frequency of about 3 MHz without leaving the realm of wafer-cut composites.

WP 4: Investigation of the coil design

In mechanical modes of antiphase motion, the changes in magnetic flux in a single coil winding spanning the whole oscillator may lead to partial or perfect cancellation of the induced voltage signal. Preliminary studies show this case for the U2 mode in Fig. A7-14. A mechanical node in the oscillation leads to the induced voltage being antiphase; this results in partial cancellation of the voltage signal. In these cases, the use of segmented pickup coils is expected to yield an amplitude increase by either reversing partial windings or by separate amplification of partial windings and subsequent phase-correct adding of the partial signals.

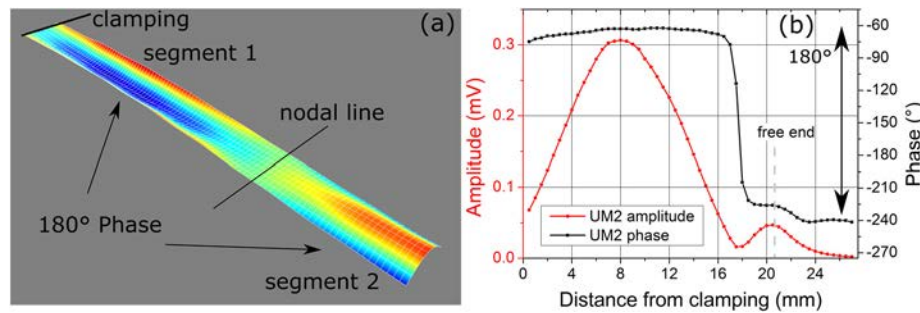


Fig. A7-14: Local induction measurement along the cantilever axis for U2 mode. (a) Vibrometry displacement measurement of U2 mode, color code indicating antiphase motion. (b) Locally induced voltage with a tiny slidable pickup coil along the cantilever axis. The tip region of the cantilever shows induced voltage with opposite phase.

The use of litz wire for the coil construction, especially for high frequencies, is anticipated to yield lower losses due to less AC resistance at medium wave frequencies in the conductor. By this, a gain of up to 30 % in coil quality factor is anticipated, which will yield more intrinsic amplification.

(1) Matching the resonance frequencies of coil and resonator

Fig. A7-4b showed that tuning the pick-up coil by a capacitor in order to match the pick-up coil resonance with the mechanical resonator resonance results in an amplification of the sensor output. A further increase is expected if the tuning is done by the inductance (number of turns) of the pick-up coil. This will be investigated for resonators with different resonance frequencies.

(2) Limiting the coil to the homogeneous part of the resonance mode

Vibrational analysis as well as modelling has revealed that in the present design, the single side clamped cantilever, the stress or deflection is highly inhomogeneous along the cantilever's long axis, Fig. A7-2a. The expectation is that limiting the extension of the coil to the homogeneous part in the case of the U1 mode or even taking two coils and compensating the 180° phase difference in the case of the U2 mode should enhance the signal and reduce noise created by different stress states in different parts of the resonator. The evaluation will include the use of a very small pick-up coil of sub-mm length to characterize the sensor's response with high spatial resolution. In such a set-up for local converse ME measurements, a tiny coil can be axially or transversely slid along the cantilever while recording frequency and amplitude sweeps. Especially local phase relations can be revealed with this tool in conjunction with a lock-in amplifier, which will aid coil design.

(3) Investigation on the filling factor

In the present design, the cross-sectional area of the coil is 32 mm², and thus the magnetic fraction (cross-section of the magnetic core: 0.005 mm²) is only 0.016 %. Within this work package approaches to evaluate and, if necessary, to increase the filling factor of the pickup coil will be studied. Simulations in conjunction with A8 should find an optimum filling factor. It is anticipated that the filling factor will have an effect on the sensitivity, but may keep the sensor signal-to-noise ratio unaffected.

WP 5: Combination of the approaches of WP 2 – 4

Based on, guided by, and included in the comprehensive SNR model of WP1, the tasks of the work packages WP2 to WP4 with regard to magnetic material, resonance mode and frequency, and pickup coil design were performed and evaluated independently. The task of this work package is now the combination of the most promising approaches. In some cases, this will require new solutions because, for example, the coil design will depend on the resonator lay-out, which might also have an influence on the choice of the magnetic layer system.

Besides the approach of combining the most promising findings of WP 2 - 4 into a sensor offering the best LOD, this work package will be explicitly used to evaluate and further improve the SNR model of WP1 via the experimental studies on the combined approaches. Finally, this work package will include redesigns of the electrically modulated ME magnetic field sensors based on modelling results obtained in **A8**, **A10**, and **B1**. The final “optimum” design and layout of this sensor will then be used in WP 6 for further miniaturization.

WP 6: Miniaturization of the sensors

Taking into account the results of the WP 1-4 in terms of the magnetic layer system, resonator and coil design concepts for miniaturization of these sensors using the bulk Si micromachining process of **Z1** will be investigated. The motivation of this work package is manifold: (1) Smaller sensors will increase the spatial resolution, (2) they are a prerequisite for sensor arrays planned for in the third funding period, and (3) they might offer a $\sqrt{N}$ improvement of the sensor performance if N sensors are used in parallel. This step is strongly dependent upon modelling results obtained by **A8** and **A10**. If modelling indicates that miniaturization of the sensors will degrade performance, then a branching will occur: arrays employing traditionally sized sensors and measurements of inhomogeneous field conditions to determine achievable spatial resolution are planned.

(1) Wafer-cut process

In this work package, the fabrication will be performed as described in Fig. A7-10 but with significantly reduced dimensions of the resonator, down into the mm regime. The full evaluation of the sensor performance, especially noise measurements with **B1**, will determine any possible dependence of the sensor performance on the overall size of the sensor.

(2) Bulk Si micromachining

Depending on the results of WP 1, this work package can be used for further miniaturization using and adapting the bulk Si micromachining process of **Z1**. Further challenges and tasks besides miniaturization are the full integration of the clamping (compare WP 3a) into the fabrication process and the transfer of the magnetostrictive layer concept (compare WP 2) to the different fabrication processes and the smaller overall dimensions. This work is an important prerequisite for any miniature sensor array fabrication which will be one of the major tasks of the third funding period. A method of fabricating small sub-mm coils is presented by [Kr10]: an air coil formed around an SU-8 photoresist bobbin. A modified wire bonder automatically fabricates these air inductors with microscopic to mesoscopic dimensions as required for this project. This step will only be investigated if the wafer-cut sensors show sufficient LODs. Otherwise, this partial WP will be used to determine the optimum compromise between sensitivity and special resolution based on wafer-cut sensors as described before.

Prospects

Electrically modulated ME sensors was a new topic started in 2016. It was based on successful work on magnetically modulated ME sensors [A7-7] and motivated by the much lower power consumption, less cross-talk between the sensors, and much higher possible resonance frequencies needed for higher bandwidth applications. This research was very successful and resulted in one of the most sensitive sensor concepts of the CRC, with properties similar to the best delta-E effect sensors (**A4**) or surface acoustic wave sensors (**A9**). They also profit very much from the work on magnetically modulated ME sensors, as the best results were obtained for APEB multilayers developed in **A1**.

Based on the present status and taking into account the envisaged improvements in the second funding period, it is very probable that these sensors can be used for many biomagnetic applications planned within the CRC. Consequently, the last 18 months of the second funding period will be spent on further miniaturization and integration, which is considered to be a prerequisite for sensor arrays. These sensor arrays will be the major task for the third funding period, which was already predicted in the funding proposal four years ago.

3.5 Role within the Collaborative Research Centre

The Collaborative Research Centre 1261 “Magnetoelectric Sensors: From Composite Materials to Biomagnetic Diagnostics” spans a wide range of projects: from materials research to sensor concepts to signal processing and finally to applications. Because this project deals with one of the sensor concepts, it is fully integrated within this research chain and we will have intense collaborations with materials research, sensor systems, and especially with the transfer project. Specifically, this sensor concept reaches all secondary requirements demanded by applications such as high bandwidth, acoustic immunity, and no required bias field, which makes it particularly relevant to **T1**.

- A1** Exchange biased multilayers
- A8** Modelling of the sensors

A10	Modelling of the noise, in operando MOKE measurements
B1	Analog electronics, noise floor characterization, LOD measurements
B2	If branching in WP6 occurs, multichannel acquisition and digital signal processing
T1	Support by using electrically modulated ME sensors for DBS measurements
Z1	Sensor miniaturization and fabrication, vibrometry measurements
Z2	Instrumentation and sensor characterization
A6	Microstructural characterization of deposited piezoelectric layers

3.6 Delineation from other funded projects of the principal investigator(s)

No other funded projects deal with magnetoelectric composites or magnetic field sensing.

3.7 Project funds

3.7.1 Previous funding

The project A7 was funded from 1.7.2016 – 30.6.2020.

3.7.2 Funds requested

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum
Doctoral researcher, 100 %	1	34.2	1	68.4	1	68.4	1	68.4	1	34.2
Total		34.2		68.4		68.4		68.4		34.2

Direct costs	Sum	Sum	Sum	Sum	Sum
Equipment up to k€ 10, software, consumables	4.5	7.0	8.0	8.0	2.5
Total	4.5	7.0	8.0	8.0	2.5
Total	4.5	7.0	8.0	8.0	2.5

(All figures in k€)

3.7.3 Staff

	No	Name, academic degree, position	Field of research	Department of university or non-university institution	Commitment in hours/ week	Category	Funded through:
Available							
Research staff	1.	Quandt, Eckhard, Prof. Dr.-Ing. Professor	Functional Materials	IMS	4		Core support
	2.	Malave, Antonio, Dr., Senior Researcher	Functional Materials	IMS	4		Core support
	3.	Meyners, Dirk, Dr., Senior Researcher	Functional Materials	IMS	2		Core support
Non-research staff	4.	Metzing, Thomas, Dipl. Ing., Technician		IMS	4		Core support
Requested							

Research staff	5.	N.N., Doctoral Researcher	Functional Materials	IMS		E13	

Job description of staff (supported through available funds):

1. Prof. Dr.-Ing. Eckhard Quandt is responsible for the coordination and the scientific management of the project A7 and represents the project within the CRC and to the outside. He advises the scientific staff in the planning and execution of the work within the project and in the interpretation of the obtained results.
2. Dr. Antonio Malave is the responsible scientist for the operation and maintenance of the Kieler Nanolabor. He will support the doctoral researcher on this project in the selection, planning, and execution of the MEMS processes.
3. Dr. Dirk Meyners, the Scientific Leader of the Kieler Nanolabor, will support the doctoral researcher in the realization of the thin film deposition processes, especially with the deposition and characterization of the magnetic thin film and multilayers.
4. Dipl.-Ing. Thomas Metzger will support the doctoral researcher in all issues regarding maintenance of different devices.

Job description of staff (requested):

5. The Doctoral Researcher will be in charge of the work packages as described in the proposal. She/he will closely collaborate with the Doctoral Researchers of the projects A1, A8, A10, B1, T1 and with the Postdoctoral Researchers of Z1 and Z2 (compare 3.5).

3.7.4 Direct costs

(All figures in k€)	2020/2	2021	2022	2023	2024/1
Funds available	1.5	3.0	3.0	3.0	1.5
Funds requested	4.5	7.0	8.0	8.0	2.5

Equipment up to k€ 10, software, consumables for 2020/2

Sensor processing consumables (photoresist, etching solutions)	k€	0.5
FeCoBSi target	k€	2.0
Standard and special silicon wafers	k€	1.0
Electronic consumables (for read-out electronics, coil, and characterization setups)	k€	1.0

Equipment up to k€ 10, software, consumables for 2021

Sensor processing consumables (photoresist, etching solutions)	k€	1.0
Lithography masks (a set of four for a redesign)	k€	2.0
Standard and special silicon wafers	k€	1.0
Targets (1x Al (8"))	k€	2.0
Electronic consumables (for read-out electronics, coil, and characterization setups)	k€	1.0

Equipment up to k€ 10, software, consumables for 2022

Sensor processing consumables (photoresist, etching solutions)	k€	1.0
Lithography masks (a set of four for a redesign)	k€	2.0
Single crystals (as alternative substrates of the resonator)	k€	4.0
Electronic consumables (for read-out electronics, coil, and characterization setups)	k€	1.0

Equipment up to k€ 10, software, consumables for 2023

Sensor processing consumables (photoresist, etching solutions)	k€	1.0
Lithography masks (a set of four for a redesign)	k€	2.0
SOI wafers (for miniaturization of sensors)	k€	3.0
Electronic consumables (for read-out electronics, coil, and characterization setups)	k€	2.0

Equipment up to k€ 10, software, consumables for 2024/1

Sensor processing consumables (photoresist, etching solutions)	k€	0.5
Electronic consumables (for read-out electronics, coil, and characterization setups)	k€	2.0

3.1 General information about Project A8

3.1.1 Project title: Modelling of Magnetoelectric Sensors

3.1.2 Research area(s):

407-02 Measurement Systems; 408-02 Theoretical Electrical Engineering

3.1.3 Project leader(s)

Gerken, Martina; Prof. Dr.
24.01.1973; German

Integrated Systems and Photonics
Institute of Electrical Engineering and Information Technology
Christian-Albrechts-Universität zu Kiel (CAU)
Kaiserstr. 2, D-24143 Kiel
Phone: +49 (0) 431 880 6250
E-Mail: mge@tf.uni-kiel.de

Is the employment of the project leader(s) at the institution(s) indicated contractually fixed for the duration of the proposed funding period? no

Do any of the abovementioned persons hold fixed-term positions? no

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

The aim of this project is a theoretical investigation of the behavior of magnetoelectric sensors and sensor arrays based on piezoelectric and magnetostrictive composite materials in inhomogeneous biomagnetic fields. In prior research, analytical and numerical methods for both static and resonant sensor operation were developed while a linearized small-signal behavior with constant material parameters was assumed. The signal-to-noise ratio is calculated by combining the methods with the noise model from **B1**. In the next funding period, the first research focus is on the modelling of surface-acoustic-wave (SAW) sensors (cooperation with **A9**) and electrically modulated cantilever sensors (cooperation with **A7**). Here, an aspect of particular importance is the development of methods for the numerical simulation of sensor geometries with high aspect ratios and anisotropic material properties. The simulation will be implemented by employing the finite element method (FEM). In numerical studies, geometry-dependent and material-dependent effects in magnetoelectric sensors will be evaluated with the aim of achieving better sensor performance. The second focus is on the modelling of magnetoelectric sensors and sensor arrays in inhomogeneous magnetic fields as they are found in biomagnetic applications. The deep-brain-stimulation system including sensors in a sensor array as well as the head properties will be investigated in a multiscale simulation (cooperation with **T1**). The aim is to determine the transfer function of the magnetoelectric sensor system as an input for solving the inverse problem. This project will collaborate closely on the sensor design with the groups in research area **A**. For the system aspects, it will be done in close cooperation with the corresponding projects in research area **B**.

3.3 Project progress to date

3.3.1 Report and current state of research

In the first funding period, a theoretical investigation of the behavior of magnetoelectric (ME) sensors as well as small arrays of these sensors was conducted. The objective was to develop simulation methods to calculate the behavior of resonant and non-resonant ME sensors and employ these to design sensors with a high signal-to-noise ratio (SNR) that are suitable for biomedical applications. The research was based on previously established analytic [Kr13] and numeric [Gu13, Ge13, Go12] simulation methods for calculating the small-signal behavior of ME sensors at the working point. Equations (A8-1) to (A8-3) present the coupled system of linearized material equations.

$$T_{ij} = c_{ijkl} S_{kl} - d_{kij} E_k - d_{kij}^m H_k \quad (\text{A8-1})$$

$$D_i = d_{ijk} S_{jk} + \epsilon_{ij} E_j \quad (\text{A8-2})$$

$$B_i = d_{ijk}^m S_{jk} + \mu_{ij} H_j \quad (\text{A8-3})$$

Here, $\mathbf{T}$ and $\mathbf{S}$ are the tensors of mechanical stress and strain, $\mathbf{E}$, $\mathbf{D}$, $\mathbf{H}$ and $\mathbf{B}$ are the field vectors of the electric field, the electric displacement, the magnetic field, and the magnetic flux density. They are coupled by the position-dependent material parameters (stiffness tensor $\mathbf{c}$, piezoelectric coefficient tensor $\mathbf{d}$, piezomagnetic coefficient tensor $\mathbf{d}^m$, permittivity tensor ϵ , permeability tensor μ). The direct ME effect may be neglected for the materials employed and is therefore not included in the equations. In a common approximation, the electric field $\mathbf{E}$ and the magnetic field $\mathbf{H}$ are derived from scalar potentials V and V_m as $\mathbf{E} = -\nabla V$ and $\mathbf{H} = -\nabla V_m$. Assuming furthermore that space charges and conduction currents are negligible [BI08], the behavior of ME sensors is described by Newton's second law (A8-4) and the Maxwell equations (A8-5) and (A8-6).

$$T_{ij,j} = \rho \ddot{u}_i; \quad i=1,2,3 \quad (\text{A8-4})$$

$$\nabla \cdot \mathbf{D} = 0 \quad (\text{A8-5})$$

$$\nabla \cdot \mathbf{B} = 0 \quad (\text{A8-6})$$

Here, $\mathbf{u}$ is the mechanic displacement vector connected to the strain tensor elements by $S_{ij} = (u_{i,j} + u_{j,i})/2$. ρ is the material density. Equations (A8-4) to (A8-6) present a system of five coupled differential equations for the five variables u_1 , u_2 , u_3 , V , and V_m (with directions $x=1$, $y=2$, and $z=3$).

Two types of sensors were investigated in detail – resonant cantilever-type sensors and surface acoustic wave (SAW) sensors. The SAW sensor modelling was performed instead of ΔE -effect sensor modelling in agreement with A4. In A4, a theoretically interested doctoral researcher was employed who conducted the ΔE theoretical study. This allowed the investigation of the highly promising SAW sensor concept here. Numerical studies were carried out on small sensor arrays of 3x1 sensors considering homogeneous and inhomogeneous magnetic excitation fields. These studies revealed that the ME sensor behavior in an inhomogeneous excitation field is much more complex than in homogeneous excitation fields with long-distance interactions between sensors due to magnetic field concentration effects. A point-sensor approximation is not valid for mm- to cm-sized ME sensors in biomagnetic fields. In the following, the research results on resonant cantilever sensors, SAW sensors, and sensor arrays are presented in detail.

We developed analytic methods for calculating the behavior of strain-coupled ferroic composite cantilevers operated in resonance-enhanced bending. Here, we considered single magnetic domain magnetostrictive layers and magnetostrictive exchange bias multilayer stacks in different stacking schemes with piezoelectric and substrate layers. Eddy currents [He97] are the dominating loss mechanism in thick magnetostrictive layers. Support losses are important but may be prevented by fixing the cantilever in nodes of the bending mode instead of fixing it at one end. Models for noise sources [Ja13, A8-4] are implemented, including Johnson-Nyquist noise from dielectric losses in the piezoelectric layer and capacitances in the preamplifier and other amplifier-intrinsic noise as well as thermal vibrations [Sa97, Du17]. Most models were extended to include higher vibration modes for cantilevers with one fixed end and one free end as well as cantilevers with free-free boundary conditions supported in the vibration mode nodes. In addition, segmented electrodes were investigated to collect strain-induced charges of different polarity. Magnetic field detection limits are calculated for differently configured magnetoelectric composite cantilevers [A8-4, A8-7, A8-10].

Figure A8-1(a) depicts an example cantilever structure in the first bending mode and the employed noise model. Figure A8-1(b) shows the resulting limit of detection (LOD) for cantilevers at three constant resonance frequencies and three constant quality factors Q_f . The total active layer thickness (sum of magnetostrictive and piezoelectric layers) is set to 2 μm . The substrate thickness is scaled to obtain the constant resonance frequency.

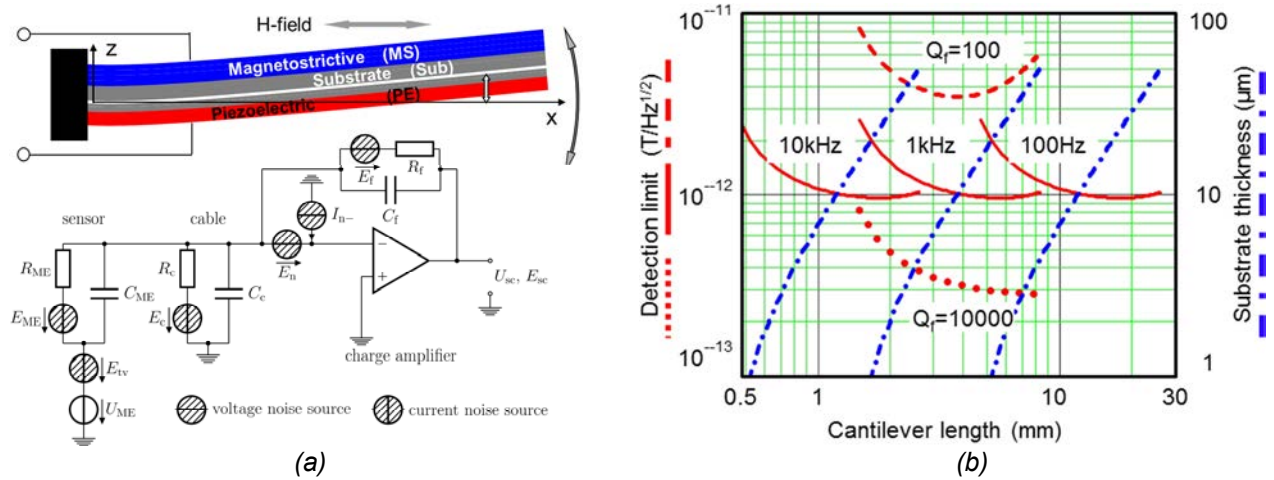


Figure A8-1: (a) ME cantilever, amplifier, and noise sources. (b) Example result of LOD vs. size scaling for FeCoBSi-Si-AlN cantilevers of length = $3 \times$ width with constant functional layer thicknesses of $1.8 \mu m$ FeCoBSi and $0.2 \mu m$ AlN. The substrate thickness is scaled to obtain the LOD at constant measurement frequencies of 10 kHz, 1 kHz, and 100 Hz at a quality factor of $Q_f=1000$ (solid red lines). Also shown are the results for a quality factor of 100 (dashed red line) and 10 000 (dotted red line) at a resonance frequency of 1 kHz.

Important findings of the systematic analytic investigation of the ME-response, sensitivity, different loss mechanisms, different noise components, resulting magnetic field detection limits, and associated scaling behavior of FeCoBSi-Si-AlN cantilevers are as follows: Sensitivity, noise, and resulting detection limits display different behavior with functional and substrate layer thicknesses. Thermal vibrations are found to dominate all investigated noise sources for practical ME composite sizes except at low quality factors where amplifier-intrinsic noise dominates [A8-7]. For constant functional layer thicknesses, resonance frequency, and Q-factor Q_f , the detection limit decreases with increasing cantilever size until a minimum is reached, as observed in the example in Figure A8-1(b). The detection limit minima scale with $Q_f^{-1/2}$, essentially independent of size for constant resonance frequency f , and are independent of f for constant Q_f with cantilever size scaling as $f^{-1/2}$. The results agree with the experimentally observed effect that many different cantilever designs have a limit of detection on the order of $1 pT/Hz^{1/2}$ for a $Q_f \approx 1000$. For an improved limit of detection, a higher Q_f or thicker functional layers are necessary. At constant f and Q_f , we find the detection limit minima scaling inversely with functional layer thicknesses and $1/length^2$ – assuming that the width is scaled proportional to the length and functional layers with properties corresponding to the thin layers can be fabricated.

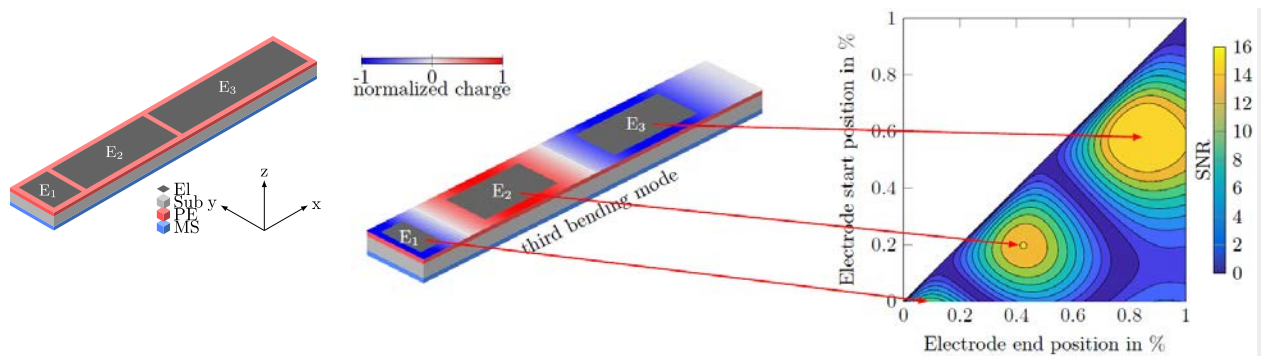


Figure A8-2: (a) Electrode design for the third flexural mode of a magnetolectric cantilever. The disconnections are located at the zeros of the strain along the cantilever to prevent the charges from cancelling each other. (b) Optical measurement of cantilever deflection at different positions along the cantilever length for the first three modes. (c) Signal-to-noise ratio (SNR) magnitude for different electrode start and end positions along the cantilever length x for the first three modes. For the first mode, the optimal electrode starts at the beginning of the sensor and ends at around 60%.

For higher-mode operation, a study was conducted investigating segmented electrodes. In numeric simulations the charge distribution along the cantilever is calculated for the first six bending modes. For such higher modes, there is a change of sign in the charge distribution along the cantilever and an electrode which connects regions of different charge signs drastically reduces the sensor output. To prevent this and obtain maximum performance, sensors with segmented electrode have been designed, as depicted in Figure A8-2. An SNR analysis has been carried out on the effect of the electrode design. By adjusting the start and end positions of the three electrodes, an SNR improvement is obtained as areas with low induced charge provide

little signal but add to the noise. In addition, magnetic flux concentration effects were investigated [A8-5]. Magnetolectric ZnO microrod composites were investigated numerically in a collaboration with **A6** [A8-3].

As a new approach within this CRC, surface-acoustic-wave (SAW) sensors are investigated and a new FEM model for SAW sensors has been implemented to calculate the mode profile and wave velocity of Love waves. The FEM model of a magnetostrictive layer on a delay-line SAW was verified by Julius Schmalz (PhD student in A8) in his external research stay in the group of Prof. Kaltenbacher at TU Wien. Figure A8-3 shows the experimental structure from **A3** and the model together with a 2D simulation result. With this model a basic understanding of such a sensor has been acquired and several parameter variations have been calculated to find parameters to improve the sensitivity of the SAW device [A8-2, A8-9]. The sensitivity is increased by choosing a higher frequency as shown in Figure A8-3(d), which would lead to a wave that is more concentrated at the surface and more sensitive to elastic property changes of the magnetostrictive layer. Alternatively, a thicker magnetostrictive layer can be chosen as depicted in Figure A8-3(d).

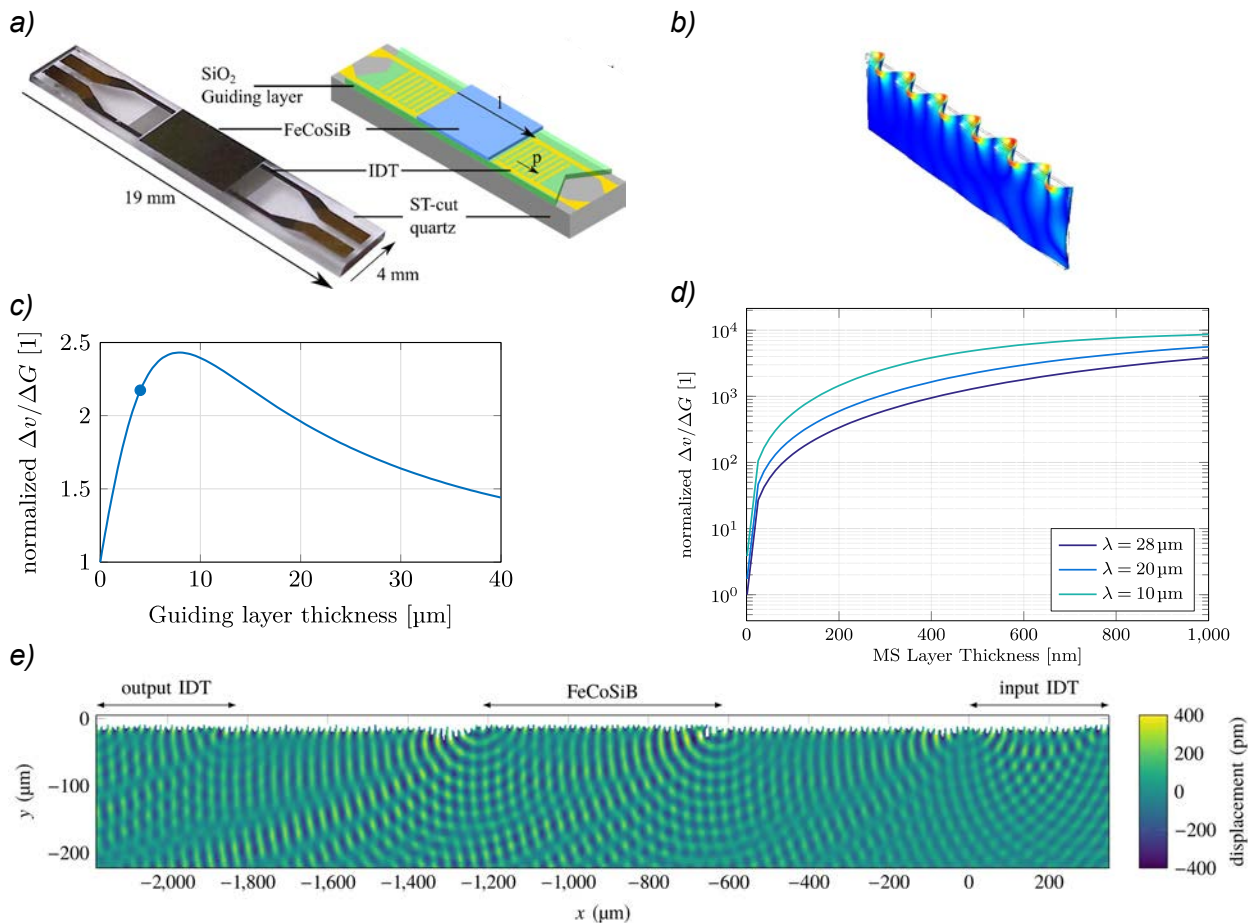


Figure A8-3: (a) Love-wave SAW sensor based on ST-cut quartz substrate and a $4.5 \mu\text{m}$ SiO_2 guiding layer. The 200 nm magnetostrictive (MS) material FeCoSiB is deposited on top of the 3.8 mm long delay line. (b) FEM result of SAW device, showing the displacement of the Love wave. (c) Simulation of normalized sensitivity for different guiding layer thicknesses and a 200 nm thick magnetostrictive layer. The blue dot represents the fabricated device. (d) Normalized structural sensitivity for different MS layer thicknesses and different periodicities of the interdigital transducers (IDTs) [A8-2]. (e) FEM result of a Love-wave propagation in complete sensor with input IDT, delay line, magnetostrictive layer, and output IDT. Reflections and interference patterns are visible at each boundary discontinuity (displacement is clipped to 400 pm for better visibility) [A8-6].

1D, 2D, 2.5D, and 3D FEM models for Love wave propagation in ME sensors were established allowing for calculation of the ME response at the working point of the magnetostrictive material [A8-6]. Together with the magnetic model from **A4**, the results are compared to measurements from **A3** [A8-2]. Experimental results from **A3** confirm that SAW sensors with lower IDT pitches and thus higher frequencies have a higher sensitivity. With the higher frequency and staying at the same guiding layer thickness, there are higher order Love waves. Their frequencies are even higher, but their sensitivity is lower compared to their fundamental mode both in simulations and in experiment [A8-8]. From simulations, it is observed that the wave energy is not as concentrated at the surface for the higher modes and thus has less overlap with the magnetostrictive layer.

A 3D simulation of the full delay line of 3.8 mm length with interdigital transducers and the magnetostrictive layer was conducted to investigate effects neglected in a reduced simulation [A8-6]. The full simulation required more than 750 GB of memory. The results show interface reflections along the delay line as seen in Figure A8-3(e) (the displacement is clipped to reveal these effects causing the “fuzzy” upper edge with the clipped region of high displacement above). Every change in the layer stack leads to small reflections and standing waves. A similar effect is observed by applying a magnetic field due to the change in the stiffness components of the magnetostrictive layer. In collaboration with the group of Prof. McCord (A1), a first investigation of Rayleigh wave propagation was carried out [A8-1]. Simulation results were compared to experimental results for wave excitation due to the movement of a domain wall. The simulated wavelength matches the observed wavelength of MOKE measurements. The methods established for conducting 3D simulations and investigating Rayleigh wave propagation are preliminary work for the next funding period.

Relevant new results on individual ME sensor design in the literature present a nonlinear ME composite model (nonuniform magnetostrictive and piezoelectric effects in layers) for alternating MS/PE layer composites excited in L-T mode (no bending) [Zh19], a model for high surface to volume ratios for nano cantilevers with MS-Sub-PE bending mode ME effects and additional surface effects [Yu15] as well as a discussion of a suitable figure of merit for ME sensors [Ya17]. A cantilever ME sensor employing metglas with an LOD of 37 pT/Hz^{1/2} at 244 Hz is presented in [Tu18]. Recently presented SAW ME sensors in the literature include: a Love-type SAW resonator using self-biased FeCoSiB with a resonant frequency around 220 MHz, a sensitivity of 663.98 Hz/μT, and good linearity [Li18]; a lithium niobate based sensor using multilayered TbCo₂/FeCo with a sensitivity of around 5e⁻⁴ °/Oe [Ma18]; and SAW devices with micro-dotted FeCo films for suppression of hysteresis effects [We18]. This comparison to results achieved in other groups shows that our sensors are among the world's best magnetoelectric sensors suitable for uncooled and unshielded operation.

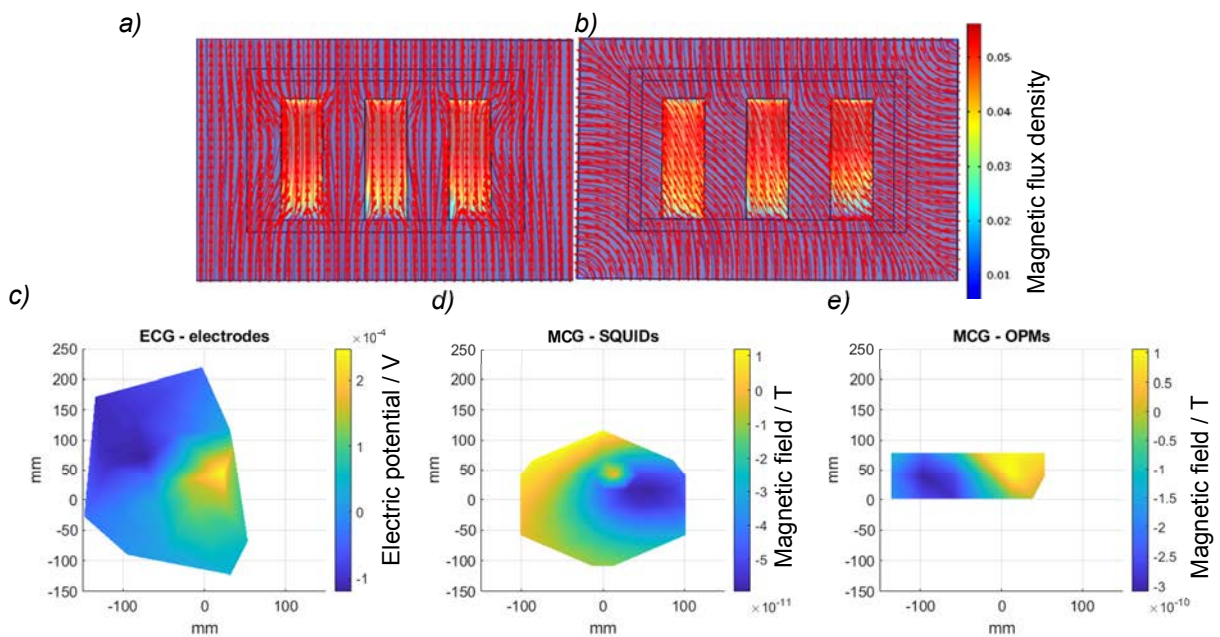


Figure A8-4: Simulated ME sensor array with magnetic flux density inside the magnetostrictive layer and corresponding arrow lines in the surrounding medium (air). An applied homogeneous (a) and inhomogeneous (b) magnetic field results in different flux density distributions for the individual sensors based on location in the array and shape of the applied magnetic field. c) to e) give examples of surface body potential and magnetic field measurements from B3, in cooperation with PTB Berlin.

The research on sensor crosstalk in sensor arrays was started as planned. First, mechanical simulations of side-by-side sensors in a single substrate frame in vacuum and air were carried out. These revealed the strength of the mechanical coupling and coupling by air movement. Next, the response of magnetoelectric sensors in a homogeneous time-variant magnetic field was considered. Close placement of several sensors leads to a different magnetic field amplitude in each sensor, as the total magnetic field is distributed onto the individual sensors. An example of this effect is shown in Figure A8-4(a). This effect was already studied previously for a pair of sensors [Li12]. Another effect that is visible in Figure A8-4(a) is that the outer sensors effectively see an inhomogeneous field that is weaker towards the middle. With this effect in mind, we started simulations of ME sensors in inhomogeneous fields, first considering artificially generated fields such as the one in Figure A8-4(b). These simulations reveal that the magnetic field has a different distribution in the sensor for different excitation fields. In Figure A8-5(b), for example, the left sensor experiences a rather homogenous

excitation field while the excitation is concentrated towards the tip in the right sensor. It was observed that the sensor response does not scale simply with the average excitation intensity. Figure A8-4(c-e) shows real cardiac magnetic fields measured in **B3** together with the PTB Berlin. Variations on the mm-scale are clearly visible and limited by the measurement resolution. Therefore, our typically mm- to cm-sized ME sensors in the CRC will experience an inhomogeneous excitation.

To analyze the effect of an inhomogeneous excitation, we conducted simulations of localized excitation by a small coil at different positions along the sensor axis, as shown in Figure A8-5(a,b). The simulations predict a rich excitation-position-dependent and frequency-dependent response behavior as shown in Figure A8-5(c). This is particularly true for excitation at 1200 Hz. The normalized mean electric potential induced by the coil excitation has a maximum near the clamped end, exhibits a zero around 16 mm, and a subsequent second maximum. This behavior is linked to the previously investigated Fano-type resonance in resonant ME sensors [Ge13]. The local magnetostrictive strain and the strain caused by resonance excitation are superimposed in the sensor and cause constructive and destructive interference effects. These effects are visible in the locally induced electric potential shown in the insets of Figure A8-5(c) for different excitation frequencies. To verify that these effects are indeed as strong as expected from the simulations, in **Z2** a measurement setup was realized with a sliding mechanism for a small excitation coil as shown in Figure A8-5(b). The normalized ME voltage from measurement is depicted in Figure A8-5(d) and confirms the simulation results qualitatively.

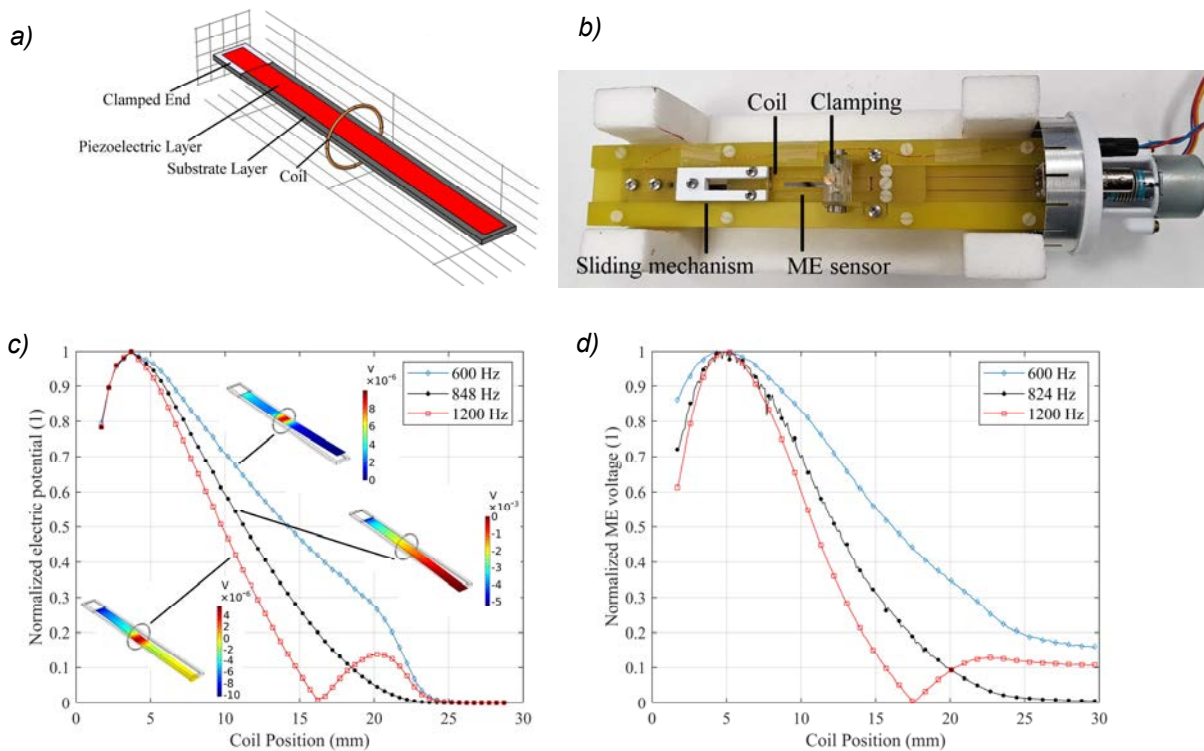


Figure A8-5: (a) ME cantilever sensor with a total free length of 26.25 mm and excitation coil in simulation setup. (b) Measurement setup for the ME sensor from **Z2**. (c) Simulated and normalized averaged electric potential on the surface of the piezoelectric layer and (d) measured normalized ME voltage for frequencies at resonance (848 Hz sim. / 824 Hz meas.), below (600 Hz) and above (1200 Hz) resonance.

The complex response behavior of ME sensors in inhomogeneous magnetic fields is of great importance for practical applications of these mm- to cm-sized sensors for biomagnetic applications. For the next funding period, a detailed study of these effects is proposed. In engineering, a common approach to describe the response behavior of a linear system is the derivation of a suitable transfer function. The transfer function mathematically connects the output signal to each possible combination of input signals. For example, the optical transfer function is employed to describe the spatial image formation in optical systems for arbitrary excitation signals. It is based on a spatial Fourier decomposition of signals [Go05]. A transfer function approach will be considered as one possible approach to handle the response of ME sensors in inhomogeneous fields.

References

- [BI08] J. F. Blackburn, M. Vopsariou, M. G. Cain, Verified finite element simulation of multiferroic structures: Solutions for conducting and insulating systems. *J. Appl. Phys.* **104**, 074104 (2008).
- [Du17] P. Durdaut, S. Salzer, J. Reermann, V. Robisch, P. Hayes, A. Piorra, D. Meyners, E. Quandt, G. Schmidt, R. Knöchel, M. Höft, Thermal-Mechanical Noise in Resonant Thin-Film Magnetoelectric Sensors. *IEEE Sens. J.* **17**, 2338–2348 (2017).
- [Ge13] M. Gerken, Resonance line shape, strain and electric potential distributions of composite magnetoelectric sensors. *AIP Adv.* **3**, 062115 (2013).
- [Go05] J. W. Goodman, *Introduction to Fourier optics* (Roberts and Company Publishers, 2005).
- [Go12] B. Gojdka, V. Hrkac, J. Xiong, M. Gerken, L. Kienle, T. Strunskus, V. Zaporozhchenko, F. Faupel, A critical evaluation of the 0–3 approach for magnetoelectric nanocomposites with metallic nanoparticles. *J. Appl. Phys.* **112**, 044303 (2012).
- [Gu13] J. L. Gugat, M. C. Krantz, M. Gerken, Two-Dimensional Versus Three-Dimensional Finite-Element Method Simulations of Cantilever Magnetoelectric Sensors. *IEEE Trans. Magn.* **49**, 5287–5293 (2013).
- [He97] G. Herzer, Magnetomechanical damping in amorphous ribbons with uniaxial anisotropy. *Mater. Sci. Eng. A.* **226–228**, 631–635 (1997).
- [Ja13] R. Jahns, A. Piorra, E. Lage, C. Kirchhof, D. Meyners, J. L. Gugat, M. Krantz, M. Gerken, R. Knöchel, E. Quandt, Giant Magnetoelectric Effect in Thin-Film Composites. *J. Am. Ceram. Soc.* **96**, 1673–1681 (2013).
- [Ka04] V. Kalinin, in *Proceedings. 2004 IEEE Radio and Wireless Conference (IEEE Cat. No.04TH8746)* (IEEE; <http://ieeexplore.ieee.org/document/1389104/>), pp. 187–190.
- [Ka11] M. Kadota, S. Ito, Y. Ito, T. Hada, K. Okaguchi, *Jpn. J. Appl. Phys.*, in press, doi:10.1143/JJAP.50.07HD07.
- [Ki13] C. Kirchhof, M. Krantz, I. Teliban, R. Jahns, S. Marauska, B. Wagner, R. Knöchel, M. Gerken, D. Meyners, E. Quandt, Giant magnetoelectric effect in vacuum. *Appl. Phys. Lett.* **102**, 232905 (2013).
- [Kr13] M. C. Krantz, J. L. Gugat, M. Gerken, Resonant magnetoelectric response of cantilevers with magnetostrictive and piezoelectric layers on opposite sides of the substrate. *AIP Adv.* **3**, 062135 (2013).
- [Li12] M. Li, Y. Wang, J. Gao, D. Gray, J. Li, D. Viehland, Dependence of magnetic field sensitivity of a magnetoelectric laminate sensor pair on separation distance: Effect of mutual inductance. *J. Appl. Phys.* **111**, 033923 (2012).
- [Li18] X. Liu, B. Tong, J. Ou-Yang, X. Yang, S. Chen, Y. Zhang, B. Zhu, Self-biased vector magnetic sensor based on a Love-type surface acoustic wave resonator. *Appl. Phys. Lett.* **113**, 082402 (2018).
- [Ma18] A. Mazzamurro, A. Talbi, Y. Dusch, O. Elmazria, P. Pernod, O. B. Matar, N. Tiercelin, Highly Sensitive Surface Acoustic Wave Magnetic Field Sensor Using Multilayered TbCo₂/FeCo Thin Film. *Proceedings.* **2**, 902 (2018).
- [Na08] Y. Nazirizadeh, U. Lemmer, M. Gerken, Experimental quality factor determination of guided-mode resonances in photonic crystal slabs. *Appl. Phys. Lett.* **93**, 261110 (2008).
- [Pa17] M. Paulsen, L. T. Neustock, S. Jahns, J. Adam, M. Gerken, Simulation methods for multiperiodic and aperiodic nanostructured dielectric waveguides. *Opt. Quantum Electron.* **49**, 107 (2017).
- [Pa13] W. Pabst, E. Gregorová, Elastic properties of silica polymorphs—a review. *Ceram. - Silikaty.* **57**, 167–184 (2013).
- [Po00] A. Pohl, A review of wireless SAW sensors. *IEEE Trans. Ultrason. Ferroelectr. Freq. Control.* **47**, 317–332 (2000).
- [Sa97] M. V. Salapaka, H. S. Bergh, J. Lai, A. Majumdar, E. McFarland, Multi-mode noise analysis of cantilevers for scanning probe microscopy. *J. Appl. Phys.* **81**, 2480–2487 (1997).
- [Sc96] H. Scherr, G. Scholl, F. Seifert, R. Weigel, Quartz pressure sensor based on SAW reflective delay line. *Proc. IEEE Ultrason. Symp.* **1**, 347–350 (1996).
- [Se05] M. Seger, G. Fischer, R. Modre, B. Messnarz, F. Hanser, B. Tilg, Lead field computation for the electrocardiographic inverse problem—finite elements versus boundary elements. *Comput. Methods Programs Biomed.* **77**, 241–252 (2005).
- [Tu18] A. V. Turutin, J. V. Vidal, I. V. Kubasov, A. M. Kislyuk, M. D. Malinkovich, Y. N. Parkhomenko, S. P. Kobeleva, A. L. Kholkin, N. A. Sobolev, Low-frequency magnetic sensing by magnetoelectric metglas/bidomain LiNbO₃ long bars. *J. Phys. D: Appl. Phys.* **51**, 214001 (2018).
- [We18] Wen; Yana; Xufeng; Yong and Zhaofu.: Magnetostrictive effect in micro-dotted FeCo film coated surface acoustic wave devices, *Smart Mater. Struct.* **27** (2018) 105040.
- [Wo04] C. H. Wolters, L. Grasedyck, W. Hackbusch, Efficient computation of lead field bases and influence matrix for the FEM-based EEG and MEG inverse problem. *Inverse Probl.* **20**, 1099–1116 (2004).
- [Ya17] L. Yang, J. Ma, C. Fang, M. Yao, W. Di, X. Zhao, H. Luo, Theoretical modeling of detectivity of magnetoelectric magnetic sensor and ultra-high magnetic detectivity of Metglas/PMNT/Metglas laminates. *Phys. status solidi.* **214**, 1700016 (2017).

- [Yo92] N. Yokokawa, S. Tanaka, T. Fujii, M. Inoue, Love-type surface-acoustic waves propagating in amorphous iron-boron films with multilayer structure. *J. Appl. Phys.* **72**, 360–366 (1992).
- [Yu15] G. Yu, H. Zhang, Y.-X. Li, Modeling of magnetoelectric composite nano-cantilever beam with surface effect. *Compos. Struct.* **132**, 65–74 (2015).
- [Zh19] J. Zhang, C. Fang, G. J. Weng, Direct and converse nonlinear magnetoelectric coupling in multiferroic composites with ferromagnetic and ferroelectric phases. *Proc. R. Soc. A Math. Phys. Eng. Sci.* **475**, 20190002 (2019).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [A8-1] R. B. Holländer, C. Müller, J. Schmalz, M. Gerken, J. McCord, Magnetic domain walls as broadband spin wave and elastic magnetisation wave emitters. *Sci. Rep.* **8**, 13871 (2018).
- [A8-2] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, F. Faupel, E. Quandt, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Sci. Rep.* **8**, 278 (2018). A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz and B. Spetzler contributed equally to this work.
- [A8-3] S. B. Hrkac, C. T. Koops, M. Abes, C. Krywka, M. Müller, M. Burghammer, M. Sztucki, T. Dane, S. Kaps, Y. K. Mishra, R. Adelung, J. Schmalz, M. Gerken, E. Lage, C. Kirchhof, E. Quandt, O. M. Magnussen, B. M. Murphy, Tunable Strain in Magnetoelectric ZnO Microrod Composite Interfaces. *ACS Appl. Mater. Interfaces.* **9**, 25571–25577 (2017).
- [A8-4] J. L. Gugat, M. C. Krantz, J. Schmalz, M. Gerken, Signal-to-Noise Ratio in Cantilever Magnetoelectric Sensors. *IEEE Trans. Magn.* **52**, 7005005 (2016).
- [A8-5] J. L. Gugat, J. Schmalz, M. C. Krantz, M. Gerken, Magnetic Flux Concentration Effects in Cantilever Magnetoelectric Sensors. *IEEE Trans. Magn.* **52**, 7403008 (2016).

b) Other publications

- [A8-6] J. Schmalz, B. Spetzler, F. Faupel, F. M. Gerken, Love wave magnetic field sensor modeling - from 1D to 3D model, Proceeding of International Conference on Electromagnetics in Advanced Applications (ICEAA) (2019). Peer-reviewed conference publication.
- [A8-7] M. Krantz, M. Gerken, Fundamental thermal limits for detection of biomedical magnetic fields by resonant magnetoelectric composite sensors, Today's Noise Tomorrow's Signal 2019, Berlin (2019). Abstract.
- [A8-8] J. Schmalz, A. Kittmann, P. Durdaut, B. Spetzler, F. Faupel, M. Höft, E. Quandt, M. Gerken, Comparison of the fundamental and higher order Love waves' sensitivities in a SAW based magnetic field sensor. SAW Symposium 2018, Dresden (2018). Abstract.
- [A8-9] J. Schmalz, F. Faupel, M. Gerken, A. Kittmann, E. Quandt, E. Yarar and S. Zabel, Influence of a magnetostrictive layer on the mode shape and wave velocity of Love-wave based SAW-device, Euro Intelligent Materials 2017, Kiel (2017). Abstract.
- [A8-10] M. Krantz, M. Gerken and J. Schmalz, Magnetoelectric cantilever theory: Effect of elastic seed and adhesion layers and multi-domain concepts on response of exchange bias multilayer sensors, Euro Intelligent Materials 2017, Kiel (2017). Abstract.

c) Patents

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3.4 Project plan

Objectives

Research in the first funding period has revealed that the response behavior of mm- to cm-sized magnetoelectric sensors in an inhomogeneous magnetic field is much more complex than for a homogeneous excitation field. Their electric amplitude and phase responses depend strongly on the exciting magnetic field position, orientation, and frequency, which lead to spatial and temporal interference effects upon superposition of signals. The overall objectives of this project are to

- (1) develop an understanding of the response behavior of magnetoelectric sensors and sensor arrays in inhomogeneous magnetic excitation fields by carrying out theoretical investigations and
- (2) develop design rules for sensors and sensor arrays suitable for biomagnetic applications.

Our working hypothesis is that detrimental effects of the complex ME sensor response in an inhomogeneous field may be countered with the following approaches:

- (1) detailed knowledge of the sensor transfer function and inclusion of this knowledge in the solution of the inverse problem
- (2) miniaturization of sensor size in comparison to the biomagnetic signal inhomogeneity such that the inhomogeneity effect is negligible
- (3) utilization of a sensor mode that exhibits a spatially homogeneous response in the ME sensor and thus reduces superposition effects to simpler constructive interference effects

The following intermediate objectives are defined, which are addressed in the listed work packages (WP):

- develop simulation method for delay-line SAW sensors (WP1), acoustic superlattices (WP2), and resonator SAW sensors (WP3) and derive design rules
- develop simulation methods for electrically modulated ME sensors and derive design rules (WP4)
- establish systematic understanding of ME sensor behavior under point excitation and develop sensor transfer functions (WP5)
- combine sensor and system results to investigate deep-brain-stimulation system in detail (WP6) and extend results to sensor arrays (WP7).

Proposed research methods

This is a theory project investigating the behavior of sensors and systems in theoretical investigations and developing the necessary simulation methods. The analytic and finite element method (FEM) simulation methods developed in prior work form the basis for the project. A linearized material model for the small-signal excitation at the working point is considered. Anisotropic material properties are included in all simulation models. Material properties are obtained from or derived in close collaboration within the CRC. In particular, magnetoelectric and piezoelectric layer properties are obtained from **A1** and **Z1**, permeability values and phenomenological noise models from **B1**, and magnetic noise models from **A10**. Overall and local magnetic layer behavior is simulated in **A10**, while whole sensor and sensor system models from the μm - to cm-scale are developed here by assuming effective material properties. We implement the physical models in the equation modus of COMSOL Multiphysics®, where all equations are included by the user such that full control is maintained, while exploiting the computer-aided design (CAD), meshing and solver utilities of COMSOL Multiphysics®. Smaller simulations are carried out on the CRC simulation server, while larger simulations are parallelized for computation on the University computer cluster. The developed simulation methods will be verified continuously through close cooperation with the experimental groups and comparison of theoretical and experimental results.

Work plan

In the following, the seven work packages (WP) are described in detail, which includes the collaboration within the CRC. WP1 to WP4 are to be conducted by a postdoctoral researcher and WP5 to WP7 by a doctoral researcher. Funding for both positions is requested here. WP1 and WP5 are started at the beginning of the CRC to achieve first insights and deliver inputs to the experimental projects. They are continued at a later point with the knowledge of experimental results. WP2 and WP3 are shown in parallel at the end of the CRC. Here, the focus will be put on one of the two work packages, depending on the achieved results. The type of sensor used in WP5 to WP7 will be based on which sensors appear most promising at the time of these work packages.

Nr.	Work packages	2020		2021				2022				2023				2024	
		III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
1	SAW delay-line sensors																
2	Acoustic superlattices																
3	SAW resonator sensors																
4	Electrically modulated sensors																
5	ME sensor response for point excitation																
6	Multiscale analysis of system model																
7	ME sensor arrays in inhomogeneous fields																

Postdoctoral researcher

Doctoral researcher

WP1: SAW delay-line sensors

This work package is dedicated to the development of theoretical models and to performing numerical FEM simulations of single-crystal and thin-film delay-line SAW sensors and is based on the methods developed in the first funding period. It is conducted in close cooperation with **A1**, **A9**, and **A10**. Previous work has shown that simulation results and measurements match well in terms of the wave propagation in the quartz and SiO_2

guiding layer due to the well-known material properties [Pa13]. The effective mechanical and magnetic properties of the magnetostrictive layer, on the other hand, are very sensitive to fabrication conditions, surface roughness, magnetization, magnetic microstructure, and domain wall positions. Thus, their material properties are fitted to measurements using the micro-magnetic model developed in **A4**. In the first part of this WP, the model derived in **A4** will be integrated with the mechanical simulation. This integration in combination with an iterative fitting procedure allows the extraction of the effective magnetic properties in the full device geometry. First design rules for single-crystal SAW delay-line sensors will be given to **A9** after 6 months.

Next, the acoustic attenuation of the quartz substrate, the guiding layer, and the magnetostrictive layer will be included in the model. The mechanical properties of the magnetostrictive (MS) layer are similar to the properties of the guiding layer, which makes the MS layer a guiding layer. An increased MS layer thickness slows down the wave and leads to a wave that is more concentrated at the surface and therefore implies an increased sensitivity. This is shown in Figure A8-6(a) [A8-2]. Measurements confirm this for layer thicknesses below 400 nm (Figure A8-6(b)). With higher layer thicknesses, the wave damping is increased and the sensitivity rise stagnates. The increased magnetic losses may be reduced by using a multilayer approach as shown by [Yo92], where the signal increased linearly with the number of stacked layers, while the losses are nearly constant (Figure A8-6(c,d)). At every material interface along the delay line, small reflections occur. With increased MS layer thickness, these reflections lead to an energy loss of the travelling wave and therefore to damping. This is another factor which must be included. By simulating the complete SAW sensor, these effects will be investigated.

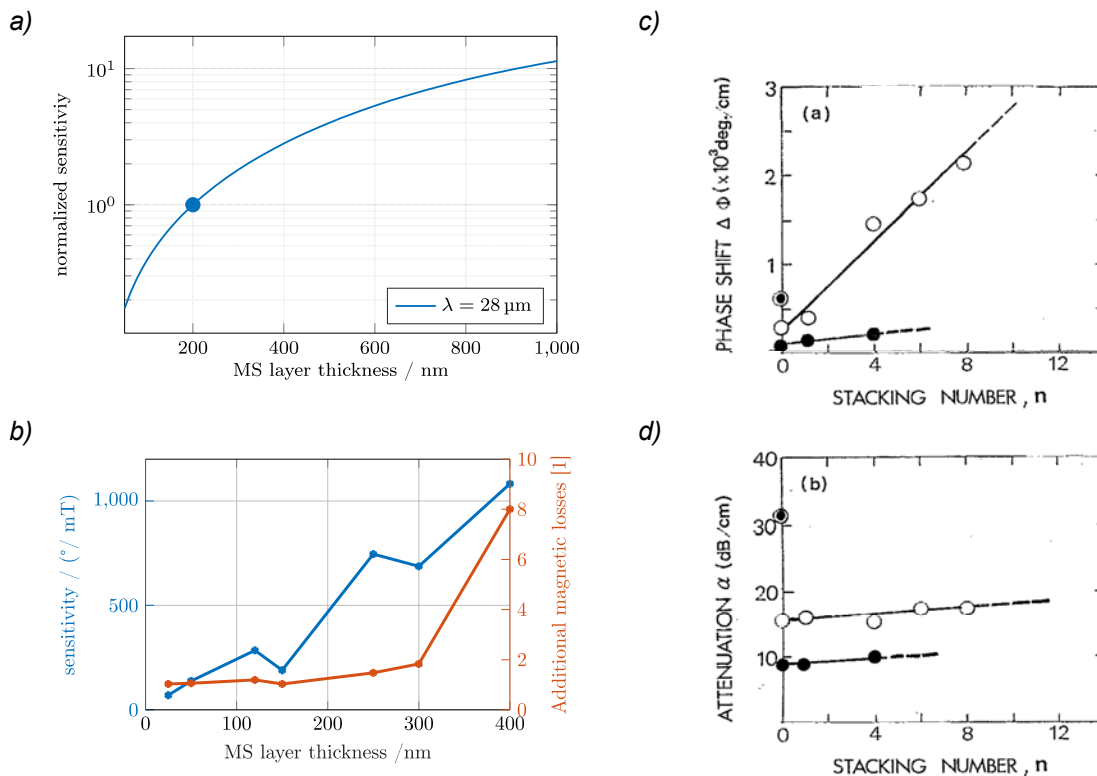


Figure A8-6: (a) Normalized sensitivity for different magnetostrictive (MS) layer thicknesses, showing increased sensitivity for thicker MS layers [A8-2]. (b) Corresponding measurement from project **A3** for different magnetostrictive layer thicknesses up to 400 nm, showing increasing sensitivity as well as increasing magnetic losses. (c/d) Phase shift and attenuation of Rayleigh (●) and Love (○) waves for different numbers of magnetostrictive layer stacks (reproduced from [Yo92]).

Surface acoustic wave simulations in full-sensor devices, including reflection effects, will be carried out for **A10**. In the third project year, the new models developed in **A10** will be combined with the full-sensor simulation implemented here. To eliminate the need for an external bias field, exchange-biased magnetostrictive layers are considered in collaboration with **A10** and their properties are included in the FEM simulations.

Thin-film SAW delay-line sensors will be investigated together with **A9**. SAW devices based on both thin-film AlScN on a silicon substrate and a magnetostrictive layer will be modeled as the starting point. These thin-film SAW devices open new opportunities for high-frequency operation and alternative acoustic modes. With high-frequency operation, a miniaturization of the SAW sensors is possible, which is advantageous for the analysis of inhomogeneous biomagnetic fields. The sensor performance with additional guiding layers (e.g. SiO_2) as

well as other materials (e.g. polymer thin films) will be calculated and design rules will be developed. Wave types other than Love waves will be investigated as alternative routes for increasing the sensitivity. Preliminary work on the simulation of Rayleigh waves with FEM has been conducted in the first funding period [A8-1].

The results achieved in this work package will be validated in comparison to experimental results in **A9**. This is the basis for realistic simulation results and a better understanding of sensor behavior. With this enhanced model, new sensor designs are investigated and design rules for delay-line SAW sensors will be supplied to **A9**. The behavior of these sensors in inhomogeneous magnetic fields will be studied in WP5.

WP2: Acoustic superlattices

In cooperation with **A9**, acoustic superlattices will be investigated by employing the polarization-switching property of AlScN with a high Sc content. This allows the use of coplanar electrodes and is another strategy for achieving high frequency operation and miniaturization of devices. The simulation model will be extended to investigate periodically poled ferroelectric domains.

As a second approach, the generation of acoustic superlattices by patterning of the magnetostrictive layer will be investigated. The band structure of the resulting phononic crystals may be tailored by the addition of lattice “defects” or by employing a more complex superlattice beyond pure periodicity. The Gerken group has been working on photonic crystals for more than ten years. Figure A8-7 (a-c) gives an example of a hexagonal photonic crystal structure and the corresponding band structure investigated in experiment and simulation. Figure A8-7 (d) depicts the results of a comparison of three different numeric simulation methods: Finite element method (FEM), rigorous coupled wave analysis (RCWA), and finite difference time domain (FDTD) method. All simulation methods agree in the resulting spectrum but differ in the simulation time. The measurement result differs due to uncertainties in the material parameters and the fabrication. It has not been fitted.

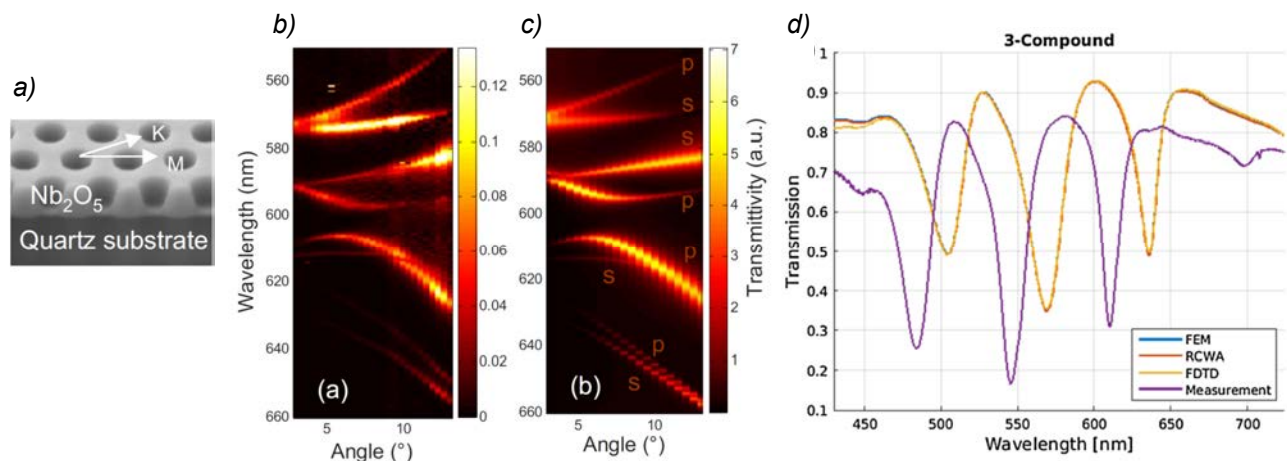


Figure A8-7: (a) Photonic crystal slab of hexagonal holes with a periodicity of 360 nm in a Nb_2O_5 waveguide layer of 221 nm thickness [Na08]. (b) Experimentally measured band structure. (c) Band structure simulated with finite-difference time-domain (FDTD) method. (d) Example of a tailored 0° incidence angle band stop characteristic obtained by a nanostructure with three grating components of different periodicity [Pa17].

Based on these simulation methods developed for photonic crystal structures, here phononic band structures will be designed to achieve an increased interaction of the magnetic field with the magnetostrictive layer and thus an improved efficiency.

WP3: SAW resonator sensors

Here, resonator structures will be investigated to achieve an increased interaction of the magnetic field with the magnetostrictive layer. This is an exploratory investigation at the end of the second funding period for experimental work in the third funding period. This work package will be conducted in parallel to WP2 with the same aim of achieving an improved efficiency and miniaturized devices. Depending on the results obtained in the initial simulations of WP2 and the experimental results of **A9**, the focus will be set on WP2 or WP3. Here, the use of reflective SAW structures based on IDTs will be investigated. Reflective SAW structures have been employed successfully to realize one-port SAW sensors as depicted schematically in Figure A8-8(a) for a delay-line sensor with two reflectors and in Figure A8-8(b) for a delay-line sensor with three reflectors and a resonator design [Sc96, Po00, Ka04]. In the literature, SAW sensors using resonator structures and first designs for magnetic sensing have been demonstrated [Ka11].

A simulation model will be developed based on the results of WP1 and WP2, the literature as well as the noise considerations of **A10**. Sensor designs based on interdigital reflectors as well as designs based on reflections at material interfaces such as the beginning and the end of a thick magnetostrictive (multi-)layer will be investigated and compared. In particular, the quality factor of resonator SAW sensors will be investigated. A high quality factor is beneficial for miniaturizing the sensor size. On the other hand, it influences the transient behavior. This effect must be considered while reducing the SAW size by using resonator structures. A parametric theoretical study of the behavior of different types of SAW sensors with reflective structures will be conducted. SAW resonator sensors in particular promise a reduced sensor size, which is beneficial for array configurations of these sensors. If the concept of acoustic superlattices does not deliver the expected improvement in the limit of detection, this work forms the basis for experimental research employing resonator SAW sensors in the third funding period of the CRC. This work package contributes to the objective of designing sensors for inhomogeneous biomagnetic fields by targeting small sensor sizes below 1 mm.

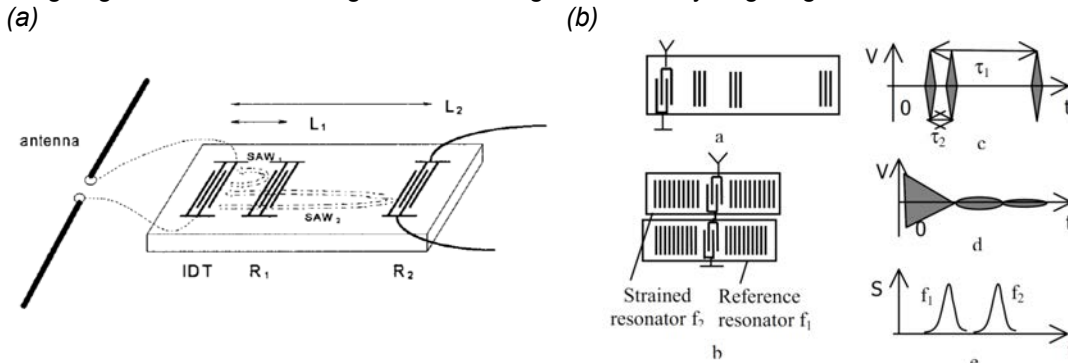


Figure A8-8: (a) Passive one-port delay-line SAW sensor with two reflectors R1 and R2 (reproduced from [Po00]). (b) Comparison of reflective delay line sensor and resonant SAW sensor regarding impulse response and spectrum of resonator response (reproduced from [Ka04]).

WP4: Electrically modulated sensors

In this work package, a cumulative theoretical model of the electrically excited converse ME effect sensor investigated in **A7** will be developed. Weak, low frequency biomagnetic fields are detected with great sensitivity by nonlinear mixing with the high frequency magnetic carrier field produced by electric excitation of ME composites whereby the mixing occurs in the magnetostrictive phase. A schematic sensor setup is depicted in Figure A8-9(a,b). While basic mechanics simulations are conducted in **A7**, here the full model including all layers will be implemented. This is particularly important for thin cantilevers where the mechanical behavior is not dominated by the substrate. The work involves establishing parametrized models for the resonant converse ME effect in layered and possibly segmented magnetoelectric composites, in particular for high resonance frequency and low aspect ratios of U-modes such as the one shown in Figure A8-9(c). ME cantilever response models beyond the Euler Bernoulli approximation, i.e., FEM models will be implemented. Magnetic concentrator structures will be included.

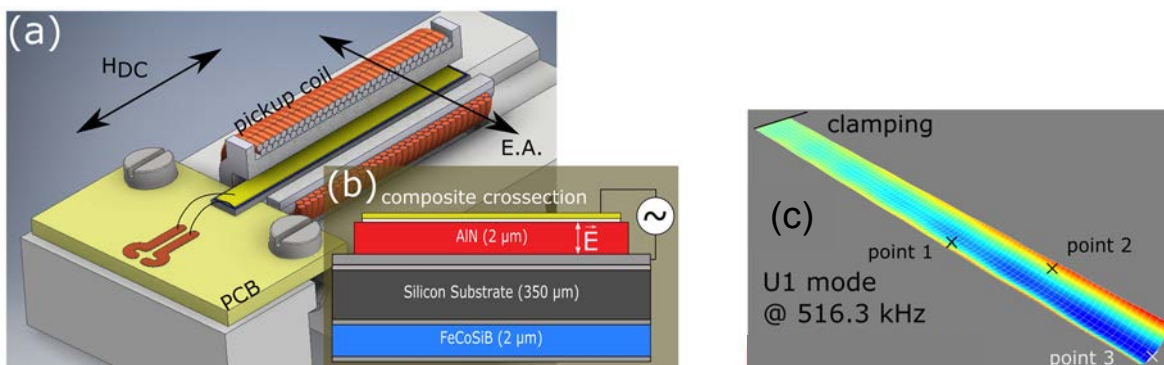


Figure A8-9: Schematic setup for electrically modulated ME sensors (see **A7**). (a) Magnetolectric cantilever in pick-up coil. (b) Cross-sectional view of a typical composite. (c) Currently employed inhomogeneous U-mode of cantilever sensor.

The signal model derived here will be combined with the noise model developed in **B1** to calculate the resulting limit of detection. Scaling laws of the above will be investigated and detection limits given by fundamental effects or engineering design derived. The influence of the filling factor of the coil, i.e. the coil core area compared to the coil area, will be investigated. The influence of the length and the positioning of the coil relative to the resonator's position will be calculated. With this insight, a specific focus will be on the investigation of

composite resonator designs yielding low strain inhomogeneities. The results will be provided to **A7** and compared to experimental results.

WP5: ME sensor response for point excitation

As described in the report section, we observed a rich position- and frequency-dependent ME sensor response behavior in inhomogeneous magnetic excitation fields. This work package aims at understanding the ME sensor response for point magnetic vector excitation at a particular position, with a particular orientation and a particular frequency. In the first project year, cantilever sensors will be investigated, while other sensor types will be included in the study in the third project year based on the sensor models developed in WP1 and WP4 and on the experimental results achieved in the CRC. In the preliminary work, models for the simulation with small coil excitation were established as these may be realized easily in experiments. Simulations were verified in experiments for the case of on-axis coil excitation. An in-depth theoretical study will be performed in this work package to evaluate the ME sensor response for coil excitation with various positions, orientations, and frequencies and the geometry-dependent sensitivity behavior. Figure A8-10(a,b) shows two example excitation fields obtained for coils with different orientations. The theoretical work will be accompanied by experimental studies in **Z2**.

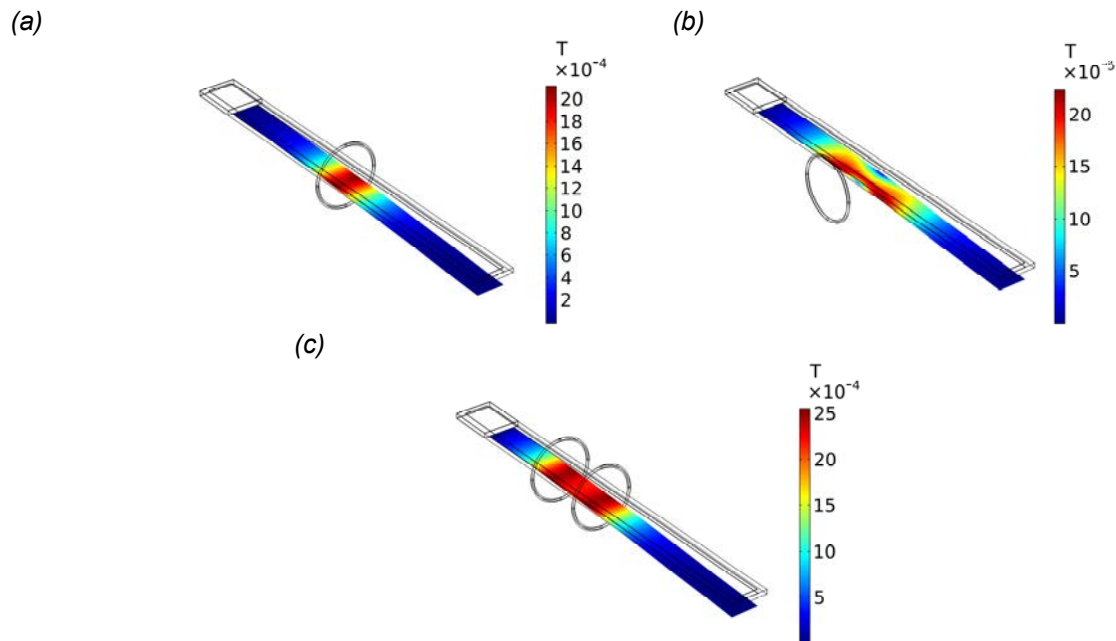


Figure A8-10: Simulation results showing magnetic flux density on the surface of the magnetostrictive layer of a cantilever sensor with excitation coil (a) along the axis of the ME sensor, (b) perpendicular to the ME sensor axis, and (c) two excitation coils.

The hypothesis behind performing point-wise excitation is that the system behaves linear in the small-signal case at the working point and that the superposition principle holds. Thus, we expect that a combination of two excitations such as depicted in Figure A8-10(c) may be calculated by phase-correct addition of the individual-coil responses. A detailed investigation will be carried out on the experimental validity range of the superposition principle. If the superposition principle holds, the sensor response for excitation with an arbitrary inhomogeneous excitation field may be obtained by linear superposition of the point-excitation solutions. The coil depicted in Figure A8-10(a) approximates a point excitation, while a single coil is not a good model for a point approximation from the side as seen in Figure A8-10(b). For the linear regime, mathematical transfer functions will be established for the different sensor types of high CRC interest, linking arbitrary magnetic input fields to the expected sensor output. Simulations will be carried out to calculate the response as a function of coil orientation and position. From these simulations, we plan to deduce a function-based transfer function. For example, the initial results for cantilever sensors show that the sensitivity along the axis may be described by a Fano function. Thus, only a few grid points need to be calculated. A first sensor model based on the most sensitive sensor areas will be supplied to the projects in project area **B** after the first year. Together with these projects, the influence of the sensor sensitivity behavior on the construction of measurement systems will be investigated. This includes providing the supporting simulations for the projects in project area **B**.

WP6: Multiscale analysis of system model

In this work package, a method for the multiscale analysis of a deep-brain stimulation (DBS) system including a DBS excitation electrode, a head model, and different sensor models will be established. The starting point for this investigation is the joint simulation of DBS electrode, head, and sensor in a single, fully coupled FEM

computation. In the first funding period we developed the method of parallel computation of large models with magnetostrictive and piezoelectric functional layers on the University computer cluster and applied it to compute full SAW delay-line sensors as depicted Figure A8-5(e). It is planned to incorporate the head model in the form of a voxel model with different tissue types and anisotropic properties to approximate the magnetic field propagation and secondary-source effects due to conductivity. The preliminary work for this approach has been carried out in **T1**. From the full simulation result, we will evaluate the reciprocal effects between stimulation and measurement. This fully coupled FEM simulation will provide insights into expected inhomogeneous magnetic field distributions distorted by the ME sensor, magnetic fields caused by the ME sensor in the head as well as resonant strain in the magnetostrictive layer generating secondary magnetic fields. Placing artificial point sources within the brain allows the calculation of the leadfield matrix [Wo04, Se05] for a given sensor geometry. New compared to the work conducted in **T1** in the first funding period is the inclusion of the full sensor model in the calculation.

In the second part of this work package, approaches will be investigated for partitioning this multiscale problem of the sensor with features on the μm - to mm-scale, the brain with the DBS electrode, and features on the 100 μm to cm-scale into the subsystems “sensor”, “brain”, and “DBS electrode”. The different scales will be coupled using scale coupling equations. For the case of successful implementation of sensor transfer functions in WP5, here the fully coupled solution will be compared to the solution decoupling the magnetic field propagation in the skull from the sensor properties. As an alternative, the effect of approximating sensors by point detectors will be analyzed. An improved sensor model will be supplied to research area **B** in 2023. The results will be further utilized together with project area **B** for developing methods for solving the inverse problem of source localization.

WP7: ME sensor arrays in inhomogeneous fields

This work package is dedicated to the analysis of ME sensor arrays in inhomogeneous biomagnetic fields. Based on the multiscale simulation methods developed in WP6, here the behavior of larger sensor arrays, e.g. with 100 sensors, will be evaluated by using segmentation of the problem and order reduction techniques. This will be based on the evaluation of cross sensitivities over the sensor array. It is expected that it is sufficient to analyze the full sensor density only over a certain range while the effect of sensors situated further away may be included as effective properties causing, e.g. a joint magnetic flux steering. Models for arrays based on the most promising ME sensors developed in the first three years of the funding period will be established. The joint sensor behavior and crosstalk characteristics will be analyzed. The overall array size is determined by the application of interest. A particular focus will be on answering the question if 500 smaller sensors on a given surface or 50 larger sensors are more promising. Using smaller sensors promises a better spatial resolution. On the other hand, larger sensors offer improve magnetic flux concentration. Different approaches of assembly in single- and double-layers (for gradient measurements) will be compared. Finally, the placement and orientation of sensors in the array for biomagnetic measurements will be investigated in collaboration with the application-oriented projects in project area **B**.

Prospects

In the third funding period, this project will continue the research in the area of theoretical investigations. After successful implementation of sensor simulation methods in the first funding period and the analysis of the behavior of sensors and sensor arrays in inhomogeneous magnetic fields in the second funding period, the third funding period is planned to include actuators into the theoretical investigation and to study closed-loop sensor-actuator systems, e.g. for real-time adjustment of the DBS stimulation field. This project will continue to provide simulations on the physical level. Material properties will be obtained from other projects in research area **A** and simulations will include material models based on input from **A10**. Systems will be designed in close cooperation with the signal processing groups in research area **B**.

3.5 Role within the Collaborative Research Centre

This project will collaborate closely on the sensor design with the technology groups in research area **A** and on inhomogeneous field effects with research area **B**. Specifically, the following collaborations are planned:

- A1** Magnetostrictive material parameters obtained from **A1**.
- A7** Sensor design rules for electric modulation are provided to **A7**. A comparison of experimental and theoretical results is employed to enhance the simulation method and provide better predictions.
- A9** SAW sensor design rules are provided to **A9**. A comparison of experimental and theoretical results is employed to enhance the simulation method and provide better predictions.
- A10** Magnetic noise model obtained from **A10**. Layer deformation and full sensor calculations provided to **A10**.

B1 Noise models developed in **B1** will be integrated into the simulation and SNR values for complex sensor geometries will be provided to **B1**.

B2/B7/B9/B10 Sensor models delivered. Transfer function implementation established together.

T1 The DBS system model will be implemented in close collaboration with **T1**.

Z2 Experimental studies on local coil excitation of ME sensors supplied by **Z2**.

Exchange on modelling topics with other projects will take place in the focus group “Modelling,” which is headed by Prof. Gerken. This project will join focus groups “Concepts based on ΔE -effect” and “ME Sensors” for the development of sensors as well as the group “Biomedical applications” to discuss the link of the sensor properties to the applications. This project will support the dissemination activities in **SOP** and the doctoral researchers will be active in the **IRTG**.

3.6 Differentiation from other funded projects

No other funded projects deal with a theoretical investigation of magnetoelectric sensors and sensor arrays.

3.7 Project funding

3.7.1 Previous funding

Funding of this project within the Collaborative Research Centre started in 07/2016. Previously, it was funded under a different DFG programme from 01/2015 to 06/2016 (GE1636/10-1 and GE 1636/12-1).

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum
Postdoctoral researcher, 100 %	1	37.1	1	74.1	1	74.1	1	74.1	1	37.1
Doctoral researcher, 100 %	1	34.2	1	68.4	1	68.4	1	68.4	1	34.2
Total		71.3		142.5		142.5		142.5		71.3

Direct costs	Sum	Sum	Sum	Sum	Sum
Equipment up to k€ 10, software, consumables	0	0	0	0	0
Total	0	0	0	0	0
Total	0	0	0	0	0

(All figures in k€)

3.7.3 Requested funding for staff for the new funding period

	No	Name, academic degree, position	Field of research	Department of university or non-university institution	Commitment in hours/ week	Category	Funded through:
Available							
Research staff	1.	Prof. Dr. Martina Gerken, professor	Electrical Engineering	Electrical and Information Engineering (EIE)	4		Core support

	2.	Doctoral researcher	Electrical Engineering	EIE	6		Core support
Non-research staff	3.	Jülf Buschmann, engineer		EIE	4		Core support
Requested							
Research staff	4	Dr. Matthias Krantz	Electrical Engineering	EIE		Postdoctoral researcher	
	5	Mesut-Ömür Özden, M.Sc.	Electrical Engineering	EIE		Doctoral researcher	

Job descriptions of staff for the proposed funding period (supported through existing funds):

1. Prof. Dr. Martina Gerken is responsible for the coordination and the scientific management of the project A8. She represents the project within the CRC and to the outside. She advises the scientific staff in the planning and execution of the modelling as well as in the interpretation of the results.
2. This doctoral researcher complements the CRC team with a position financed by existing funds. He/she is supporting the numerical simulation of ME sensors and sensor arrays employing FEM.
3. Jülf Buschmann is responsible for the operation of the simulation computers as well as for the installation and service of simulation software.

Job descriptions of staff for the proposed funding period (requested funds):

4. Dr. Matthias Krantz has contributed in the last years significantly to the development of simulation methods for magnetoelectric sensors. With a doctoral degree in physics and many years of industry experience, he supports the project with a comprehensive knowledge both on physical fundamentals as well as on application aspects. He is responsible for establishing models and conducting analytic and numeric simulations of SAW sensors and electrically modulated sensors in WP1 to WP4. The successful execution of the work packages within the set time frame requires an in-depth knowledge of physical ME sensor principles that includes the modelling of piezoelectric and magnetostrictive material properties as well as profound experience in carrying out sensor simulations. Therefore, the position cannot be filled with a doctoral researcher. Dr. Krantz is responsible for the planning, execution, and evaluation of work packages WP1 to WP4 and will assist in the other WPs.
5. Mesut-Ömür Özden is a doctoral researcher carrying out the analysis of the ME sensor response in inhomogeneous excitation scenarios. He is already employed on the CRC topic and will finish his PhD after the first year of the second funding period. A new doctoral researcher will be employed for the subsequent 3 years of the second funding period. This position is responsible for implementing a full-system simulation, and analyzing ME sensor arrays in inhomogeneous fields as described in WP5 to WP7. Mesut-Ömür Özden and his successor are responsible for the planning, execution, and result evaluation of these work packages.

3.7.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/1
CAU	2	4	4	4	2
Sum of existing funds	2	4	4	4	2
Sum of requested funds	0	0	0	0	0

(All figures in k€)

3.7.5 Requested funding for instrumentation for the new funding period

N/A

3.1 General information about project A9(N)

3.1.1 Project title: Surface Acoustic Wave Magnetic Field Sensors

3.1.2 Research areas:

406-02 Synthesis and Properties of Functional Materials, 407-03 Microsystems

3.1.3 Project leaders

Quandt, Eckhard, Prof. Dr.-Ing.
05.04.1960

Lofink, Fabian, Dr. rer. nat.
05.09.1977

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Do the above mentioned persons hold fixed-term positions? no

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no

3.2 Summary

As part of the research in **A3** in the previous funding period, it was shown that surface acoustic wave (SAW) sensors using the ΔE -effect can be used for very sensitive, broadband magnetic field sensing. These sensors are based on a patented approach using shear horizontal acoustic surface waves that are guided by a fused silica layer (Love waves) with an amorphous magnetostrictive FeCoSiB thin film on top. The velocity of these waves follows the magnetoelastic-induced changes of the shear modulus according to the magnetic field present. The delay line operation of the SAW sensor translates these changes into a phase shift. With an extremely low magnetic noise level of approximately $70 \text{ pT/Hz}^{1/2}$ at 10 Hz, a bandwidth of 50 kHz and a dynamic range of 120 dB, this magnetic field sensor system shows outstanding characteristics. In addition to piezoelectric bulk crystals, polycrystalline thin-film AlScN on a silicon substrate will be investigated as a possible alternative, since its electro-acoustic coupling coefficient is clearly superior, especially in the high frequency domain.

A main objective is to derive a comprehensive model for the sensitivity and the noise of magnetic field SAW sensors. This work will be performed in close collaboration with **A1** on the magnetostrictive film, with **A8** on modelling of design parameters as well as of the acoustic wave propagation, with **A10** on magnetic noise modelling and characterization, and with **B1** on the overall noise models. The major questions will include the concept and realization of the magnetostrictive component and investigations on the frequency, which is of course not independent from the magnetostrictive material of choice.

Besides this general objective, the following sub-objectives will guide the corresponding work packages, while the major results will be included in the signal-to-noise model:

- (1) For single crystalline SAW sensors, the choice of the piezoelectric single crystals and the material and layout of the guiding layer will be investigated as important parameters for the sensors' performance;
- (2) for thin film SAW sensors, the acoustic mode and the layout of the sensor will be investigated and compared to our reference single crystalline SAW sensors; and
- (3) for phononic crystals, acoustic band gaps with defect-induced transmission windows as well as the micromagnetic fine-structure of the individual magnetic lattice elements will be investigated.

3.3 Project progress to date

3.3.1 Report and current state of research

The report contains three chapters covering single crystal substrate-based SAW sensors, thin film based SAW sensors, and AlScN thin films as the main parts of the proposal. It is restricted to aspects important for magnetic field sensing and contains results obtained in A3 in the first funding period.

(1) Single Crystal SAW Sensors

The principle of SAW sensors is based on the generation of acoustic waves by applying a high frequency electric voltage to interdigital transducers (IDTs) placed on a piezoelectric surface. Due to the inverse piezoelectric effect, an alternating displacement of the piezoelectric crystal is induced, leading to an excitation of elastic waves [Wh65]. One concept to detect these waves is the so-called delay line setup, where the travelling wave is picked up by a second pair of IDTs and is transformed back into an electrical signal using the direct piezoelectric effect after propagating over a defined distance, the delay line. A measurable, additional phase change between output and input signal occurs when an alteration of the wave velocity by an external influence takes place. Additionally, any externally induced change in the wave amplitude could be recorded. SAW devices have been applied as sensors for a wide range of quantities: the sensing of gases [Ra17], pressure [Sc96], temperature [Re03], humidity [Ca93], biological molecules in liquids [A9-9], and magnetic fields [A9-4][Li18]. The last is based on the change of elastic moduli with applied magnetic field of a magnetostrictive layer placed on the delay line. This is known as the ΔE -effect (compare **A4**) for the change of Young's modulus [A9-10]. The ΔE -effect leads to a magnetic field dependence of the acoustic wave propagation velocity, and thus an additional phase difference occurs.

A comparison of different SAW magnetic field sensors developed over the years is given in Tab. A9-1. In the table only the obtained sensitivities are shown, since in none of the publications, besides our work, noise behavior was discussed. Thus, limits of detection (LOD) are not known for these sensors.

Tab. A9-1: Comparison of different SAW magnetic field sensors.

Substrate	Wave type	Design	Magnetic layer	Frequency	Effect size/Sensitivity	Ref.
Y LiNbO ₃	Rayleigh	Delay line	Ni	70 MHz	80° at 130 mT	[Ga75]
Y LiNbO ₃	Rayleigh	Delay line	TbFe ₂	42 MHz	$\Delta V/V = 0.27\%$ at 400 mT	[Ya80]
ZnO	Rayleigh	Delay line	Garnet film	105 MHz	700 Hz/mT	[Ha87]
ST Quartz	Love	Delay line	FeB-SiO ₂ ML	120 MHz	2300 °/cm	[In92]
ST Quartz	Love	Delay line	FeCoSiB	148 MHz	2000 °/mT	Our work
ST Quartz	Love	Resonator	FeCoSiB	221.8 MHz	664 Hz/ μ T	[Li18]

Love waves (horizontal surface shear waves) only occur in layered structures exhibiting a large difference in shear modulus G and/or density ρ of each layer. These differences lead to different phase velocities v of the acoustic waves, which forces the waves to propagate in the low velocity layer, thus termed the guiding layer. Increasing the difference in velocity between the layers leads to a stronger confinement of the acoustic energy to the surface of the guiding layer. Depending on the type of acoustic wave present, different elastic moduli are affected. Love waves perform a shear motion parallel to the plane of the magnetic film and are thus more sensitive to changes of the shear modulus G . The change of shear modulus with magnetic field has shown to be more pronounced than Young's modulus [Sa00]. Since the acoustic wave is strongly confined to the surface in Love wave devices, the sensitivity to changes of shear modulus is greater compared to Rayleigh or bulk shear horizontal waves. Therefore, SAW sensors using Love waves turned out to be more suitable for magnetic field sensing. In our own prior work, this type of sensor was previously established as biosensors in liquid environments due to their lower damping in fluids compared to Rayleigh waves. Additionally, the protection of the IDTs by the dielectric guiding layer is provided and generally higher sensitivities to mass loading are achieved [A9-9].

Fig. A9-1 depicts the Love wave device used for magnetic field sensing in **A3** in the preceding phase of the

CRC. It is based on a 500 μm ST-cut quartz substrate with 300 nm Au split finger IDTs and a 4.5 μm thick SiO_2 guiding layer. A 200 nm thick amorphous magnetostrictive $(\text{Fe}_{90}\text{Co}_{10})_{78}\text{Si}_{12}\text{B}_{10}$ layer acts as the sensitive element.

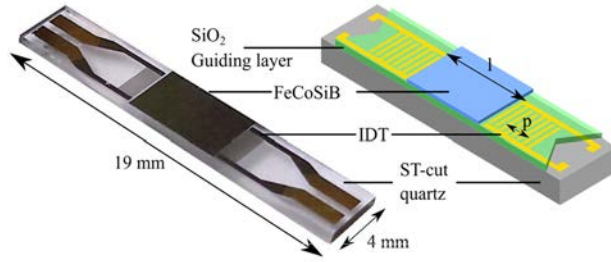


Fig. A9-1: Image and schematic of the Love wave SAW sensor based on an ST-cut quartz substrate and a 4.5 μm SiO_2 guiding layer. The 200 nm layer of magnetostrictive FeCoSiB is deposited between the transducers on top of the delay line with a length l of 3.8 mm. The interdigital transducers have a periodicity p of 28 μm providing the wavelength of the generated acoustic waves and thus the synchronous frequency of the sensor.

The sensitivity of the sensor is governed by three contributions: The sensitivity of the magnetic layer S_{mag} , i.e. the change of shear modulus with magnetic field $\partial G/\partial H$, the structural sensitivity S_{str} , i.e. the change of wave velocity with change in shear modulus $\partial v/\partial G$, and the geometric sensitivity S_{geo} , i.e. the phase change with change in wave velocity $\partial \phi/\partial v$. Thus, the overall sensitivity S of the sensor is defined as the phase change with applied magnetic field:

$$S = \frac{\partial \phi}{\partial H} = \frac{\partial G}{\partial H} \cdot \frac{\partial v}{\partial G} \cdot \frac{\partial \phi}{\partial v} = S_{\text{mag}} \cdot S_{\text{str}} \cdot S_{\text{geo}} \quad (1)$$

Since the phase change is a continuous function of the applied magnetic field, a point of maximum slope exists, which is the point of highest sensitivity. The direct measurement of the sensitivity is shown in Fig. A9-2 (a) as a function of applied magnetic bias field. Here, from the highest maxima a maximum sensitivity of $S = 2000^\circ/\text{mT}$ is obtained at a static bias field of 0.1 mT. At this point the change of shear modulus induced by an external AC magnetic field is maximized. The total maximum phase shift amounts to 380° in the magnetic remanent state at 0 bias field.

To fully characterize the sensor and estimate its performance capabilities in measuring magnetic fields, it is necessary to evaluate possible noise contributions. They will, with reduced magnitude of the magnetic field, progressively limit the sensor's ability to detect such fields. The measure which quantifies the smallest measurable magnetic field is the limit of detection (LOD). If a sinusoidal carrier signal is injected into the sensor with a frequency within the SAW device's passband, phase noise around this signal will occur. Methods for the suppression of the phase noise have been developed within the CRC [A9-3]. In Fig. A9-2 (b), the SAW sensor's magnetic noise floor is shown measured inside a magnetically and mechanically shielded chamber [Ja11]. At 10 Hz a LOD of $70 \text{ pT}/\text{Hz}^{1/2}$ and at 100 Hz a LOD of $25 \text{ pT}/\text{Hz}^{1/2}$ were achieved. These values are well within the $100 \text{ pT}/\text{Hz}^{1/2}$ range of thin-film ΔE -effect sensors [A9-7], but with a far higher bandwidth of 50 kHz. It can be seen that the limiting factor so far is the $1/f$ noise in the low frequency regime. A lower phase noise would directly lead to an improved LOD.

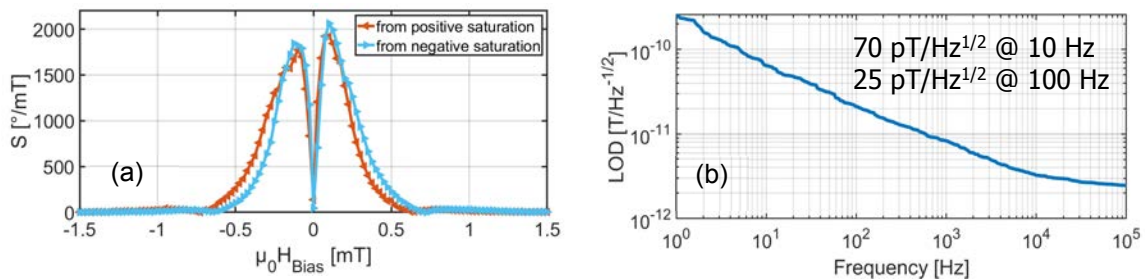


Fig. A9-2: (a) Measured sensitivity of the SAW device as a function of magnetic field. (b) Equivalent magnetic noise floor of the output signal shows the frequency dependent LOD. At 10 Hz a LOD of $70 \text{ pT}/\text{Hz}^{1/2}$ and at 100 Hz a value of $25 \text{ pT}/\text{Hz}^{1/2}$ are achieved.

A potential biomedical application of surface acoustic wave magnetic field sensors is the localization of the electrode during deep brain stimulation (DBS) in cooperation with **T1**. Preliminary measurements with **B5** have already demonstrated the potential for using SAW sensors for the measurement of magnetic fields of a commercial DBS electrode. A bipolar DBS signal at a fundamental frequency of 160 Hz with 8 V_{pp} (equivalent to 90 pT) was applied and showed the possibility of measuring not only the fundamental frequency but also

higher harmonics over a wide frequency range (Fig. A9-3). It was shown that the sensitivity of the SAW sensor is constant in the frequency range relevant for DBS [A9-1]. This not only provides the possibility of measuring at higher frequencies, thus at a lower noise level, but also shows that higher harmonics can be further used for digital signal processing to further improve the signal-to-noise ratio (see T1).

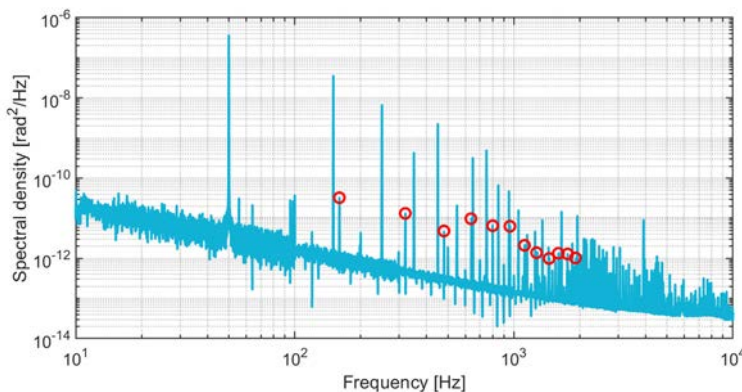


Fig. A9-3: Preliminary measurement of deep brain stimulation (DBS) using a bipolar signal at a fundamental frequency of 160 Hz with 8 V_{pp}. The marked signals refer to the bipolar excitation; the large signals are multiples from 50 Hz.

(2) Thin-film based SAW sensing

Today, ZnO and AlN are the predominant materials for piezoelectric thin-film SAW devices. The main applications are frequency filters for mobile applications and development with respect to future acoustic biosensors, acoustofluidics, and lab-on-a-chip devices [Fu17, Oz10, Wa14]. To date, there is only one working group at Northeastern University/Boston that has investigated the suitability of an acoustic wave in a thin-film bulk acoustic resonator (FBAR) for measuring magnetic fields reaching a limit of detection of 800 pT/Hz^{1/2} [Li17].

Major motivations to switch from piezoelectric bulk crystals to a thin-film approach are flexibility in substrates especially with respect to compatibility to CMOS and MEMS technology, a reduction of the chip size below 1 mm², and the possibility of tailoring and improving device performance via a clever multilayer design. Different layered stacks have been used in thin film acoustic devices to improve temperature stability, phase velocity, and electromechanical coupling [Ka03]. Yet it is not only the physical properties which count but also the thicknesses of each layer which significantly impacts the performance, e.g. a thickness-optimized layered structure can significantly increase the confinement of acoustic energy in the surface layer and thus improve sensitivity and coupling [Xu18]. However, a known issue with multi-layered thin-film acoustic wave devices is the unintentional generation of various wave modes and vibration patterns or hybrid modes [Ch10]. Hence, understanding and optimizing the acoustic propagation behavior in a multilayered thin-film device is mandatory, and finite element analysis (FEA) usually has to be applied.

Among the selection of thin-film piezoelectric materials available for acoustic wave technology, AlN has the largest wave velocity while PZT has the largest electromechanical coupling coefficient. However, PZT has several disadvantages for sensing applications such as high acoustic attenuation, low quality factor, high energy loss, low sound wave velocity, and the toxicity of Pb [Mu08].

Besides its high wave velocity, AlN has good mechanical and dielectric properties, high thermal conductivity, and high breakdown voltage [Du99]. Operation up to 700 °C and even up to 1000 °C in an inert atmosphere is possible [Au13]. Thin-film AlN enables the development of SAW devices operating at high frequencies up to several GHz which equals an improved sensitivity in sensing context [Ca03] (Compare Eq. (1)). Further, AlN is fully compatible with CMOS process technology, and thus allows a future monolithic integration of read-out electronics. Recently it was demonstrated that alloying AlN with Sc improves the electromagnetic coupling of the layer significantly, whereby the many advantages of AlN are largely retained [A9-5, Wa14, Ak09].

Aside from AlN, ZnO has also attracted great attention in the SAW community since the material has a high piezoelectric coupling coefficient, good biocompatibility, usually low film stress, and good adhesion with most substrates including glass and polymers [Oz10]. Due to its lower sound velocity compared to AlN, it is especially useful for devices operating in the lower frequency range. However, the strong reactivity of ZnO films is a major concern since it is unstable if exposed to moisture or water.

Further alternative thin-film materials are gallium nitride (GaN), gallium arsenide (GaAs), or polyvinylidene fluoride (PVDF), although they all possess a low electromechanical coupling coefficient. GaN films have frequently been used for fabricating SAW devices due to the high acoustic sound velocities for high frequency

(GHz range). Thin films of LiNbO₃, LiTaO₃, SrTiO₃, BiFeO₃, and BaTiO₃ have also been investigated for Lamb wave, SAW, BAW, or FBAR devices due to high electromechanical coupling coefficients, but they often suffer from poor control of film stoichiometry, orientation, texture, and process parameters [Sa07, Zh11, Vo14].

(3) AlScN thin films

To date, almost all reports on the fabrication of AlN-ScN solid solutions (Al_{1-x}Sc_xN) are based on reactive (pulsed) DC or RF sputter deposition. Sputtering from two metallic targets (co-sputtering) and single targets (either segmented or alloyed) was shown to be feasible, with the former being more flexible in terms of composition. The initial investigations on Al_{1-x}Sc_xN thin films were performed by Akiyama *et al.* in 2009 [Ak09]. Their layers were deposited by reactive RF co-sputtering from pure Al and Sc targets in an Ar-N₂ atmosphere directly on (100) n-type Si wafers. Measurements of the longitudinal piezoelectric coefficient d_{33} in Al_{1-x}Sc_xN

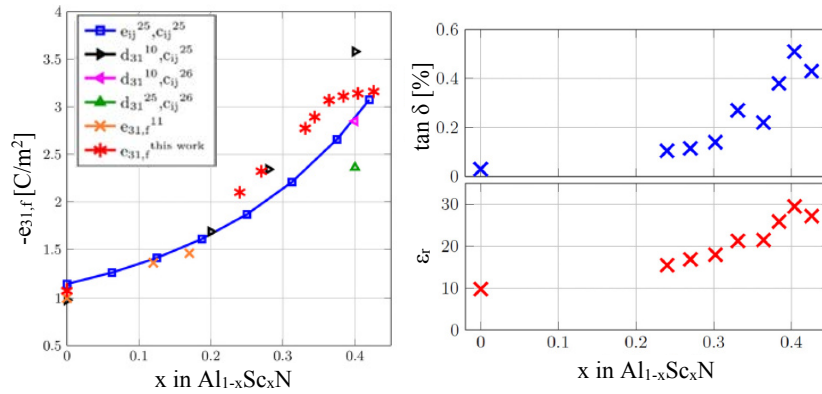


Fig. A9-4: (a) Transverse thin film piezoelectric coefficient $e_{31,f}$ over percentage of Al atoms substituted by Sc. (b) Loss tangent and relative dielectric permittivity over percentage of Al atoms substituted by Sc. [A9-5]

C/m². The slope of $e_{31,f}$ over the Sc content, however, started to decline above $x = 0.36$. We found that in selected samples of pure AlN, the dielectric loss tangent $\tan \delta$ could be below 0.04% and was regularly below 0.1%. Up to $x = 0.27$, $\tan \delta$ increased moderately to 0.11% where a better SNR $\propto \frac{e_{31,f}}{\sqrt{\epsilon_0 \epsilon \tan(\delta)}}$ than for pure AlN (or PZT) can be expected in sensory applications.

Below $x = 0.4$, numerous sources exist on investigations of the piezoelectric and dielectric properties as well as the morphology of Al_{1-x}Sc_xN. Notable groups studying Al_{1-x}Sc_xN are Mayrhofer *et al.* [Ma15], Zukauskaitė *et al.* [Zu15], Matloub *et al.* [Ma13], and as Zywitzki & Barth *et al.* [Ba16].

Experimental evidence of ferroelectric switching in Al_{1-x}Sc_xN was reported the first time in [A9-2]. Additionally, only a theoretical study with focus on Ga_{1-x}Sc_xN exists [Zh13], that does motivate the occurrence of ferroelectricity in solid solutions of AlN and GaN with ScN. Ferroelectric switching was demonstrated in Al_{1-x}Sc_xN, beginning at Sc concentrations of $x = 0.27$ [Fig. A9-5]. Between the ferroelectric switching points, the material behavior corresponds to the results of Fig. A9-4 and the piezoelectric response is highly linear and bipolar, as for pure AlN, so there is no negative impact on sensor properties. Moreover, this feature can be used in SAW devices to create acoustic superlattices by polarization domain inversion for efficient signal creation, amplification, or filtering [Yu09].

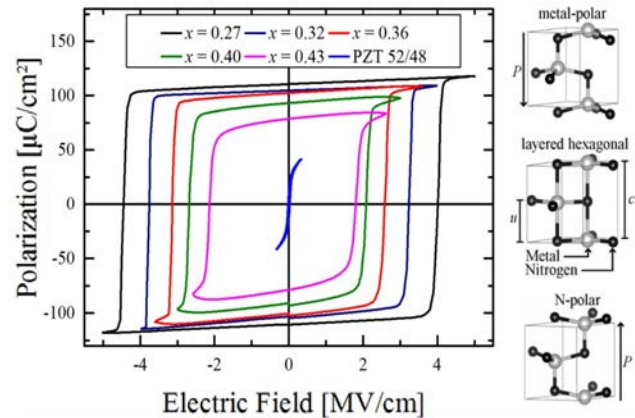


Fig A9-5: P-E loops of ferroelectric Al_{1-x}Sc_xN with Sc contents of $x = 0.27, 0.32, 0.36, 0.40$ and 0.43 as well as of PZT 52/48. To the right, the structures associated with the respective polarization states are displayed.

References

- [Ak09] M. Akiyama, K. Kano, A. Teshigahara, Influence of growth temperature and scandium concentration on piezoelectric response of scandium aluminum nitride alloy thin films. *Appl. Phys. Lett.* **95**, 162107 (2009).
- [Au13] T. Aubert, J. Bardong, O. Legrani, O. Elmazria, M. Badreddine Assouar, G. Bruckner, A. Talbi, In situ high-temperature characterization of AlN-based surface acoustic wave devices. *J. Appl. Phys.* **114**, 14505 (2013).
- [Ba16] S. Barth, H. Bartzsch, D. Glöß, P. Frach, T. Modes, O. Zywitzki, G. Suchanek, G. Gerlach, Magnetron sputtering of piezoelectric AlN and AlScN thin films and their use in energy harvesting applications. *Microsyst. Technol.* **22**, 1613–1617 (2016).
- [Be04] E. Berkenpas, S. Bitla, P. Millard, M. P. da Cunha, Pure shear horizontal SAW biosensor on langasite. *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.* **51**, 1404–1411 (2004).
- [Ca93] C. Caliendo, E. Verona, A. D'Amico, A. Furlani, G. Iucci, M. V. Russo, Surface Acoustic Wave Humidity Sensor. *Sens and Act. B: Chem.* **16**, 288–292 (1993).
- [Ca03] C. Caliendo, P. Imperatori, High-frequency, high-sensitivity acoustic sensor implemented on ALN/Si substrate. *Appl. Phys. Lett.* **83**, 1641–1643 (2003).
- [Ch08] R.-C. Chang, S.-Y. Chu, P.-W. Yeh, C.-S. Hong, H.-H. Huang, Y.-J. Huang, An investigation of Love wave devices based on ZnO. *Sens. and Act. B: Chem.* **132**, 312–318 (2008).
- [Ch10] G.-S. Chung, D.-T. Phan, Finite Element Modeling of Surface Acoustic Waves in Piezoelectric Thin Films. *J. Korean Phy. Soc.* **57**, 446–450 (2010).
- [Du99] M.-A. Dubois, P. Murali, Properties of aluminum nitride thin films for piezoelectric transducers and microwave filter applications. *Appl. Phys. Lett.* **74**, 3032–3034 (1999).
- [Fu17] Y.Q. Fu, J.K. Luo, X.Y. Du, A.J. Flewitt, Y. Li, G.H. Markx, A.J. Walton, W.I. Milne Recent developments on ZnO films for acoustic wave based bio-sensing and microfluidic applications: a review. *Sens. and Act. B* **143**, 606 (2010).
- [Ga75] A. K. Ganguly, K. L. Davis, D. C. Webb, C. Vittoria, D. W. Forester, Magnetically tuned surface-acoustic-wave phase shifter. *Electron. Lett.* **11**, 610 (1975).
- [Ha87] S. M. Hanna, Magnetic Field Sensors Based on SAW Propagation in Magnetic Films. *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.* **34**, 191–194 (1987).
- [In92] N. Yokokawa, S.-i. Tanaka, T. Fujii, M. Inoue, Love-type surface-acoustic waves propagating in amorphous iron-boron films with multilayer structure. *Journ. of App. Phys.* **72**, 360–366 (1992).
- [Ja11] R. Jahns, H. Greve, E. Woltermann, E. Lage, E. Quandt, R. Knöchel, Magnetolectric Sensors for Biomagnetic Measurements. *IEEE Int. Workshop on Med. Meas. and Appl. proceedings*, 107–110 (2011).
- [Jo19] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. D. Toxværd, M. Höft, R. Knöchel, E. Quandt, D. Meyners, J. McCord, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors. *Appl. Phys. Lett.* **114**, 192410 (2019).
- [Ka03] K. Kalantar-Zadeh, D. A. Powell, W. Wlodarski, S. Ippolito, K. Galatsis, Comparison of layered based SAW sensors. *Sens. and Act. B: Chem.* **91**, 303–308 (2003).
- [La12] E. Lage, C. Kirchhof, V. Hrkac, L. Kienle, R. Jahns, R. Knöchel, E. Quandt, D. Meyners, Exchange biasing of magnetoelectric composites. *Nat Mater.* **11**, 523–529 (2012).
- [Li17] M. Li, A. Matyushov, C. Dong, H. Chen, H. Lin, T. Nan, Z. Qian, M. Rinaldi, Y. Lin, N. X. Sun, Ultra-sensitive NEMS magnetoelectric sensor for picotesla DC magnetic field detection. *Appl. Phys. Lett.* **110**, 143510 (2017).
- [Li18] X. Liu, B. Tong, J. Ou-Yang, X. Yang, S. Chen, Y. Zhang, B. Zhu, Self-biased vector magnetic sensor based on a Love-type surface acoustic wave resonator. *Appl. Phys. Lett.* **113**, 82402 (2018).
- [Lu02] A. Ludwig, M. Tewes, S. Glasmachers, M. Löhndorf, E. Quandt, High-frequency magnetoelastic materials for remote-interrogated stress sensors. *J. of Magnetism and Magnetic Mat.* **242-245**, 1126–1131 (2002).
- [Lu12] R. Lucklum, M. Ke, M. Zubtsov, Two-dimensional phononic crystal sensor based on a cavity mode, *Sens. and Act. B: Chem.* 171–172, 271 (2012).
- [Ma11] D. Matatagui, J. Fontecha, M. J. Fernández, M. Aleixandre, I. Gràcia, C. Cané, M. C. Horrillo, Array of Love-wave sensors based on quartz/Novolac to detect CWA simulants. *Talanta*. **85**, 1442–1447 (2011).
- [Ma13] R. Matloub, M. Hadad, A. Mazzalai, N. Chidambaram, G. Moulard, C. S. Sandu, T. Metzger, P. Murali, Piezoelectric Al_{1-x}Sc_xN thin films. *Appl. Phys. Lett.* **102**, 152903 (2013).

- [Ma15] P. M. Mayrhofer, H. Euchner, A. Bittner, U. Schmid, Circular test structure for the determination of piezoelectric constants of $\text{Sc}_x\text{Al}_{1-x}\text{N}$ thin films applying Laser Doppler Vibrometry and FEM simulations. *Sens. and Act. A: Phys.* **222**, 301–308 (2015).
- [Mu08] P. Muralt, Recent Progress in Materials Issues for Piezoelectric MEMS. *J. Am. Cer. Soc.* **91**, 1385–1396 (2008).
- [Oz10] Ü. Özgür, D. Hofstetter, H. Morkoç, ZnO Devices and Applications. *Proc. IEEE*. **98**, 1255–1268 (2010).
- [Ra17] L. Rana, R. Gupta, M. Tomar, V. Gupta, ZnO/ST-Quartz SAW resonator. *Sens. and Act. B: Chem.* **252**, 840–845 (2017).
- [Re03] L. Reindl, I. Shrena, S. Kenshil, R. Peter, Wireless measurement of temperature using surface acoustic waves sensors. *IEEE International Frequency Control Symposium and PDA Exhibition Jointly with the 17th European Frequency and Time Forum*, 935–941 (2003).
- [Sa07] G. N. Saddik, D. S. Boesch, S. Stemmer, R. A. York, DC electric field tunable bulk acoustic wave solidly mounted resonator using SrTiO_3 . *Appl. Phys. Lett.* **91**, 43501 (2007).
- [Sa00] Z. Sárközi, K. Mackay, J. C. Peuzin, Elastic properties of magnetostrictive thin films using bending and torsion resonances of a bimorph. *J. Appl. Phys.* **88**, 5827–5832 (2000).
- [Sc96] H. Scherr, G. Scholl, F. Seifert, R. Weigel, Quartz Pressure Sensor based on SAW Reflective Delay Line. *IEEE Ultrasonics Symposium proceedings* (1996).
- [Sc09] U. Schürmann, A. Gerber, A. Kulkarni, F. Hettstedt, V. Zaporozhchenko, R. Knöchel, F. Faupel, E. Quandt, Fabrication of Toroidal Microinductors for RF Applications. *IEEE Trans. Magn.* **45**, 4770–4772 (2009).
- [Vo14] A. Vorobiev, M. Löffler, E. Olsson, S. Gevorgian, Effect of growth conditions on microstructure of BiFeO_3 - 0.33BaTiO_3 films and performance of bulk acoustic wave resonators. *J. Appl. Phys.* **115**, 84105 (2014).
- [Wa14] W. Wang, P. M. Mayrhofer, X. He, M. Gillinger, Z. Ye, X. Wang, A. Bittner, U. Schmid, J. K. Luo, High performance AlScN thin film based surface acoustic wave devices with large electromechanical coupling coefficient. *Appl. Phys. Lett.* **105**, 133502 (2014).
- [Wh65] R. M. White, F. W. Voltmer, Direct Piezoelectric Coupling to Surface elastic waves. *Appl. Phys. Lett.* **7**, 314–316 (1965).
- [Xu18] Z. Xu, Y. J. Yuan, Implementation of guiding layers of surface acoustic wave devices: A review, *Biosens. Bioelectron.* **99**, 500 (2018).
- [Ya80] M. Yamaguchi, K. Hashimoto, H. Kogo, M. Naoe, Variable SAW delay line using amorphous TbFe_2 film. *IEEE Trans. Magn.* **16**, 916–918 (1980).
- [Yu09] D. Yudistira, S. Benchabane, D. Janner, V. Pruneri, Surface acoustic wave generation in ZX-cut LiNbO_3 superlattices using coplanar electrodes. *Appl. Phys. Lett.* **95**, 052901 (2009).
- [Zh13] S. Zhang, D. Holec, W. Y. Fu, C. J. Humphreys, M. A. Moram, Tunable optoelectronic and ferroelectric properties in Sc-based III-nitrides. *J. Appl. Phys.* **114**, 133510 (2013).
- [Zh11] C. Zhou, Y. Yang, J. Zhan, T. Ren, X. Wang, S. Tian, Surface acoustic wave characteristics based on c-axis (006) LiNbO_3 /diamond/silicon layered structure. *Appl. Phys. Lett.* **99**, 22109 (2011).
- [Zu15] A. Žukauskaitė, C. Tholander, F. Tasnádi, B. Alling, J. Palisaitis, J. Lu, P. O.Å. Persson, L. Hultman, J. Birch, Stabilization of wurtzite $\text{Sc}_{0.4}\text{Al}_{0.6}\text{N}$ in pseudomorphic epitaxial $\text{Sc}_x\text{Al}_{1-x}\text{N}/\text{In}_y\text{Al}_{1-y}\text{N}$ superlattices. *Acta Materialia* **94**, 101–110 (2015).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [A9-1] J. Labrenz, A. Bahr, P. Durdaut, M. Höft, A. Kittmann, V. Schell, **E. Quandt**, Frequency Response of SAW Delay Line Magnetic Field/Current Sensor, *IEEE Sensors L.* **3**, 1500404 (2019).
- [A9-2] S. Fichtner, N. Wolff, **F. Lofink**, L. Kienle, B. Wagner, AlScN : A III-V semiconductor based ferroelectric. *J. Appl. Phys.* **125**, 114103 (2019).
- [A9-3] P. Durdaut, A. Kittmann, A. Bahr, **E. Quandt**, R. Knochel, M. Höft, Oscillator Phase Noise Suppression in Surface Acoustic Wave Sensor Systems. *IEEE Sensors J.* **18**, 4975–4980 (2018).
- [A9-4] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, F. Faupel, **E. Quandt**, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Sci Rep.* **8**, 278 (2018).
- [A9-5] S. Fichtner, N. Wolff, G. Krishnamurthy, A. Petraru, S. Bohse, **F. Lofink**, S. Chemnitz, H. Kohlstedt, L. Kienle, B. Wagner, Identifying and overcoming the interface originating c-axis instability in highly Sc enhanced AlN for piezoelectric micro-electromechanical systems. *Journal of Applied Physics.* **122**, 35301 (2017).

- [A9-6] **F. Lofink**, A. Philippi-Kobs, M. R. Rahbar Azad, S. Hankemeier, G. Hoffmann, R. Frömter, H. P. Oepen, Domain Walls in Bent Nanowires. *Phys. Rev. Applied.* **8** (2017).
- [A9-7] S. Zabel, C. Kirchhof, E. Yarar, D. Meyners, **E. Quandt**, F. Faupel, Phase modulated magnetoelectric delta-E effect sensor for sub-nano tesla magnetic fields. *Appl. Phys. Lett.* **107**, 152402 (2015).
- [A9-8] S. Fichtner, T. Reimer, S. Chemnitz, **F. Lofink**, B. Wagner, Stress controlled pulsed direct current co-sputtered $\text{Al}_{1-x}\text{Sc}_x\text{N}$ as piezoelectric phase for micromechanical sensor applications. *APL Materials.* **3**, 116102 (2015).
- [A9-9] M. D. Schlensog, T. M.A. Gronewold, M. Tewes, M. Famulok, **E. Quandt**, A Love-wave biosensor using nucleic acids as ligands. *Sensors and Actuators B: Chemical.* **101**, 308–315 (2004).
- [A9-10] A. Ludwig, **E. Quandt**, Optimization of the ΔE effect in thin films and multilayers by magnetic field annealing. *IEEE Trans. Magn.* **38**, 2829–2831 (2002).

b) Issued Patents

- [A9-P1] A. Kittmann, S. Zabel, E. Yarar, F. Faupel, R. Knöchel, M. Höft, P. Durdaut, E. Quandt, Sensorelement für Magnetfelder mit hoher Frequenzbandbreite, DE 10 2016 123 274 B4.

c) Pending Patents

- [A9-P2] S. Fichtner, D. Kaden, B. Wagner, F. Lofink, Ferroelektrisches Material, MEMS-Bauteil mit einem ferroelektrischen Material, MEMS-Vorrichtung mit einem ersten MEMS-Bauteil, Verfahren zur Herstellung eines MEMS-Bauteils und Verfahren zur Herstellung eines CMOS-kompatiblen MEMS-Bauteils, DE 10 2018 203812.
- [A9-P3] S. Fichtner, B. Wagner, F. Lofink, Ferroelektrische Halbleitervorrichtung und Verfahren zur Herstellung einer Speicherzelle, DE 10 2018 212736.

3.4 Research Plan

Objectives

Experiments within the scope of **A3** (Figs. A9-1 to A9-3, Tab. A9-1) have shown that surface acoustic wave devices – especially Love wave sensors – exhibit magnetic sensing properties that are very promising for the envisaged biomagnetic applications. These experiments were performed with modified Love wave sensors, which were originally developed for biochemical experiments in fluids. Furthermore, extensive noise investigations performed within **B1** have revealed that the present performance is limited by magnetic noise, as uncoated or magnetically saturated SAW sensors exhibit a 20dB lower noise level in the relevant frequency range. The first investigations to improve the performance with respect to the initial experiments have revealed that the effect size often scales as expected, e.g. the sensitivity increases with increasing magnetostrictive film thickness. Nevertheless, the gain in limit of detection (LOD) is mostly neglectable as the noise increases in a similar way. Furthermore, noise calculations for SAW sensors by **B1** have shown that under certain conditions, the LOD is dependent on the real and imaginary part of the permeability of the magnetostrictive sensing layer but independent of the sensitivity. Additionally, preliminary experiments have demonstrated the feasibility of using thin-film SAW devices of AlScN film on Si wafers as magnetic field sensors, which will widen the experimental possibilities towards very high frequency devices and alternative acoustic modes. Based on these results as well as on results obtained for magnetic frequency conversation (**A1**) or electrically modulated sensors (**A7**), the following hypotheses for evaluating the full potential of SAW devices as magnetic field sensors are derived.

- 1) Using magnetostrictive materials with pure rotational processes instead of domain wall motions upon excitation should enhance the signal-to-noise (SNR) ratio.
- 2) The optimum SAW frequency will be identified as a compromise between sensitivity enhancement and increase in magnetic losses (increase in the imaginary part of the permeability) with increasing frequency.
- 3) The best acoustic mode and the specific sensor layout will depend critically on the fraction of acoustic energy being concentrated in the magnetostrictive film.
- 4) The optimum working point with respect to, for example, excitation amplitude or magnetic bias field has to be identified, as it will in general not be identical to the maximum sensitivity conditions (Fig. A9-6).

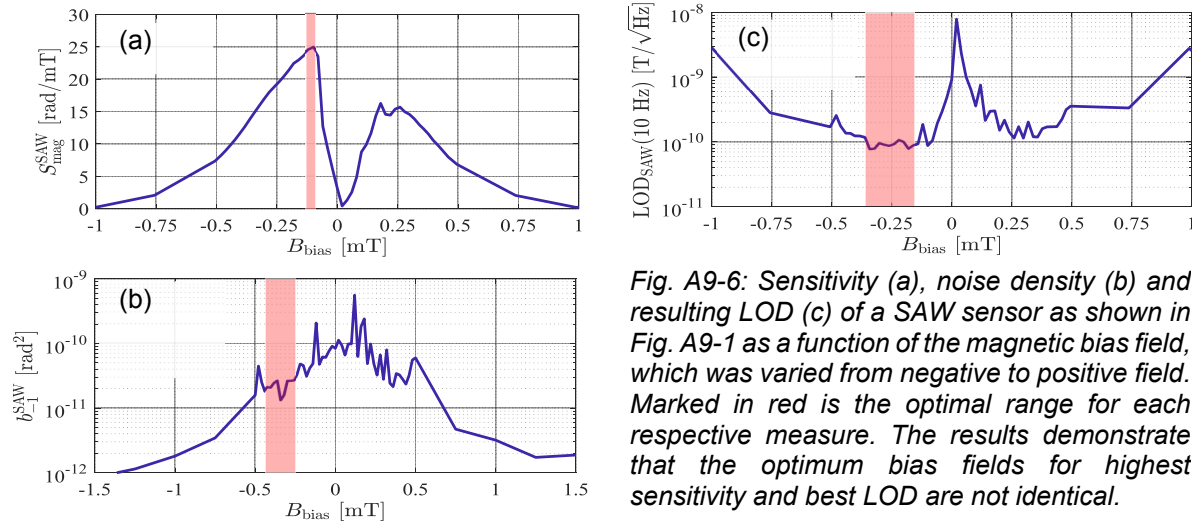


Fig. A9-6: Sensitivity (a), noise density (b) and resulting LOD (c) of a SAW sensor as shown in Fig. A9-1 as a function of the magnetic bias field, which was varied from negative to positive field. Marked in red is the optimal range for each respective measure. The results demonstrate that the optimum bias fields for highest sensitivity and best LOD are not identical.

Proposed research methods

(1) Processing

For the fabrication of SAW magnetic sensors, methods and techniques of micro- and nanotechnology will be applied. For this work, the cleanroom of the Kieler Nanolab of the CAU and the MEMS cleanroom of Fraunhofer ISIT are available. The combination of both facilities offers extensive options of different equipment and methods for depositing and etching of thin film materials and high-resolution stepper lithography (> 350 nm) while preserving experimental flexibility regarding new material systems and processes. More details are provided in the description of WP1.

(2) Functional Characterization

The magnetic measurements will be performed in the center of a solenoid providing a homogenous field. The magnetically induced phase shift and the derivative of that, the corresponding sensitivity (°/mT), will be measured at the sensor's center frequency with a lock-in amplifier (Zurich Instruments UHFLI). To measure the scattering parameters of the SAW sensor, a vector network analyzer E8361A from Agilent Technologies will be used. Prior to the measurements, both ports of the sensor will be matched to 50 Ω by means of a parallel capacitor and a series inductor (as seen from the 50 Ω ports into the sensor ports). Measurement of the phase noise floor and thus the sensors limit of detection (LOD) will be done by using a Rohde & Schwarz FSWP phase noise analyzer. More details, especially regarding the equivalent magnetic noise floor measurement, are given in **B1**. The magnetostrictive properties will be measured in a custom-built cantilever deflection setup, which allows monitoring of the deflection of cantilevers coated with the magnetostrictive film. Magnetic domain characterization will be performed using static and time-resolved magneto-optical Kerr effect (MOKE) microscopy in cooperation with **A10**. A large-view MOKE microscope is used for analysis of domain states and anisotropy of the whole magnetic delay line, and a high resolution time-resolved MOKE is used for dynamic characterization, where the interaction between acoustic waves and domain walls will be investigated. Magnetic induction-based set-ups, namely vibration sample magnetometer (VSM) and a BH-looper, will be further used for the investigation of magnetic properties on different substrates.

(3) Structural Characterization

In collaboration with **A1**, the structural characterization of the magnetostrictive films will be done by X-ray diffraction, scanning electron microscopy, and transmission electron microscopy with a Tecnai F30 STwin microscope (300 kV, field-emission gun). Compositions will be determined by energy-dispersive X-ray analysis (EDX). Chemical and structural analysis of AlScN will be investigated via TEM and X-Ray in tight cooperation with **A6**. For structural properties, SEM with EDX on wafer scale and on chip scale will be used. Surface properties can be determined by AFM, MFM, and White Light Interferometry.

Work plan

The objectives of the project will be addressed in seven work packages. An overview on the duration of each work package is given in Table A9-2.

Table A9-2: Work schedule - Main work done by: red: CAU, blue: ISIT, purple: both.

	2020		2021				2022				2023				2024	
	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP1: SAW Fabrication																
WP2: SNR model																
WP3: Single Crystal SAW																
WP4: Thin Film SAW																
WP5: Combination																
WP6: Acoustic Superlattices																
WP7: Characterization																

In the following, the key tasks, challenges, and approaches of the work packages will be described in detail including the collaboration within the project and within the CRC.

WP 1: SAW Fabrication

Resp.	Cross section	Description
CAU ISIT		Substrates • Options are Si, quartz, LiNbO ₃ , LiTaO ₃ or langasite
CAU ISIT		Interdigital transducers (IDTs) • Deposition of Al or Au (300 nm) • Standard or Sub- μ m Stepper Lithography • Ion beam etching (IBE) or chlorine based dry etching
ISIT CAU		Bonding pads and acoustic reflectors (optional) • Sputter deposition of Cr(10 nm)/Au (300 nm) • Sub- μ m stepper lithography • Wet chemical etching of Au and Cr
ISIT		Piezoacoustic thin film layer (optional) • Sputter deposition of AlScN (0.5 – 1 μ m)
ISIT CAU		Acoustic guiding layer • PECVD deposition of (3 - 6) μ m SiO ₂ or spin coating of polymeric PMMA, polyimide or BCB • Chemical mechanical polishing (CMP) • Standard photolithography (pad opening) • Fluorine-based dry etching of SiO ₂ • Chlorine-based dry etching of AlScN
CAU		Magnetically sensitive layer • Negative resist-based lift-off • Lithography (stepper lithography at ISIT for optional patterning of magnetic layer as phononic crystal) • Sputter deposition of magnetostrictive layer (e.g. FeCoSiB)

Fig. A9-7: Cross-sectional description of the fabrication sequence of SAW magnetic field sensors. Left column gives the responsibility for the corresponding process steps, center column depicts the cross section and right column describes the function associated with the step and the corresponding central technological aspects.

start of the project, this will be the fabrication sequences of the SAW magnetic field sensor based on ST-cut quartz and without reflector, piezo-acoustic thin film and patterned magnetic layer. This includes mainly the PECVD deposition of SiO₂ with subsequent chemical mechanical polishing (CMP) which is to be supplied as a process module from **Z1**. The technological focus in this work package is therefore mainly on the use of new substrates, the integration of a piezoacoustic thin film and reflector electrodes as well as the patterning of the magnetic layer.

WP 2: Signal-to-noise Model of SAW Magnetic Field Sensors

This work package will start based on the information gathered in the preceding funding period within the scope of **A3**, **A8**, and **B1** [A9-1, A9-3, A9-4]. In general, two models will be derived from the experiments and the modelling, both in close collaboration with **A1**, **A8**, **A10**, and **B1**. The easier model will describe the sensors' sensitivity as a function of the design and operational parameters as, e.g., the ΔE -effect of the magnetostrictive

This work package focuses on the fabrication process of the SAW magnetic field sensors. The general process-flow in Fig. A9-7 shows the major processing steps and their responsibilities both for WP2 and WP3. It is planned to combine the fabrication opportunities of ISIT and CAU in the best possible way. If both partners are specified, the process can be executed by either, which creates additional flexibility. This ensures meeting the specific requirements, gaining from the results between the different work packages, and to getting the best overall performance. Consequently, this technology must allow fabricating sensors based on different substrate types (Si, quartz, LiNbO₃, LiTaO₃, langasite) and wafer diameters (4", 6", and 8"). Furthermore, IDT technology down to sub- μ m resolution has to be available for delay-line configurations (magnetostrictive layer next to the IDTs) as well as for one-port resonators (magnetostrictive layer on IDTs) with or without reflectors. For the investigations in WP3, the integration of a piezoacoustic thin film (AlScN) must be possible. To guarantee the best possible quality of the magnetically sensitive layer, special attention must be paid to the condition of the surface (roughness, stress, ...) for the growth of the magnetic layer. In addition, it should be possible to pattern the magnetic layer with a resolution of down to 1 μ m.

Since the fabrication of sensors is very time-consuming, established fabrication modules have to be handed over to **Z1** if possible. At the

material, the frequency of the acoustic waves, the wave mode, the geometry of the sensor, and the choice of the different materials. The second, significantly more advanced model will focus on the correct understanding and description of the sensors' noise behavior. In the next funding period, the main aspect will be the magnetic noise, as this has proven to be the most prominent contribution [A9-4].

The starting point for a model of magnetic noise will be a simple model (compare **B1**) relating the $1/f$ noise to the imaginary part of the permeability of the magnetostrictive film. This is particularly true for hysteretic noise created by domain wall motion and has to be extended to the favored rotational magnetization processes that will be realized in future, more advanced magnetostrictive multilayer concepts [La12][Jo19] in collaboration with **A1**. For this, **B1** will set up a thin film permeameter (similar to [Lu02]) that will allow the determination of the real and imaginary part of the permeability as a function of frequency and magnetic bias field. Besides this approach, further extensions and improvements of the model are expected by the modelling and characterization of the corresponding SAW magnetic field sensors in **A10**, which will initially focus on simpler models with a few wavelengths to simulate, e.g., interactions with domain walls. Later these models will be applied on the actual sensor concept. Furthermore, this work package will also continuously incorporate the findings of the work packages WP3 to WP5 regarding wave mode, sensor layout, and materials selection, where the experiments will be evaluated with modelling and simulations carried out in **A8**. Essential for all of this work is the correlation to the analogue read-out electronics used and their noise behavior, which is the main objective of **B1** (compare WP2 of **B1**).

WP 3: Single Crystal SAW Investigation

So far our investigations on single crystal bulk substrates for magnetic sensing focused on quartz due to its common application for Love wave biosensors [A9-9]. In the case of biosensors, a high temperature stability is necessary; however, in magnetic sensing temperature is of less importance since, for the most part, the sensors operate at room temperature. Thus, substrates that are less temperature stable but have higher electromechanical coupling coefficients K^2 can also be used, such as the ferroelectric single crystals 36° Y-cut lithium tantalate (LiTaO_3) and 64° Y-cut lithium niobate (LiNbO_3) [Ch08]. A higher K^2 value leads to lower insertion losses due to higher electromechanical conversion and thus to a better performance of the sensor. Additionally, the electromechanical coupling of quartz is reduced at elevated frequencies, which is not the case for LiTaO_3 and LiNbO_3 , thus making it suitable for high frequency applications. Investigating the high frequency sensitivities will be part of this work. Another promising substrate is the quartz isomorph langasite ($\text{La}_3\text{Ga}_5\text{SiO}_{14}$) [Be04] which so far is utilized predominantly as a SAW pressure sensor at elevated temperatures due to its high phase transition temperature. Its less anisotropic and low thermal expansion coefficients makes it attractive for magnetic field applications. This enables the possibility of doing magnetic field annealing of the magnetostrictive phase for easier alignment of magnetic anisotropy. The anisotropic thermal expansion of piezoelectric substrates leads to a uniaxial stress acting on the magnetic film and is inducing a uniaxial anisotropy, which makes the films hard magnetic (Fig. A9-8) if the resulting stress is too high. The thermal expansion coefficients of langasite are more similar to those of silicon; thus due to magnetic field annealing, stress relaxation takes place which leads to softer magnetic films, and annealing in magnetic fields enables the possibility of advanced low noise magnetic multilayers based on FeCoSiB layers or on FeGaB (Iron-Gallium-Boron) and FeGaC (Iron-Gallium-Carbon) in cooperation with Nian X. Sun from Northeastern University.

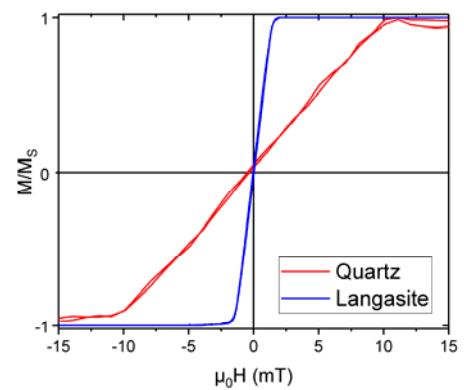


Fig. A9-8: Hard axis loops of 200 nm FeCoSiB on ST-cut quartz (red) and (euler angles $0^\circ, 22^\circ, 90^\circ$) langasite (blue). Both were annealed in a magnetic field at 270°C with the magnetic field being parallel to the SAW propagation direction.

The horizontal shear wave velocity of amorphous SiO_2 is about half that of crystalline quartz. A greater difference in acoustic phase velocity leads to a stronger confinement at the surface of the guiding layer, yielding a potentially lower limit of detection. Thus, polymeric guiding layers which have a low Young's modulus and correspondingly a low phase velocity become attractive. Polymer guiding layers have not been investigated for SAW magnetic field sensing applications so far. However, polymers have a higher acoustic damping, so the maximum film thickness is limited [Ma11]. The optimum thickness needs to be investigated. Potential materials for guiding layers are polymethylmethacrylate (PMMA), polyimide, or benzocyclobutene (BCB). The last has additionally the advantage of a high surface smoothness and a planarization of the surface [Sc09] which makes it attractive for magnetic film deposition. These polymers are typically deposited by spin coating with a subsequent curing at elevated temperatures for cross-linking. Additionally, multilayer approaches by the combination of SiO_2 and a polymeric material are possible and have shown in the case of mass sensitivity a

better performance than single layer wave guides. The optimum film thickness ratio of SiO₂ and the polymer will be investigated, also by simulation in cooperation with A8.

WP 4: Thin Film SAW Investigation

In this work package, SAW sensors based on thin-film AlScN on silicon substrates are investigated. The fabrication is based on silicon technology (WP1). The acoustically active area consists of an AlScN layer (excited by IDT) a few μm thick, an optional further guide layer (e.g. SiO₂), and the magnetostrictive phase (Fig. A9-9 (a)). The propagation behaviour of the acoustic wave as well as the excitation efficiency of different modes can be specifically adjusted by selecting the layer thicknesses and combining it with other thin film materials (e.g. SiO₂) of higher or lower acoustic velocities. The first numerical calculations show that it is possible to efficiently excite an acoustic mode with strong confinement at the surface by a proper selection of the layer thickness ratios (Fig. A9-9 (b)). With respect to the sensor response of a magnetic field sensor as in Fig. A9-9 (a), the use of the Love-like thin-film mode from Fig. A9-9 (b-III) should be superior to the use of a Rayleigh or Sezawa wave mode. Hence, a focal point of this work package is the investigation of the different modes in thin-film SAW devices (Rayleigh, Sezawa, Love-like, ...) and the evaluation of their suitability for use in magnetic field sensors. Further to the acoustic two-layer system (AlScN/SiO₂), studies on multi-layer systems with $N > 2$, comprising different fast and slow acoustic materials, will be also part of this package.

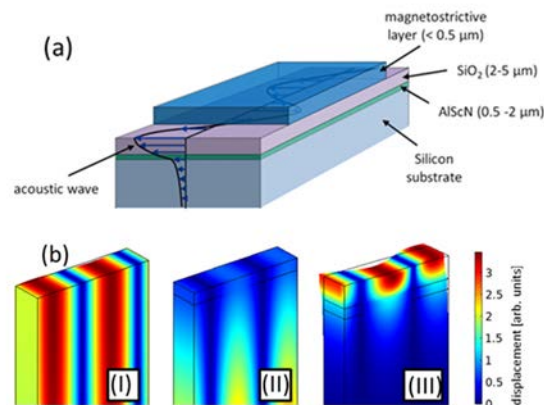


Fig. A9-9: (a) Sketch of thin-film SAW based on AlScN. (b) Propagation of acoustic wave in (I) Si bulk (267 MHz), (II) AlN(2 μm)/Si (268 MHz) and (III) SiO₂(4.5 μm)/AlN(2 μm)/Si (238 MHz). The configuration in (III) enables a high surface confinement of the acoustic wave such as for Love waves, whereas in (I) and (II) the acoustic energy is predominantly located in the substrate.

In addition to selecting the most suitable acoustic mode for magnetic sensing, an enhancement of the sensitivity can also be achieved by increasing the frequency. Especially AlScN has an advantage over quartz single crystal (SC) substrates in this respect since its electroacoustic coupling increases significantly with increasing amount of Sc and for higher frequencies (Fig. A9-10). In the scope of this work package, thin-film SAW devices with frequencies between 500 MHz and 3 GHz will be investigated and compared with identical designs on quartz-SC substrates. Since the ferromagnetic resonance of FeCoSiB is at about 2 GHz (stress and thickness dependent), the investigation of this frequency range is of special interest, as a significant signal increase is expected.

WP 5: Combination of different approaches

Although the idea of WP2 is to derive a comprehensive model of the signal-to-noise ratio of the SAW magnetic field sensor, the combination of the different findings of the work packages WP2 to WP4 regarding magnetic material, frequency, wave mode, sensor layout and materials, the combination of these different approaches remains a challenge because many of these parameters are not independent. Depending on the results obtained with single crystal or thin film SAW magnetic field sensors (WP3 and WP4, respectively) the decision will be taken which combination of the different approaches will be selected that promises the highest probability of achieving the LOD goals within the CRC. For example, the features of the magnetic material are known to depend critically on roughness and thermal expansion coefficients of the underlying material; furthermore, the right choice will most probably also depend on the selected wave mode and the frequency of operation. If, for instance, the sensor performance of the thin-film devices stays significantly below their single crystalline counterparts, this approach will not be continued in the second half of the project, but other tasks, e.g. the acoustic superlattices (WP6), then move further into focus.

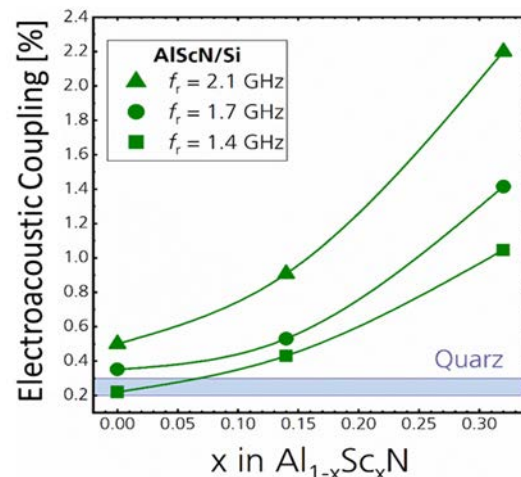


Fig. A9-10: Electroacoustic coupling versus Sc concentration for different wave velocities for a Rayleigh mode in a 1 μm thin-film AlScN-layer. For comparison, the value for the electroacoustic coupling in quartz SC is given.

In addition to the approach to combine the most promising findings into a kind of “optimum” sensor, this work package will be explicitly used to evaluate and further improve the overall sensor model of WP2 via extensive experimental studies. Newly established processes of this WP will be incorporated in this general process flow (WP1) once having been positively evaluated. Characterization of the different sensors will be performed within WP7.

Finally, this work package will include redesigns of the SAW devices based on modelling results obtained in **A8** and **A10**. Furthermore, the chopping approach of **B1** will be supported by designing and fabrication of SAW sensors suited for this work.

WP 6: Acoustic Superlattices

(a) Ferroelectric Interdigital Transducer

Besides having very attractive piezoelectric properties, recent studies [A9-2] have proven that its polarization can be switched ferroelectrically for compositions with a Sc content exceeding 27 at.%. This property enables the creation of artificial acoustic superlattices (ASL) by the generation of periodically inversely polarized AlScN structures as sketched in Fig. A9-11. In such an ASL structure, acoustic waves can be generated with coplanar electrodes instead of interdigital electrodes (IDT), which already is a benefit if the entire measuring system is considered (e.g. for impedance matching). By applying an external AC electric field to this structure, the domains are subjected to periodic deformations, which thus effectively act as localized sound sources and generate elastic waves. In contrast to IDT arrangements, in which only a very near-surface volume experiences piezoelectric excitation, here the entire thickness of the piezoelectric layer will be used to generate and detect the sound wave, which should be accompanied by a signal increase. Another advantage of an ASL-based transducer with respect to fabrication is that the elastic wavelength is given directly by the period Γ_{Ferro} of the grating $f = v_p/\lambda \equiv c/\Gamma_{\text{Ferro}}$ (v_p : phase velocity) and not by $f = v_p/\lambda \equiv c/2\Gamma_{\text{IDT}}$, as is the case for IDT electrodes. In order to generate such piezoelectric gratings, this work package will investigate how precise and up to what lateral size domains in AlScN can be created. Lateral domain sizes of 1 μm are targeted in order to realize center frequencies of up to 3 GHz. Numerical studies to investigate periodically ferroelectric domains will be carried out by **A8**.

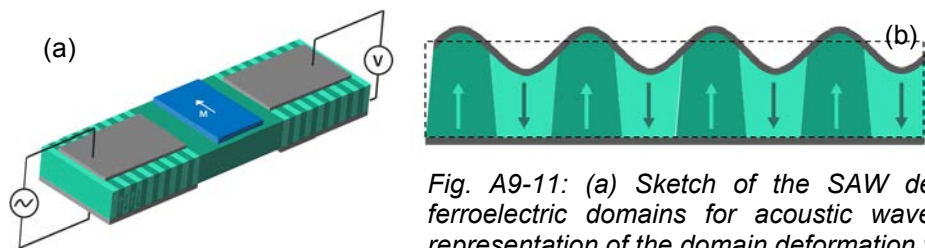


Fig. A9-11: (a) Sketch of the SAW device with periodically poled ferroelectric domains for acoustic wave generation. (b) Schematic representation of the domain deformation with applied AC voltage.

(b) Phononic Crystals

Another type of ASL can be created by a patterned magnetic layer, e.g., a 2D periodic array of magnetic (FeCoSiB) circular disks, ellipses, or rectangles in the area of the delay line instead of the closed film (compare A9-11 (a)). If such an acoustic grid modulates the elasticity or the speed of sound on the scale of the wavelengths, it acts as a phononic crystal. For center frequencies of 100 MHz to a few GHz, the size of the diameter of the magnetic discs has to be in the range of 1 to some 10 μm . With such a phononic crystal, acoustic band gaps are created. Within the band gap, a defined bandpass can be introduced by the intentional incorporation of lattice defects. The frequency position of the transmission window created shifts depending on the magnetically induced change in elasticity of the lattice elements. Hence, this phononic-crystal structure can be used to measure the external magnetic field. Since this approach is already successfully applied to increase the sensitivity of SAW sensors for the detection of concentrations in liquids [Lu12], the suitability for enhancing the performance of the magnetic sensor (A9-11 (a)) will be investigated within the scope of this work package. A second advantage of using such small magnetic structures ($d < 20 \mu\text{m}$) is that the anisotropy and thus the orientation of the magnetization can be adjusted via the shape of the individual array elements [A9-6]. This enables very precise control of the magnetic alignment, and thus also the precise adjustment of the optimal operating point. Numerical studies on phononic crystals will be carried out by **A8**.

WP 7: Characterization

The work package on characterization will include both functional and structural characterization using methods as described in the section “Proposed Research Methods”. The functional characterization will be performed in collaboration with **A10** (characterization of the magnetic phase) as well as with **B1** and **Z2** (electrical characterization including noise measurements). The structural characterization will include a collaboration with **A6**. Furthermore, this work package allows direct comparison between the Love wave sensors with piezoelectric single crystals and the thin film SAWs based on AlScN by using exactly the same characterization methods and devices. Some of the core measurements for the characterization of SAW

properties are the measurements of scattering parameters for the determination of the sensors working frequency, magnetic bias field-dependent measurements for the determination of potential working points and phase noise measurements to determine the sensors' limit of detection. For understanding the underlying noise contributions, time-resolved MOKE imaging in cooperation with **A10** will be used to determine the effect of magnetic domains and domain walls on the propagation of acoustic waves and how they contribute to magnetic noise. For this, different domain states and different delay line structures will be investigated with respect to their magneto-acoustic properties. In collaboration with **B1**, a set-up for the measurement of the magnetic permeability will be used to investigate the influence of loss mechanisms, expressed by the complex permeability μ'' , in the generation of magnetic noise. Especially the deduction of the origin of these loss mechanisms will be the main focus.

Prospects

Surface acoustic wave sensors are a new topic for the second funding period. Very successful preliminary work was performed under the scope of **A3** "Resonant ME sensors". This research has already resulted in one of the most sensitive sensor concepts of the CRC, with properties similar to the best ΔE -effect sensors (**A4**) or electrically modulated sensors (**A7**). Analogous to **A4**, it uses the ΔE -effect, but uses a different read out scheme based on piezoelectrically generated and detected acoustic waves. Being operated at very high frequencies (100 MHz – few GHz), it offers a very high frequency bandwidth and is DC-capable. It has already been demonstrated that these sensors can be used for measurements of deep brain stimulation (DBS), which were performed in **B5** and will be continued in **T1**. Based on the present status and taking into account the envisaged improvements and the potential of thin film SAW sensors, it is predicted that these sensors can be used for many biomagnetic applications planned within the CRC. Accordingly, sensor arrays will be the major task for the third funding period, which will also benefit from further miniaturization of the SAW sensors.

3.5 Role within the Collaborative Research Centre

The CRC 1261 spans a wide range of projects: from materials research to sensor concepts to signal processing and finally to applications. Because this project deals with one of the sensor concepts, it is fully integrated within this research chain and we will have intense collaborations with materials research, sensor systems, and even with applications, especially with the transfer project. The last collaboration includes mainly the support of **T1** in its measurements using SAW sensors for the localization of deep brain stimulation (DBS) and using the derived data and information for further improvement of the sensors for this application. In particular, the following close collaborations with other projects are planned:

- A1:** Application of advanced magnetic multilayers to SAW sensors
- A6:** Chemical and structural analysis of AlScN
- A8:** Modelling of SAW sensor parameters and designs as well as of acoustic superlattices
- A10:** Numerical studies on noise and in operando time-resolved MOKE measurements
- B1:** Analog electronics, noise floor characterization, LOD measurements, chopper approach
- B2:** Setup of specifically tailored read-out schemes for SAW sensors
- B7:** SAW sensors for MSPM and magnetorelaxometry experiments
- T1:** DBS measurements using SAW sensors
- Z1:** Support in SAW sensor fabrication
- Z2:** Support with sensor characterization and DBS measurements

3.6 Delineation from other funded projects of the principal investigator(s)

Within the BMBF project SALSA (Lofink), the research is dedicated to ferroelectric thin-film AlScN, its switching behavior, and an application in micro speakers and high electron mobility transistors. As the requirements are completely different, the design and materials selection differs from the approaches in the CRC.

All other funded projects of the principal investigators deal neither with SAW sensors nor with AlScN.

3.7 Project funding

3.7.1 Previous funding

None

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum
Doctoral researcher, 100 %	2	68.4	2	136.8	2	136.8	2	136.8	2	68.4
Total		68.4		136.8		136.8		136.8		68.4

Direct costs	Sum	Sum	Sum	Sum	Sum
consumables	6.0	13.0	8.5	7.5	5.0
Total	6.0	13.0	8.5	7.5	5.0
Total	6.0	13.0	8.5	7.5	5.0

(All figures in k€)

Dr. Lofink does not apply for a grant regarding consumables. He agrees to allocate the consumables for this Project A9 from internal resources of Fraunhofer ISIT.

3.7.3 Requested funding for staff for the new funding period

	No	Name, academic degree, position	Field of research	Department of university or non-university institution	Commitment in hours/week	Category	Funded through:
Available							
Research staff	1.	Prof. Dr. Eckhard Quandt, Professor	Functional Materials	IMS	4		Core support
	2.	Dr. Fabian Lofink, Senior Researcher	MEMS	ISIT	4		Core support
	3.	Dr. Antonio Malave, Senior Researcher	Functional Materials	IMS	2		Core support
	4.	Dr. Erdem Yazar, Senior Researcher	MEMS	ISIT	2		Core support
	5.	Simon Fichtner, Researcher	Micro Systems Technology	ISIT	4		Core support
Non-research staff	6.	Metzing, Thomas, Dipl. Ing., Technician		IMS	4		Core support
Requested							
Research staff	7.	Viktor Schell / N.N., Doctoral Res.	Functional Materials	IMS		E13	
	8.	Jingxiang Su / N.N., Doctoral Res.	MEMS	ISIT		E13	

Job description of staff (supported through available funds):

1. Prof. Dr.-Ing. Eckhard Quandt is responsible for the coordination and the scientific management of the CAU part of the project A9 and represents together with Dr. Lofink the project within the CRC and to the outside. He advises the scientific staff of the CAU in the planning and execution of the work within the project (single crystal SAW sensors) and in the interpretation of the results obtained.

2. Dr. rer. nat. Fabian Lofink is responsible for the coordination and the scientific management of the ISIT part of the project A9 and represents together with Prof. Quandt the project within the CRC and to the outside. He advises the scientific staff of the ISIT in the planning and execution of the work within the project (thin film SAW sensors) and in the interpretation of the results obtained.
3. Dr. Antonio Malave is the responsible scientist for the operation of the Kieler Nanolabor. He will support the doctoral researcher in the selection, planning, and execution of the MEMS processes in Kiel.
4. Dr. Erdem Yazar will support the doctoral research at ISIT with respect to SAW characterization and integration of magnetostrictive material.
5. Simon Fichtner will support the doctoral research at ISIT with respect to ferroelectric AlScN.
6. Dipl.-Ing. Thomas Metzging will support the doctoral researcher in all issues regarding maintenance of different devices.

Job description of staff (requested):

7. Viktor Schell/N.N. will be responsible for part of the scientific work within this project. This person will work at the CAU (Prof. Quandt) and will be in charge of the work packages related with SC SAW sensors.
8. Jingxiang Su/N.N. will be responsible for part of the scientific work within this project. This person will work at the ISIT (Dr. Lofink) and will be in charge of the work packages related to thin film SAW sensors.

3.7.4 Requested funding for direct costs for the new funding period

(All figures in k€)	2020/2	2021	2022	2023	2024/1
Funds available CAU	1.5	3.0	3.0	3.0	1.5
Funds available ISIT	10.0	20.0	20.0	20.0	10.0
Funds requested CAU	5.0	13.0	11.5	7.0	3.5
Funds requested ISIT	0.0	0.0	0.0	0.0	0.0

Equipment up to k€ 10, software, consumables for 2020/2

Chemicals for polymeric guiding layer (PMMA)	k€	1.0
Lithography masks (a set of three)	k€	1.5
Quartz wafer (20 pcs)	k€	1.0
LiNbO ₃ wafer (20 pcs)	k€	1.5

Equipment up to k€ 10, software, consumables for 2021

Chemicals for polymeric guiding layer (BCB resin)	k€	3.0
Lithography masks (two sets of three)	k€	3.0
Quartz wafer (20 pcs)	k€	1.0
Langasite wafer (15 pcs)	k€	6.0

Equipment up to k€ 10, software, consumables for 2022

FeGaB- und FeGaC-Targets	k€	6.0
Lithography masks (two sets of three)	k€	3.0
Quartz wafer (20 pcs)	k€	1.0
LiTaO ₃ wafer (20 pcs)	k€	1.5

Equipment up to k€ 10, software, consumables for 2023

LiNbO ₃ wafer (20 pcs)	k€	1.5
Lithography masks (a set of three)	k€	1.5
Al Target (10")	k€	2.0
Electronic consumables (for readout and characterization setups)	k€	2.0

Equipment up to k€ 10, software, consumables for 2024/1

Electronic consumables (for readout and characterization setups)	k€	2.0
Lithography masks (a set of three)	k€	1.5

3.1 General information about Project A10(N)

3.1.1 Project title: Magnetic Noise of Magnetoelectric Sensors

3.1.2 Research area: 406-02 Synthesis and Properties of Functional Materials

3.1.3 Project leaders

McCord, Jeffrey, Prof. Dr.-Ing.
06.10.1965, German

Wulfinghoff, Stephan, Prof. Dr.-Ing.
23.12.1982, German

Nanoscale Magnetic Materials – Magnetic Domains
Institute for Materials Science
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Computational Materials Science
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E-Mail: swu@tf.uni-kiel.de

Do any of the abovementioned persons hold fixed-term positions? No.

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

A detailed understanding of magnetic noise behavior in magnetoelectric (ME) sensor structures is of fundamental interest for the realization of magnetic field sensors with ultra-low detection limits, as many promising sensor approaches of the CRC are presently limited in their performance due to magnetic noise. The aim of this project is to comprehend and quantify the influence of geometrical and physical imperfections as well as the connected magnetic microstructure on the magnetic noise of ME sensors. Defects of magnetic relevance include physical and geometrical deviations, which differentiate the real system from an idealized one. The nucleation and the behavior of magnetic domains and domain walls are highly related to the defect structure of the system. Examples of imperfections are local geometrical errors, non-uniform magnetic material properties, and local eigenstresses, all of which will influence the magnetic structure of the magnetic layers and its ME response characteristics.

To achieve the aforementioned goal, dedicated experimental methods, for example, time-resolved in-situ magneto-optical magnetic domain response analysis and local noise measurements, will be combined with high-resolved and adaptive micromagnetomechanical simulations including adaptive discretization approaches and scale transition methods. For the modelling, transfer functions will be derived, revealing the influence of geometrical and physical imperfections on the measured noise. The influence of material properties, sensor designs, and fabrication processes will be investigated numerically and experimentally. Different ME sensor concepts under consideration within the CRC (electrically modulated, surface acoustic wave, and soft composite-based sensors) will be covered in combination with magnetic domain, general magnetic, and noise investigations on well-defined model structures exhibiting artificial imperfections and tailored micromagnetic features. Our strategy will permit achieving accurate and direct insights into the exact influence of imperfections on the magnetic domain behavior and thus the magnetic noise. From comparing the results, a fundamental understanding of the role of different scales in time, depending on the operational

frequency, and space will be developed. From the relevance to the magnetic noise behavior, we will derive targeted strategies for noise reduction as well as identify possible feasibility limits.

3.3 Research rationale

3.3.1 Current state of research and preliminary work

Correlation of micromagnetic activity with sensor noise

Magnetic domain activity is a significant factor determining the performance of magnetic layer-based magnetic field sensors. From magnetoresistive sensor applications, it is known that the signal-to-noise ratio (SNR) of such sensors is strongly dominated by the activity of magnetic domains and domain walls [Ts81, Pu07]. Magnetic domain fluctuations lead to a $1/f$ -noise dependence [Wa98]. The sensitivity of the magnetic sensors to domain behavior is based on the occurrence of local rearrangement processes of the domains as well as interactions of the domain walls with defects or inhomogeneities within the magnetic layers. Such discontinuous or erratic rearrangement processes can be detected by magnetooptical (MO) measurement techniques [Ca01, Pi05, Ry07], but have so far mostly been measured inductively. General discussions on magnetic noise mechanisms, magnetic losses, and magnetic domain effects and its interconnection can be found in [Be98, Ji15]. The effects do not only depend on the basic domain structure but are also determined by the type of magnetic domain walls, which can be seen, e.g., in the magnetic layer thickness dependence of Barkhausen jumps, which correlate with the changes in the domain wall structure [Wi77, Pu07]. For recording heads, a connection between shield domain activity and sensor noise [Na99, Mc03] exists, which is related to magnetic hysteresis effects and domain activity in the magnetic shields.

The use of magnetostrictive layers for sensor applications, as in the case of ME film sensors, complicates the situation. In such systems magnetoelastic effects together with locally varying stress contributions play a crucial role for the resulting magnetic domain or microstructure [Mc04a, Ur14]. For magnetoelectric sensors, magnetic noise has become the major obstacle to achieve better SNR. For exchange biased cantilever-based sensors with magnetic domain stabilization [La14], a thickness limit for the ferromagnetic layer was established [A10-6, A10-10] that suggests a connection to magnetic domain formation for the exhibited noise in the sensor structures. Magnetic domain formation is more pronounced for larger ferromagnetic layer thicknesses due to the increasing demagnetization. Other possible effects like edge effects due to patterning, increasing film roughness with increasing layer thickness, structural inhomogeneities in the amorphous phase, and other local variations of effective magnetic properties have not been considered so far. Eliminating magnetic domains through controlling the effective demagnetization has led to a strong reduction of noise [A10-2], the level of which is still not at the level needed. Despite being of high relevance, the amount or degree of noise contributions stemming from the actual magnetic inhomogeneities, magnetic domain structures, and structural imperfections is not known. Magnetooptical (MO) microscopy [A10-9, Ur16] has proven to be an essential tool for the investigation of domain activity in magnetic materials. Direct correlations of magnetic and domain activity [Qi19] can be derived by combined MO imaging and electrical measurements. MO imaging gives direct access to the magnetic domain processes, especially in magnetic films, and can be performed at all the relevant time scales [A10-9, Ur16] for existing and envisioned ME sensor devices. Overall it is known that a connection exists between details of the micromagnetic structure, particularly magnetic domain nucleation and annihilation, and the noise behavior in magnetic materials. The complementary way to address the micromagnetic structure is by modelling.

Micromagnetomechanical modelling and simulation

Most micromagnetomechanical studies present solutions of the Landau-Lifshitz-Gilbert (LLG) equation being coupled with the linear momentum balance and suitable constitutive equations. For example, Challab et al. [Ch19] use finite elements (COMSOL) for the micromagnetic modelling of nanostructures subject to heterogeneous strain fields (see also [Sr16, Zh16]). Bruckner et al. [Br18] carry out finite-element simulations of micromagnetic thermal noise based on ferromagnetic resonant modes of magnetic nanostructures and draw connections to the noise in sensors. Ryo et al. [Ry17] investigate exchange coupled nanocomposite multilayer thin films, as they are used in certain magnetoelectrical sensors. Furthermore, different authors propose to carry out micromagnetic simulations within a phase-field framework, which in most cases is nearly equivalent to approaches using the LLG equation [Wa13, Zh16]. In many cases, the application of Fast-Fourier-transforms accelerates the computations significantly, which is of particular relevance in three-dimensional multiphysical problems [Ya14]. Miehe et al. [Mi12, Et15, Sr16] present a multi-scale variational approach to micromagnetomechanics based on an incremental potential being consistent with the LLG equation (neglecting precession effects). On the numerical side, they propose to use the exponential map to meet the constraint on the magnetization vector length to be constant in time. This side-condition is also addressed by Dornisch et

al. [Do18] in their work on the modelling of multiferroic heterostructures. Further work on numerical aspects is given by Gusenbauer et al. [Gu19], who propose a procedure for automatic finite element mesh generation with adaptive mesh size, and by Hertel et al. [He19], who investigate the usage of H2-matrices to speed up the solution of the large equation systems in micromagnetics. An overview of the current state of the art in micromagnetic simulations of ferromagnetic materials and an outlook is given by Leliaert and Mulkers [Le19].

Preliminary work

Experimental characterization of magnetic noise in ME sensors induced by domain wall activity

Recently, we were able to directly connect specific magnetic domain behaviors in magnetically modulated thin film ME composite sensors to the exhibited effective noise levels. In this case, through simultaneous ME response and magneto-optical microscopy measurements as well as additional complementary noise and limit-of-detection (LOD) measurements, we were able to relate distinct magnetic domain activities to different regimes of magnetic noise. Through in situ magneto-optical domain observations in combination with ME sensor measurements, we showed how individual magnetic domain processes contribute differently to the sensors' noise density (Fig. A10-1), SNR value, and LOD. We could show that transitions between magnetic domain states with differing domain densities and local effective magnetic anisotropy perturbations directly influence the sensor signals and the effective noise levels. As a result, the LOD of the sensor deteriorates by orders of magnitude depending on the discrete magnetic domain characteristics. By this means, it became clear that the performance of magnetic field sensors is dominated by the revealed physical micromagnetic processes. We could also show that the exact nature of the hysteretic magnetic domain processes is relevant for specific noise contributions to the magnetic signal. The amount of hysteresis is directly connected to the magnetic noise. We concluded that the connected noise density is the most central figure of merit for improving sensor performance. Focusing on the removal of magnetic noise is the first choice for sensor advancement.

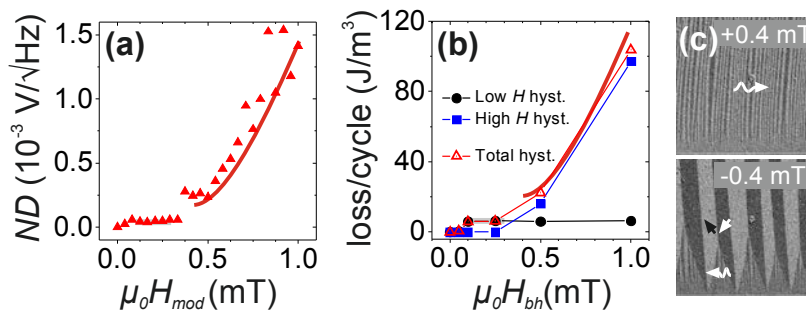


Figure A10-1: Direct connection between magnetic domain-induced magnetic hysteresis and magnetic noise. (a) Magnetic field dependency of noise density, (b) magnetic losses from hysteresis, and (c) related high field magnetic change in magnetic domain patterns responsible for the strong increase in noise for high magnetic fields.

For other ME sensor systems within the CRC, the interrelation of magnetic domain activity and magnetic imperfections is not straightforward. This is especially true for SAW sensors [Ki18] (A9), which operate at frequencies where magnetization dynamics, also of the magnetic domain walls, become relevant. We have long-standing experience in the imaging of magnetic domain effects at frequencies ranging from DC to GHz [A10-9, Ur16, Ho17]. With the excitation at high frequencies, magnetic resonance effects in the domain walls lead to individual, non-linear, spin-wave-like magnetization responses influencing the total magnetization behavior [Mo15]. Time-resolved MO microscopy of excited SAW-based ME sensors revealed similar micromagnetic effects (Fig. A10-2(a)).

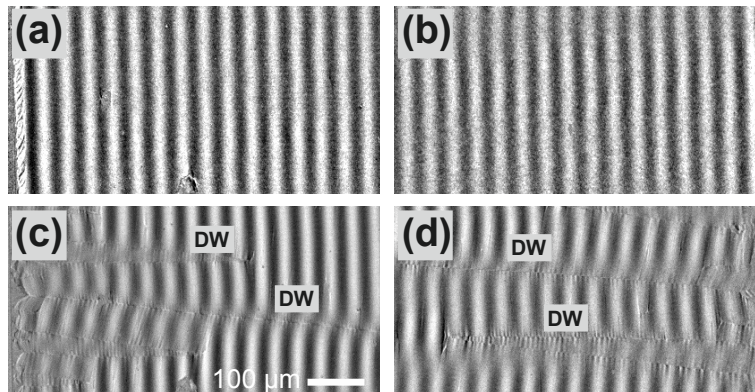


Figure A10-2: Wave propagation in a SAW sensor imaged by time-resolved magneto-optical domain imaging in a magneto-electric SAW-based sensor at 150 MHz at the left edge (a),(c) and right edge (b),(d) with and without magnetic domains (wave vector points to the right). Wave induced local magnetization rotation and lossy domain wall response are visible. Interaction with magnetic “imperfections” like magnetic domain walls exist. A local reduction of magneto-optical contrast at the domain walls relates to absorption and reflection of the surface waves.

We could show that dynamic MO imaging at operational frequencies provides direct insights into lateral shear wave propagation. Quantitative information on the wavelength and the SAW damping inside the sensor can be extracted from the MO signal. We further discovered diffraction of surface waves from physical and magnetic defects. Domain walls emit additional magnetization waves and act as sources of wave reflection (Fig. A10-2). The magnetic processes are expected to be hysteretic or lossy in character, which is also indicated

by a lateral SAW amplitude loss at the domain walls. From our first experiments with varying the magnetic domain structures in SAW sensor elements, there seems to be a strong connection between the sensor noise and domain wall activity. Yet, because the processes are different from lower frequency magnetization processes, the effects on sensor noise are not known.

Also for electric modulated sensors (A7) [Ha18], the situation is different, because no magnetic field contribution is responsible for the change of magnetization, but a periodic variation of the effective magnetic anisotropy is [Mc04]. Dynamic domain experiments show strong magnetic domain activity at electrical modulation (Fig. A10-2(b)). A quantitative evaluation of the acting magnetic hysteresis processes and their influences on noise is still missing. In order to obtain a clearer picture and to assess the influence of the various structural defects and micromagnetic effects on the sensor noise density and thus the sensor performance, modelling of the individual effects and their influence is essential. By direct comparison to experimental data, the most relevant parameters for sensor improvement can be identified, which result in recommended actions for sensor design, fabrication, and excitation. Understanding and specifically quantifying the noise contributions is crucial for achieving the sensor performance goals within the CRC.

Complex material models and multi-field problems

The functionality of ME composite sensors, as described in the previous sections, hinges on a well-coordinated interplay of magnetic, electric, and mechanical fields with highly nonlinear and history-dependent material behavior. Simulations of such systems require multi-field methods in combination with the numerically efficient modelling of complex material behavior. Results from preliminary work [A10-5, A10-7, A10-8, Wu13, Wu15] focusing on such complex multi-field models, are shown in Fig. A10-3.

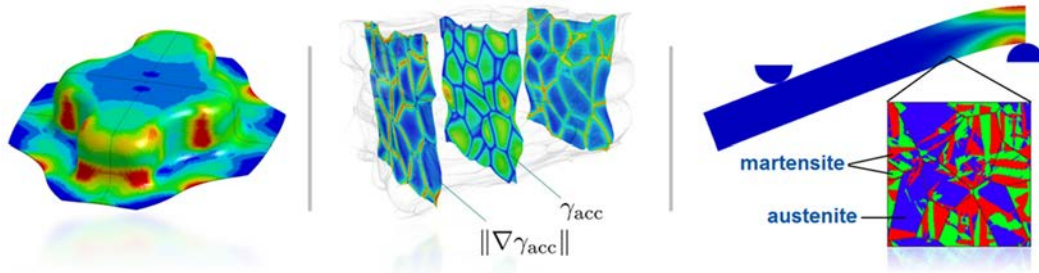


Figure A10-3: Examples of multi-field models. (a) Simulation of an electromagnetic high-speed forming process to increase forming limits based on the coupling of a conventional elastoplastic deep-drawing process with electromagnetic impulse forming (depicted is the major strain with maximum 0.37, see [A10-7]). (b) Size-dependent crystal plasticity model resolving the plastic slips within individual grains coupled with a simplified continuum dislocation model based on the gradient of the accumulated plastic slip γ_{acc} [Wu13, Wu15]. (c) Two-scale simulation of a bending process. The macroscopic stress-strain relationship at each macroscopic integration point derives from a micromechanical simulation model including austenite/martensite phase transformations (blue: austenite, green/red: martensite variants) [A10-8].

The examples show solutions of the linear momentum balance equation, which has been coupled with Maxwell's equations, with partial differential equations related to dislocation densities and with a phase-field model. The latter was embedded into a two-scale model to capture the influence of the microstructural development on the macroscopic mechanical behavior. A further recent preliminary work [A10-3] presents a new model-order reduction technique for the computational homogenization of the nonlinear behavior of composite materials (see Fig. A10-4). This approach is called 'Hashin-Shtrikman finite element method' (HSFE).

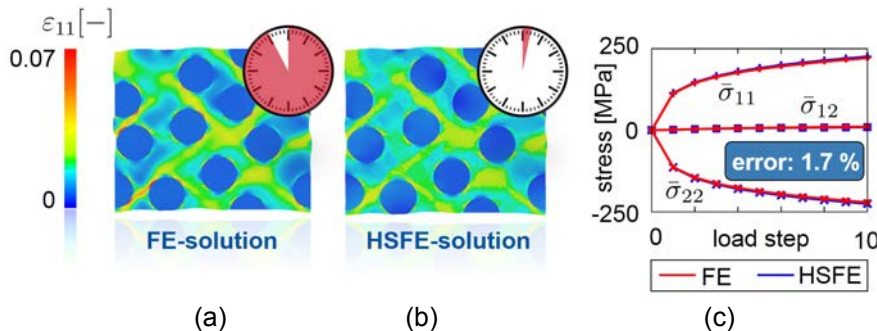


Figure A10-4: Microscopic strain distribution for (a) finite element (FE) model (~25400 degrees of freedom, ~50000 stress computations) and (b) reduced model (48 degrees of freedom, 16 stress computations, speed-up: ~700). (c) Macroscopic stress components [A10-3].

Furthermore, an implicit micromagnetic finite element formulation has been implemented into the academic FE-software FEAP [Ta18]. To meet the constraint of constant magnetization vector magnitude, the exponential map algorithm proposed by Miehe and co-workers [Mi12, Et15] has been implemented. The code has been

coupled with linear elasticity in order to enable simulations of magnetostrictive systems. In addition, an adaptive remeshing algorithm has been implemented for FEAP to dynamically adapt the local numerical resolution in each time step. Figure A10-5 shows an obtained equilibrium magnetization configuration in a thin film together with the local induced stress component σ_{xy} . The significance of stress and strain effects on magnetic domain behavior and dynamics has been shown by us in [A10-4], where we experimentally found the emission of sound waves due to magnetic domain wall oscillations in magnetostrictive materials and confirmed the general behavior by FEM modelling on a very basic scale. A connection of modeling and magnetic domain data related to the effective demagnetization field distribution in ΔE sensors was obtained in [A10-1].

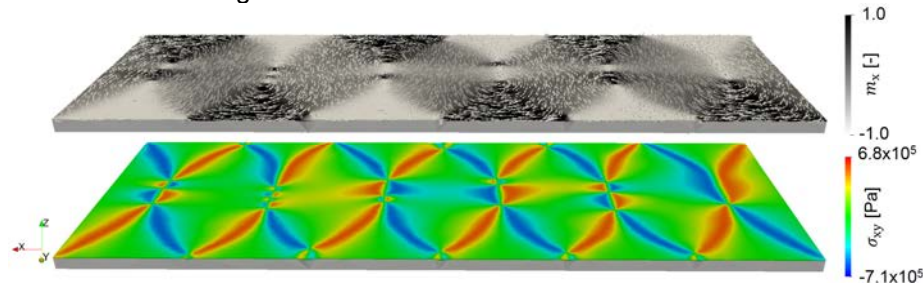


Figure A10-5: Exemplary equilibrium magnetization configuration (x-component of the magnetization direction indicated by arrows and σ_{xy} -stress component) in a thin film ($5 \text{ nm} \times 1 \mu\text{m} \times 3 \mu\text{m}$) on a substrate computed by an implicit micromagnetomechanic finite element formulation which has been implemented into the academic FE-software FEAP [Ta18]. The material parameters are those of typical magnetostrictive layers used in magnetoelectrical sensors developed in the CRC.

Linking magnetic imaging and simulations offers solutions from two sides for the comprehension of noise mechanisms in sensors. Combining magnetic imaging and modelling provides the only possibility to obtain insights into the connection between sensor noise and micromagnetic features of various kinds in a quantitative way. By tackling the micromagnetics simultaneously with experiments and modelling, an accurate understanding of relevant noise mechanisms in ME sensors will be obtained.

References

- [Be98] G. Bertotti, *Hysteresis in magnetism* (Academic press, 1998).
- [Br18] F. Brückner, M. d'Aquino, C. Serpico, C. Abert, C. Vogler, D. Suess, Large Scale Finite-Element Simulation of Micromagnetic Thermal Noise. *Journal of Magnetism and Magnetic Materials* **475**, 408-414 (2019).
- [Ca01] L. Callegaro, E. Puppini, S. Ricci, Barkhausen noise and size effects in magnetic microstructures. *Journal of Applied Physics* **90**, 2416-2421 (2001).
- [Ch19] N. Challab, A. D. Aboumassoud, F. Zighem, D. Faurie, M. Haboussi, Micromagnetic modeling of nanostructures subject to heterogeneous strain fields. *Journal of Physics D: Applied Physics* **52**, 355004 (2019).
- [Do18] W. Dornisch, D. Schrade, B.X. Xu, M.A. Keip, R. Müller, Coupled phase field simulations of ferroelectric and ferromagnetic layers in multiferroic heterostructures. *Archive of Applied Mechanics* **89**, 1031-1056 (2019).
- [Et15] G. Ethiraj, A. Sridhar, C. Miehe, Variational modeling and homogenization in dissipative magneto-mechanics. *GAMM - Mitteilungen* **38**, 75-101 (2015).
- [Gu19] M. Gusenbauer, J. Fischbacher, A. Kovacs, H. Oezelt, S. Bance, P. Zhao, T.G. Woodcock, T. Schrefl, Automated meshing of electron backscatter diffraction data and application to finite element micromagnetics. *Journal of Magnetism and Magnetic Materials* **486**, 165256 (2019).
- [Ha18] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yazar, A. Piorra, R. Knöchel, Y.K. Fetisov, E. Quandt, Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing. *Journal of Physics D: Applied Physics* **51**, 354002 (2018).
- [He19] R. Hertel, S. Christophersen, S. Börm, Large-Scale Magnetostatic Field Calculation in Finite Element Micromagnetics with H2-Matrices. *Journal of Magnetism and Magnetic Materials* **477**, 118-123 (2019).
- [Ho17] R.B. Holländer, C. Müller, M. Lohmann, B. Mozooni, J. McCord, Component selection in time-resolved magneto-optical wide-field imaging for the investigation of magnetic microstructures. *Journal of Magnetism and Magnetic Materials* **432**, 283-290 (2017).
- [Ji15] D. Jiles, *Introduction to Magnetism and Magnetic Materials* (CRC Press), (2015).
- [Ki18] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N.X. Sun, J. McCord, M. Gerken, G. Schmidt, M. Höft, R. Knöchel, F. Faupel, E. Quandt, Wide band low noise love wave magnetic field sensor system. *Scientific reports* **8**, 27 (2018).

- [La14] E. Lage, N. O. Urs, V. Röbisch, I. Teliban, R. Knöchel, D. Meyners, J. McCord, E. Quandt, Magnetic domain control and voltage response of exchange biased magnetoelectric composites, *Applied Physics Letters* **104**, 132405, (2014).
- [Le19] J. Leliaert, J. Mulkers, Tomorrow's micromagnetic simulations. *Journal of Applied Physics* **125**, 180901 (2019).
- [Mc03] J. McCord, H. Zolla, H. Grimm, Influence of magnetic properties of shields on recording head instability parameters. *IEEE Transactions on Magnetics* **39**, 2384-2386 (2003).
- [Mc04] McCord, J.; Schäfer, R.; Frommberger, M.; Glasmachers, S.; Quandt, E.: Stress induced remagnetization in magnetostrictive films. *Journal of Applied Physics* **95**, 6861-6863 (2004).
- [Mi12] C. Miehe, G. Ethiraj, A geometrically consistent incremental variational formulation for phase field models in micromagnetics. *Computer Methods in Applied Mechanics and Engineering* **245**, 331-347 (2012).
- [Mi19] MicroMagus®, <http://www.micromagus.de/>
- [Mo15] B. Mozooni, J. McCord, Direct observation of closure domain wall mediated spin-waves. *Applied Physics Letters* **107**, 042402 (2015)
- [Na99] K. Nakamoto, S. Narumi, T. Kawabe, T. Kobayashi, H. Fukui, Shield-related signal instability in magnetoresistive heads. *Journal of Applied Physics* **85**, 5846-5848 (1999).
- [Pi05] E. Pinotti, M. Zani, E. Puppini, Magneto-optical measurement of Barkhausen noise spectra. *Review of Scientific Instruments* **76**, 113906 (2005).
- [Pu07] E. Puppini, E. Pinotti, M. Brenna, Barkhausen noise in variable thickness amorphous finemet films. *Journal of Applied Physics* **101**, 063903 (2007).
- [Qi19] F. Qiu, M. Klug, M. Jovičević, G.Y. Tian, P. Hu, J. McCord, Influence of magnetic domain wall orientation on Barkhausen Noise and magneto-mechanical behavior in electrical steel. *Journal of Physics D: Applied Physics* **52**, 265001 (2019).
- [Ry07] K.S. Ryu, H. Akinaga, S.C. Shin, Tunable scaling behaviour observed in Barkhausen criticality of a ferromagnetic film. *Nature Physics* **3**, 547 (2007).
- [Ry17] H.S. Ryo, L.X. Hu, J.G. Kim, Y.L. Yang, Micromagnetic finite element study for magnetic properties of nanocomposite exchange coupled Nd₂Fe₁₄B/ α -Fe multilayer systems. *Journal of Magnetism and Magnetic Materials* **426**, 328-333 (2017).
- [Sr16] A. Sridhar, M.A. Keip, C. Miehe, Homogenization in micro-magneto-mechanics. *Computational Mechanics* **58**, 151-169 (2016).
- [Ta14] Taylor, R. L., FEAP-A finite element analysis program. (2014).
- [Ts81] C. Tsang, S.K. Decker, The origin of Barkhausen noise in small permalloy magnetoresistive sensors. *Journal of Applied Physics* **52**, 2465-2467 (1981).
- [Ur14] N. O. Urs, I. Teliban, A. Piorra, R. Knöchel, E. Quandt, J. McCord, Origin of hysteretic magnetoelastic behavior in magnetoelectric 2-2 composites, *Applied Physics Letters* **105**, 202406 (2014).
- [Ur16] N.O. Urs, B. Mozooni, P. Mazalski, M. Kustov, P. Hayes, S. Deldar, E. Quandt, J. McCord, Advanced magneto-optical microscopy: Imaging from picoseconds to centimeters - imaging spin waves and temperature distributions (invited), *AIP Advances* **6**, 055605 (2016).
- [Va14] Vansteenkiste, A., Leliaert, J., Dvornik, M., Helsen, M., Garcia-Sanchez, F., & Van Waeyenberge, B., The design and verification of MuMax3. *AIP Advances* **4**, 107133 (2014).
- [Wa98] Wallash, A.; A study of voltage fluctuation, noise and magnetic instability in spin valve GMR recording heads.; *IEEE Transactions on Magnetics* **34**, 1450-1452 (1998).
- [Wa13] J. Wang, J. Zhang, A real-space phase field model for the domain evolution of ferromagnetic materials. *International Journal of Solids and Structures* **50**, 3597-3609 (2013).
- [Wi77] N.J. Weigman, Barkhausen effect in magnetic thin films: Experimental noise spectra. *Applied physics* **12**, 157-161 (1977).
- [Wu13] S. Wulfinhoff, E. Bayerschen, T. Böhlke, A gradient plasticity grain boundary yield theory, *International Journal of Plasticity* **51**, 33-46 (2013).
- [Wu15] S. Wulfinhoff, T. Böhlke, Gradient crystal plasticity including dislocation-based work-hardening and dislocation transport. *International Journal of Plasticity* **69**, 152-169 (2015).
- [Ya14] T. N. Yang, J. M. Hu, C. W. Nan, L. Q. Chen, On the elastically coupled magnetic and ferroelectric domains: A phase-field model. *Applied Physics Letters* **104**, 202402 (2014).
- [Zh16] H. Zhang, X. Zhang, Y. Pei, A finite element based real-space phase field model for domain evolution of ferromagnetic materials. *Computational Materials Science* **118**, 214-223 (2016).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [A10-1] B. Spetzler, C. Kirchhof, E. Quandt, **J. McCord**, F. Faupel, Magnetic sensitivity of bending-mode delta-E-effect sensors, *Physical Review Applied* **12**, 064036 (2019).

- [A10-2] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. Salzer, M. Höft, E. Quandt, D. Meyners, **J. McCord**, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors, *Applied Physics Letters* **114**, 192410 (2019).
- [A10-3] **S. Wulfinhoff**, F. Cavaliere, S. Reese, Model order reduction of nonlinear homogenization problems using a Hashin–Shtrikman type finite element method, *Computer Methods in Applied Mechanics and Engineering* **330**, 149-179 (2018).
- [A10-4] R.B. Holländer, C. Müller, J. Schmalz, M. Gerken, **J. McCord**, Magnetic domain walls as broadband spin wave and elastic magnetisation wave emitters. *Scientific Reports* **8**(1), 13871 (2018).
- [A10-5] Y. Kilicar, I.N. Vladimirov, S. **Wulfinhoff**, S. Reese, O.K. Demir, C. Weddeling, A.E. Tekkaya, M. Engelhardt, C. Klose, H.J. Maier, M. Rozgić, M. Stierner, Finite element analysis of combined forming processes by means of rate dependent ductile damage modelling, *International Journal of Material Forming* **10**, 73-84 (2017).
- [A10-6] V. Röbisch, S. Salzer, N. Urs, J. Reermann, E. Yasar, A. Piorra, C. Kirchhof, E. Lage, M. Höft, G. Schmidt, R. Knöchel, **J. McCord**, E. Quandt, D. Meyners, Pushing the detection limit of thin film magnetoelectric heterostructures, *Journal of Materials Research* **32** (2017).
- [A10-7] Y. Kilicar, O.K. Demir, M. Engelhardt, M. Rozgić, I.N. Vladimirov, S. **Wulfinhoff**, C. Weddeling, S. Gies, C. Klose, S. Reese, A.E. Tekkaya, H.J. Maier, M. Stierner, Experimental and numerical investigation of increased formability in combined quasi-static and high-speed forming processes, *Journal of Materials Processing Technology* **237**, 254-269, (2016).
- [A10-8] J. Kochmann, **S. Wulfinhoff**, S. Reese, J.R. Mianroodi, B. Svendsen, Two-scale FE–FFT-and phase-field-based computational modeling of bulk microstructural evolution and macroscopic material behavior, *Computer Methods in Applied Mechanics and Engineering* **305**, 89-110 (2016).
- [A10-9] **J. McCord**, Progress in magnetic domain observation by advanced magneto-optical microscopy (Topical Review), *Journal of Physics D: Applied Physics* **48**, 333001 (2015).
- [A10-10] V. Röbisch, E. Yasar, N. O. Urs, I. Teliban, R. Knöchel, **J. McCord**, E. Quandt, D. Meyners, Exchange biased magnetoelectric composites for magnetic field sensor application by frequency conversion, *Journal of Applied Physics* **117**, 17B513 (2015).

3.4 Project plan

Objectives

The overall aim of the projects on sensor technology is to obtain ME composite sensors with sufficiently high SNR at low frequencies to enable the targeted biomagnetic measurements. In this context, project A10 concentrates on the understanding and quantification of the influence of geometrical and physical imperfections as well as the magnetic microstructure itself on magnetic noise contaminating the signals of ME sensors developed in the CRC and thereby limiting their application range. “Imperfections” denotes any physical and/or geometrical deviations which differentiate a real system from an idealized one. Structural examples are given, e.g. by shape irregularities as well as interface roughness. From the magnetic material point of view, examples are given by complex eigenstress distributions together with magnetoelastic interactions in the magnetostrictive phase or heterogeneous material properties, e.g., laterally varying amplitude and direction of easy axis of magnetization or exchange bias. The effective local magnetic properties then determine the magnetic domain structure and magnetic domain wall density, which in the above context can be viewed as a magnetic defect. The domain structure then influences the magnetic activity in the magnetostrictive phase.

The first basic working hypothesis of the project is that structural and magnetic imperfections (as defined above) determine the local reorganization processes of the magnetic microstructure. The second hypothesis is that these processes are measured as noise on a larger scale which critically limits the sensor performance. The third hypothesis is that this linkage between imperfections, magnetic microstructure, and noise can be quantified by new procedures of investigation being developed in this project based on the close interaction between experiment and theory and on starting with a common foundation of systems that are equally open to modelling and experiment. Of particular interest is the influence on the magnetic domain wall activity which may be characterized by an increased number of local switching events that contribute thus to the sensor noise. However, this local picture might be a too simple and an insufficient view. In order to gain universal insight into the topic, the research will not be restricted to a special sensor type but to three different sensor concepts that are being developed in the CRC. More specifically, the focus will be on electrically modulated sensors (coop. with **A7**), surface acoustic wave sensors (with **A9**) and sensors based on magnetostrictive soft composites (coop. with **A2**). Each of the sensor concepts comprises different types of magnetic actuation response and activity on different length and time scales. It will be investigated to what extent magnetic processes in the different sensors can be traced back to their micromagnetomechanical origin. Since the magnetic noise is considered the main limitation on the sensors’ LOD, the knowledge obtained in this project is crucial

for the derivation of sensor improvement strategies to be developed in cooperation with the other projects. The research involves the following objectives:

The **first objective** is to classify those imperfections which are expected to have the strongest impact on magnetic noise. For the modelling, this involves developing a concept for their quantification particularly based on statistical descriptors. Simple examples are given by the arithmetic average roughness R_a or the ten-point mean roughness R_z as statistical measures for the surface quality.

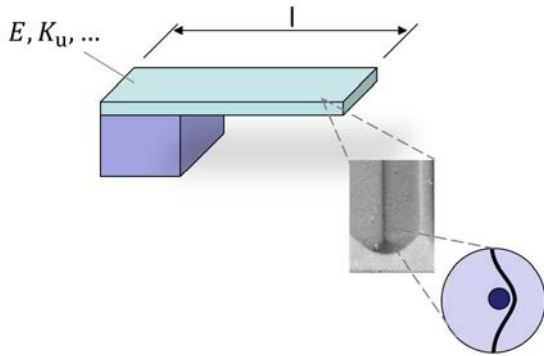


Figure A10-6: Illustration of three length scales relevant for magnetic noise: “sensor”-scale, “domain structure”-scale (MO image displaying magnetoelastic edge effects in a ME sensor from [Ur14]) and “domain wall”-scale. Possible imperfections are heterogeneous material properties (e.g. effective anisotropy K_u or Young’s modulus E) or geometrical deviations.

The **second objective** is to obtain fundamental insight about the impact of imperfections on domain reorganization processes under external stimuli, like applied magnetic field or periodic magneto-elastic excitations. The aim is to design and use experimental and simulation procedures for the comparative investigation of well-defined model systems with precisely defined properties (of imperfections).

The **third objective** is the development of noise characterization methods. In particular for the modelling part, a multiscale-like characterization method includes the identification of transfer functions which connect the fast local magnetic processes on small scales with the overall measured noise and thus bridge the scales from individual magnetic domain wall activity and microscopic imperfections to their contribution to the macroscopic sensor scale (Fig. A10-6). From an experimental point of view, this includes the development and execution of statistical domain imaging methods.

The **fourth objective** is to obtain generic insights into the dominant magnetic noise mechanisms as a function of various imperfection types by applying the developed experimental and simulation methods to different sensor types of the CRC. To generate clear and meaningful results, the aim is to first concentrate on small sections or simplified versions of the sensors and to subsequently transfer the obtained results to the actual full sensor systems.

The **fifth objective** is to characterize the influence of the materials used, the sensor design, and the fabrication process on the noise. Here, the sensitivity of the magnetic noise intensity with respect to variations of different material, design, and fabrication parameters will be investigated.

The **sixth objective** is the derivation of strategies for sensor quality improvement for magnetic noise reduction in individual sensors. The basis is the knowledge gained about the actual relevance of various imperfections and their adjustment to minimize their contribution to noise mechanisms.

Proposed research methods

Sample preparation – For the general layer and sample preparation, we rely on the projects **Z1**, **A2**, **A7**, and **A9**. Special thin films will be deposited in cooperation with **A1**. The design of the lithographic mask and the patterning of the model structures will be concluded in **A10**.

Magnetic characterization – Magnetic properties of imperfect magnetic films and sensor structures will be investigated by complementary measurements of inductive (volume) magnetization loops, e.g. fluxmetric BH loop measurements and surface layer sensitive time-resolved MO magnetometry. The local magnetic domain behavior will be analyzed by quasi-static and time-resolved MO microscopy. Domain imaging will be carried out with in situ noise measurements at the operation frequencies of ME model and device structures. Different domain imaging setups are available for the investigations which can be grouped into high-resolution MO setups with variable time-resolutions and large-view MO microscopes for the analysis of complete large sensor structures. Using MO imaging methods based on the quadratic Voigt effect [Ur16] we will draw direct conclusions on the local magnetostrictive response. The connection between domain and ME, respectively noise performance is further achieved by complementary or simultaneous measurements of the magnetic response and noise characteristics. A current limitation in our experimental setups is on time-resolved magnetic imaging, for which the relevant frequency ranges are in most cases not addressable with our current setups. An extension of the time-resolved imaging for flexible time-resolution needed for the investigation of SAW devices (**A9**) to conclude with the narrow bandwidth of electrical excitation and for future electrically modulated ME sensors (**A7**) will be implemented within this project (we apply for funding for a flexible laser illumination

source within this project). With advanced MO microscopy, a complete picture of the local micromagnetoelastic behavior will be obtained. Magnetic noise effects will be further investigated by single shot dynamic magnetic imaging that permits direct insight into the discontinuity, the irreversibility, and the reproducibility of the magnetization processes. Complementary measurements of ME properties and spectral noise densities are obtained in an acoustically and magnetically shielded setup in cooperation with **B1**.

Structure characterization – Characterization of the existing structures will be performed by optical microscopy, by atomic force microscopy (AFM), e.g., for surface roughness quantifications, and by scanning electron microscopy (SEM), e.g., for the investigations of edge effects. High resolution structural investigations on amorphous magnetic films giving insights into structural and magnetic homogeneity will be performed in cooperation with project **A6**. Internal film stresses will be characterized together with **A1**.

Modelling and simulation – A micromagnetoelastic finite element formulation has been implemented in the scientific open source code FEAP [Ta14]. It gives full control over all model details (e.g., choice of the different magnetic energy contributions and magnetoelastic coupling), its discretization, and the solution process. Different parallel solvers are readily available and already partially in use. Due to their three-dimensional, multiphysical, and nonlinear character, the intended simulations are numerically challenging. It is expected that a multitude of magnetic domain walls needs to be simulated for the planned noise investigations. We will therefore implement a new computational strategy specifically tailored to speed up micromagnetic problems involving domain wall activity, which is expected to significantly reduce the computational effort (see WP 2). For the simulations, access to the following clusters and high performance computing systems is available: (1) Hybrid NEC High Performance Computing (HPC) System including an NEC HPC-Linux-Cluster (6192 cores in total, 404.4 TFlops) and NEC SX-ACE Vector system (65.6 TFlops); (2) HLRN (North-German Supercomputing Alliance) system (87,500 cores with a total peak performance of 2.7 PFlops); (3) Two Linux-clusters (1948/280 cores). Additional simulations of certain aspects like roughness effects, local anisotropy dispersion, domain walls, and the verification of the implementation will be performed using the micromagnetic simulation packages Micromagus® [Mi19] and Mumax³ [Va14]. Multiphysics simulations on the full sensor scale will be carried out by project **A8**, providing boundary conditions for the microscopic simulations of this project. In turn, magnetic noise results will be passed back to **A8**.

Work packages

The objectives of this project will be addressed in five work packages (WPs) according to the time schedule in Table 1. The details of the individual work packages are discussed in the following.

Table 1: Work schedule - Work done by group Wulfighoffs (red) and group McCord (blue)

	2020		2021				2022				2023				2024	
	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP1: Experimental tasks – establishing preconditions for experiments																
WP2: Development of efficient magnetoelastic simulation methods																
WP3: Investigations of simple model structures																
WP4: Magn. noise of simplified/real sensors																
• Electrically modulated sensors																
• Surface acoustic wave sensors																
• Soft composites																
WP5: Sensitivity analysis and noise reduction techniques																

WP1 Experimental tasks – establishing preconditions for experiments

Within this work package we will install a laser system for the spatial and temporal magnetic response investigations of ME devices (WP4). The laser will be especially adaptable to the operational frequencies of the SAW (**A9**) and electrically modulated sensor devices (**A7**) of interest. In order to match the sharp resonance frequencies of the SAW devices, a laser system with 1 MHz repetition rate together with a timing synchronizer is needed to be integrated into the existing MO microscopes. It will also provide enough bandwidth for the planned higher excitation frequencies for electrically modulated sensors in **A7**. We ask for funding for the pulsed laser illumination source within this proposal. Flexible electronics for driving the SAW and electrical modulation devices in the MHz to GHz range during MO imaging already exist. For the investigations of model

structures (WP3), a bending and shear stage will be designed, fabricated, and implemented in the MO microscopy setups. This will permit the initial comparison of experimental and simulation results. It will further enable studying the effect of magnetic anisotropy strength [Mc04a] and variations on the micromagnetic behavior.

WP2 Development of efficient magnetoelastic simulation methods

In this work package, the simulation methods for the micromagnetomechanical noise simulations will be developed. These methods are a prerequisite to address the individual objectives in the subsequent work packages. The planned simulations comprise simple model structures in the form of mechanical specimens coated by thin magnetostrictive films (see WP3) as well as different sensor types based on magnetostrictive thin films and composite materials (coop. with **A2**, **A7**, and **A9**, see WP4). To begin, for the films we will assume constant magnetization over the thickness of the thin films which will thus be modelled as two-dimensional objects (reducing the computational effort related to the magnetization). However, the magnetic field in the surrounding free space and the mechanical specimens carrying the thin films (WP3) will be computed in three dimensions. The three-dimensional remeshing tool, mentioned in the preliminary work, will be used for a high numerical resolution of the domain walls and their environment. As a result, the high-resolution area is mainly restricted to the quasi-two-dimensional magnetostrictive thin films, thus significantly reducing the computational effort.

In WP4, different sensor concepts will be investigated. This requires the resolution of a multitude of complex interactions of domain walls with imperfections and other domain walls. To cope with these numerical challenges, plans are to develop a new adaptive discretization strategy which is particularly suited for micromagnetic simulations. It is based on the observation that, typically, the magnetic activity is concentrated in certain domain walls while the solution remains nearly constant over long time periods in large areas, namely within the domains and inactive domain walls. Primarily, the inactive domain walls are unnecessarily costly, since they need a fine mesh to be resolved. It is thus planned to exploit the hierarchical mesh structure inherent to the adaptive remeshing scheme by approximating locally the aforementioned small magnetization changes by using the shape functions of the coarser underlying mesh, but only as long as the domain walls remain nearly inactive. In this way, the fine resolution of inactive walls can be kept, while the small wall motion is captured by a reduced (and thereby numerically cheap) set of degrees of freedom. A further efficiency gain can be obtained based on a linearization of the nearly inactive wall behavior. It is roughly estimated that the new adaptive discretization method may allow speed increases up to ten-fold (depending on the problem) in addition to the large gain already obtained from the adaptive remeshing scheme. Furthermore, the coupling of mechanical and magnetic field quantities needs to be evaluated. It is expected that the coupling can be considered one-directional in some cases. This would allow for a significant reduction of the numerical costs based on one-directional numerical coupling schemes.

WP3 Investigations of model structures

The major goal of this work package is the investigation of fundamental interactions of domain walls with each other and with imperfections from an experimental and simulation point of view. The work package addresses objectives 1 (classify relevant imperfections) and 2 (obtain fundamental insights). Therefore, simplified model structures will be studied here while more complex sensor systems are investigated in later WPs. The model structures will permit clarifying fundamental aspects of magnetization-imperfection-interactions in a well-defined environment with precisely assessed imperfections. For the experiments, magnetic structures of different types will be investigated in terms of the local magnetic behavior. Relevant substructures, for instance, periodic magnetic domain patterns or certain defects, will be identified. Based on this, suitable submodels of the investigated structures will be defined for the simulations assuming, e.g. periodic boundary conditions, as the simulation of the whole magnetic microstructure is expected to be numerically too costly to be fully resolved. It is expected that the obtained insights will already be useful in deriving first measures to decrease magnetic noise, which will then be passed to the materials (**A1**) and sensor projects. Matching simulation with experiments and laying the foundations for the sensor experiments (see WP4) is in the focus of the work package.

Plans are to start the survey with patterned magnetostrictive thin films being deposited on bending specimens (like in Fig. A10-6), which thus represent a simplified version of the sensors to be analyzed in WP4. Layers will be state-of-the-art magnetostrictive layers, incorporated in the different sensors of the CRC. For the magnetic film deposition, we will rely on **A1** and **Z1**. Furthermore, shear specimens will be studied, as shear is the main loading type experienced by the magnetostrictive thin films in the surface-acoustic-wave (SAW) sensor based on the propagation of Love waves (**A9**). The intentions are to investigate specimens with different thicknesses, film stresses, different patterning dimensions and features, and also varying well-defined imperfection-types (e.g., shape irregularities, surface roughness, eigenstresses, magnetic anisotropy dispersion) and -intensities to quantify the effect of the latter on the magnetization reorganization processes. Nonuniform material properties will be estimated while also considering structural information provided by **A6** with a focus on the influence of structural and magnetic features of the magnetostrictive phase on all relevant length scales. With this, first insights on the relevance of different imperfection types for the magnetic noise will be obtained.

The most relevant length scale for the investigations is that of individual domain walls and local domain structures, the behavior of which strongly contributes to the magnetic noise. The correlation of local magnetic reorganization processes with the noise in individual sensor signals is subject of WP4. Depending on the results of WP4 and WP5, additional modified model structures will be reinvestigated.

First, it is planned to experimentally investigate and numerically reproduce the effects of film stress on micro-magnetic structures. Internal film stress, e.g. influenced by deposition and annealing procedures in conjunction with stress relaxation, play an important role here. Furthermore, from experiments it is clear that the reduction of magnetostrictive self-energy processes play an important role in the magnetic domain formation [Mc04a, Ur14]. Here, special focus will be on the role of magnetic anisotropy strength for the formation of irregular “crumpled” magnetization structures due to magnetostrictive self-energy effects [Urs14]. This will be experimentally investigated in low magnetic anisotropy samples and reproduced by the simulations. Furthermore, it is planned to investigate the effects of both heterogeneities of the easy axis direction and the degree of anisotropy (see Fig. A10-7(a)), which are partly inherent due to the sputtering process but will preferably be introduced by post annealing procedures. In addition to these dispersion effects, geometrical imperfections on different length scales will be introduced into the specimens and the simulation models. For example, the intentions are to investigate different surface roughness values and/or boundary undulations with varying wavelengths (Fig. A10-7(b)), applied to the magnetostrictive layer as well as the substrate by surface roughening and lithography patterning, which will lead to local variations in the effective field. This would result in a nonhomogeneous magnetization distribution (Fig. A10-7(c)). Arrays of patterned structures also provide periodic conditions that can be modelled with less computing effort. Roughening can be achieved by magnetic structures deposited on thick seed layers. Before the imperfections are incorporated into real specimens, they will be investigated numerically to identify reasonable ranges for specimen sizes and imperfection magnitudes.

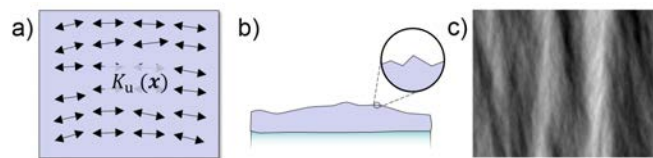


Figure A10-7: (a) Sketched top view of a magnetostrictive thin film with heterogeneous easy axis distribution. (b) Geometrical imperfections on different length scales leading to a dispersion in the effective magnetic field. (c) Calculated [Mi19] magnetization distribution of a physical property dispersive magnetic thin film (values for FeCoSiB were used for the calculations with an effective magnetic dispersion of $\Delta H = 0.1$ mT).

The effects of the different imperfections on the domain wall behavior will be characterized using MO microscopy supported by structural analysis techniques. The experimental investigations are then complemented by simulations giving details into hard-to-measure quantities, like the local magnetic field strength or the strain and stress distributions induced by magnetostriction. Here, the modification of the magnetomechanical energy landscape, as induced by the imperfections (e.g. at edges), is of particular interest. The comparisons of simulation results with experiments will also serve for the validation of the simulation methods implemented in WP2. If needed, the simulation procedures of WP2 will be modified in accordance to the experimental results. WP3 is designed to benchmark WP2. From the data of WP3, the first hints for sensor improvements will be garnered which will be evaluated with the sensor projects (in particular **A2**, **A7**, and **A9**).

WP4 Magnetic noise of simplified and real sensors

This work package aims at the extension of the fundamental investigations on simple magnetic model structures made in WP3 to actual, full sensor structures. In particular, the following objectives are addressed: objective 3 (noise characterization, derivation of transfer functions), objective 4 (obtain generic insights) and objective 5 (influence of materials, design, and fabrication). First, simplified sensor structures will be examined, and subsequently the investigations will be expanded to real ME sensors. The contribution of the magnetic microstructure to the overall sensor noise will be experimentally and numerically analyzed in detail. Similar but expanded optimization schemes, as discussed in WP3, will be applied. The work package also aims at providing the foundation for the investigations planned in WP5. WP4 is thus central to the work program planned.

Experiments have shown that certain sensor types display strong magnetic domain activity during operation and limitations in their SNR are mainly attributed to magnetic noise. Figure A10-8 displays sensor types of relevance for this project together with characteristic magnetic domain structures. The knowledge gained in this work package can be continuously transferred to the related projects to initiate steps for the improvement of the SNR. Fig. A10-8(a) illustrates a SAW sensor which exploits the ΔE effect (coop. with **A9**). Fig. A10-8(b) depicts the piezoelectrically modulated oscillation mode of a beam coated by a magnetostrictive thin film, the average magnetization of which is measured by a pick-up coil (coop. with **A7**). Both sensors induce modulations of magnetization and/or magnetic anisotropy in time and in space due to the inverse magnetostrictive effect. A connection of the related magnetization processes to the occurrence of magnetic noise is apparent.

Fig. A10-8(c) shows a sketch of a composite material which is tailored to be highly magnetoelastic by embedding magnetic particles in a mechanically soft matrix (coop. with **A2**). The application of an external field leads to a measurable elongation. The magnetization reversal modes of the particulate structure are unknown, however. The sensor concepts will be investigated according to the schedule in Table 1.

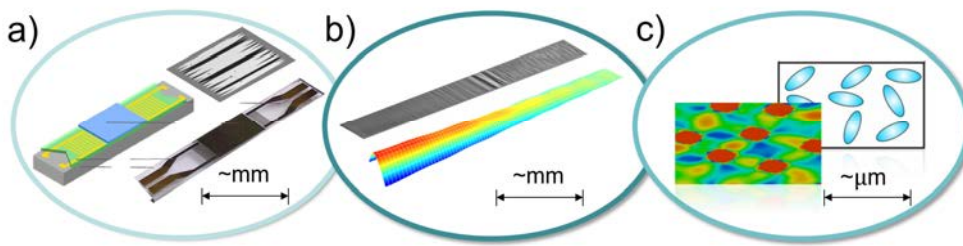


Figure A10-8: Different sensor types to be investigated in this project: (a) SAW sensor (concept and actual sensor), (b) electrically modulated sensor (depicted is the bending-oscillation mode used to trigger the inverse magnetostrictive effect) and (c) magnetostrictive soft composite. Representative, experimentally obtained magnetic domain structures in real sensors are shown in (a) and (b).

The design of the simplified sensors will be based on existing sensors structures which will be modified in such a way that the lateral dimensions of the magnetostrictive phase in all cases is within the viewing field of the MO microscope used. This will allow direct and complete identification of all micromagnetic features within the magnetostrictive layer. It will further enable complete control of varying features, e.g. the magnetic history, and thus enable an important handle with which to vary magnetic response features without changing the sensor structure. All measurements will be accompanied by a thorough electrical characterization of sensitivity, noise density, and limit of detection (in coop. with **Z2**) with varying magnetic field. From repetitive MO imaging including, if possible, single shot imaging and MO contrast analysis of the magnetic response, we will gain further insight into the reproducibility of the occurrence of certain magnetic reversal processes.

Besides the system complexity, which is now greater than in WP3, the measured sensor signals represent an additional new aspect that needs to be analyzed. As a key ingredient for the modelling, transfer functions will be established which enable the prediction of the sensor signals – sensitivity and the noise – as a function of the magnetization activity observed in the experiments and simulations. To our knowledge, this challenging task has not been addressed before in the literature. The required transfer functions can be established by coupling the developed micromagnetomechanical simulation models with additional models of the related signal-generating devices. For example, in the case of the electrically modulated sensor (see Fig. A10-8(b)), this would be a model of the pick-up coil measuring the magnetic flux modifications. Since it will be very demanding to simulate the complete magnetic structure of the sensors including all domain walls, suitable submodels will be defined by exploiting symmetries and assuming, e.g., periodic boundary conditions. With the experimental input, the relevance of the modelled features, e.g. magnetic domain segments, will be ensured. For example, in the case of the SAW sensor, we plan to restrict the simulations to a limited number of wavelengths. Furthermore, a possible submodel of the electrically modulated sensor is schematically shown in Fig. A10-9. Changes of the magnetic microstructure will then lead to noise which is captured by the pick-up coil model (not shown).

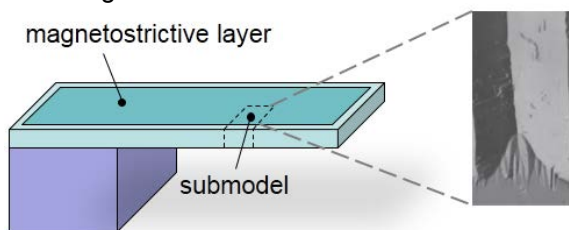


Figure A10-9: Potential submodel (dashed black line) of the electrically modulated sensor with an experimentally observed magnetic microstructure (element) from an electrically modulated ME sensor (together with A7). The time resolution for the MO experiments was 10 ns and the electrical excitation frequency was 517 kHz.

A possible submodel of the SAW-sensor is based on the introduction of a moving coordinate system that travels at the same speed as the surface acoustic waves. In this way, a subsystem consisting of a control volume including a few waves can be established (to reduce the computational cost, the lateral wave dimension may be reduced). This makes it possible to follow the waves along their way from the IDTs (interdigital transducers) across the sensor surface until they finally reach the IDTs, where the wave-induced surface deformation is measured. On their way, the waves encounter different kinds of imperfections, material property heterogeneities, and the underlying magnetic domain and domain wall structure, which are passed through the control volume and locally vary the wave speed. Thus, the interactions with the objects will lead to local distortions of the waves. Experimental indications of some of the effects already exist from MO investigations (see Fig. A10-2) that show a complex interaction pattern. When the waves reach the measuring IDTs, these distortions are measured as noise. The noisy signal can be directly deduced from the model (with an ideal

piezoelectric material model) and thus a related transfer function can be established for SAW-sensors that describes the influence of imperfections, heterogeneities, and the domain structure on magnetic noise.

Subsequently, it will be important to identify methods which allow one to conclude the overall sensor performance from the noise of the electrically modulated and SAW sensor submodels. A simple approach to achieve this is to repeat the submodel simulation several times with statistically varying imperfection configurations and to superpose the observed noise to make conclusions about the overall sensor noise spectrum. This strategy is similar to the experimental approach of imaging individual magnetic events multiple times. Experimentally, this will be achieved by the aforementioned imaging schemes but also by reinitialization of the magnetic domain structure. From differences of the noise figure with varying magnetic domain structures, further insight is expected to be gained. For the modelling, this implies the simplifying assumption that the noise predicted by the individual submodels is due to local effects and that noise interactions between the submodels can be neglected. It will then be necessary to perform a convergence study with respect to the computational domain size and number of submodel simulations to assure that no artifacts are induced into the predicted noise. The electrically modulated and SAW sensors are also simulated by project **A8** on a larger scale (complete sensor model) without resolving the magnetic microstructure. It is planned to partially use the simulation results by **A8** (e.g. as boundary conditions) for the submodels investigated in this project. For example, the vibrations of the electrically modulated sensor computed in **A8** can be used to prescribe the displacement/strain field of the submodel depicted in Fig. A10-9. The results can then directly be compared to results from dynamic MO imaging. In turn, information on the resulting magnetic noise will be passed back to **A8**.

The investigations are planned as follows. First, a basic understanding of the magnetization reorganization processes will be obtained from experiments and simulations, which need to be matched. In general, we expect more complicated behavior than for the model structures in WP3. Further knowledge will be generated by introducing well-defined imperfections into the simplified sensor models in complete analogy to the procedures applied in WP3. Identified imperfection types will be further integrated in the simulations. We will then select imperfections or features, which were observed to be dominant or of special interest. It is expected that well-defined imperfections will lead to deterministic behavior that can be probed by real-world experiments and reproduced by the computer experiments which will include standard micromagnetic simulations. In addition, frequency-dependent effects will now play a role, which were not subject to the model structures of WP3. For instance, active stimuli for the currently investigated sensor concepts vary from kHz into the hundred MHz regime (or beyond). The frequency effects in the simplified sensor structures will be probed by time-resolved MO imaging. The dynamic features revealed will be incorporated in the simulations. For the SAW sensor, further plans are to compare the noise with a continuous magnetostrictive layer and a structured layer consisting of patterned magnetostrictive islands that allow specific engineering of the magnetic domains (with **A1** and **A9**). Depending on the results on relevant defects, we will (re)investigate adjusted model structures in WP3.

Last, to establish a model for the soft composite material in Fig. A10-8(c), a periodic three-dimensional microstructural model will be formulated (coop. with **A2**). Here, it is planned to carry out purely numerical three-dimensional magnetomechanical investigations of the particles and the induced stresses and strains in the composite to identify the dependence on the parameters defining the composite. With scale transition techniques (e.g. periodic boundary conditions, field averaging), the microstructural model will be used to identify the overall magnetostrictive properties of the composite material as a function of the microstructure. This information will be used in project **A2** to design the material in terms of the matrix and particle properties such that it exhibits a preferable performance. Magnetization reversal in the composites will be probed by MO microscopy with MO indicator film techniques [A10-9] to obtain a further understanding of the possible magnetic noise effects and for comparison with the simulation results. The outcome of this work package is to explain magnetic noise based on fundamental imperfection-magnetization-domain interactions.

WP5 Sensitivity analysis and noise reduction techniques

After having established in WP4 a basic qualitative understanding of the interactions of the magnetization with various sorts of imperfections on the one hand and the consequential sensor noise on the other hand, the first scope of WP5 is to investigate the identified most noise-relevant relations in a more quantitative and systematic manner. The second scope is to exploit the newly gained knowledge for the derivation of appropriate noise reduction strategies (objective 6), which concentrate on a systematic modification of the most important factors to obtain the lowest magnetic noise. For this purpose, it is planned to determine the sensitivity of the magnetic noise intensity with respect to variations of those imperfections which have been identified in WP3 and WP4 as being most relevant, as well as variations of different parameters related to the choice of the materials, the design, and the fabrication process. In other words, it is planned to investigate the space of all parameters relevant to magnetic noise and to systematically search this space for a noise minimum. Here, one must consider the constraint that certain parameters are bounded (for example, a minimum achievable surface roughness exists). As a first step towards the search for a noise minimum, the knowledge gained in WP4 will be

used to identify a point in the parameter space, which is expected to be sufficiently close to the minimum in demand. Next, the simulation methods developed in the previous work packages will be applied to identify the sensitivities $\partial N/\partial \alpha_i$, where N denotes the noise intensity and α_i represent the system parameters controlling the noise. Based on a linearization of N , the sensitivities will then allow identifying new values α_i which are closer to the minimum by a constrained Newton-scheme. This procedure is repeated until the desired minimum is achieved, which will then be validated based on an experimental characterization of the related sensor system. The outcome of this work package is a sensor-dependent noise-minimization strategy. This derived strategy will provide a set of clear measures for the projects **A1**, **A2**, **A7**, and **A9** that indicate how tolerances, designs, materials, and fabrication processes should be defined to minimize magnetic noise. At the same time, the strategy explores the feasibility limits for noise reduction measures in the sense that it provides the minimum noise achievable. This will be especially relevant for the research in the next funding period.

Prospects

The main aim of this project is to comprehend and to quantify the exact influence of geometrical and physical effects on the magnetic noise of ME sensors. This will allow us to derive strategies for the minimization of the magnetic noise of the sensor systems developed in the CRC. It is planned that some of these new strategies will already be implemented in the upcoming CRC phase. However, the extension to further sensors systems being investigated in the CRC and the full realization of all derived steps necessary to significantly reduce magnetic noise is a long-term task which goes beyond the upcoming funding period. This route will enable further validation and continued improvement of the individual and variable knowledge-based magnetic noise reduction concepts developed in this project. In addition, the knowledge gained holds the long-term prospect of identifying those sensors which have the highest potential to satisfy prospective requirements.

3.5 Role within the Collaborative Research Centre

The global objective of our project is the research on the relevance and quantification of micromagnetic activity, contributing to the performance of the individual, pursued sensor concepts in research area A. Thereby, A10 plays a central role within the CRC to guide sensor concepts. We will strongly cooperate in sample preparation with project **Z1** and **A1**. On magnetic noise characterization we will cooperate with **B1** and **Z2**. **A10** will further contribute to the focus groups “Modelling”, “ME Sensors”, “Concepts based on ΔE effect”, and “Magnetic layers”. The doctoral researchers will be active in the IRTG. Collaborations with the following projects are planned:

- A1: Deposition of special magnetic layers. We will provide input for film requirements to A1.
- A2: Cooperation on magnetostrictive composite magnetization reversal characteristics.
- A4: Feedback on the influence of imperfections on the domain wall and noise behavior.
- A6: Structural characterization by TEM and X-ray.
- A7: Cooperation on electrically modulated magneto-electric sensor characteristics.
- A8: Combination of modelled magneto-electric sensor characteristics.
- A9: Cooperation on SAW device characteristics.
- B1: Conduction of noise density measurements.
- Z1: Fabrication of (simplified) sensor structures.
- Z2: Conduction of noise density measurements.

3.6 Differentiation from other funded projects of the project leader(s)

None of the other funded projects of the PIs deals with magnetostrictive or magnetoelectric materials.

3.7 Project funding

3.7.1 Previous funding

This project is currently not funded and no funding proposal has been submitted.

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral researcher, 100 %	2	68.4	2	136.8	2	136.8	2	136.8	2	68.4
Total		68.4		136.8		136.8		136.8		68.4
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, consumables	10.5		2.5		2.0		2.0		1.0	
Total	10.5		2.5		2.0		2.0		1.0	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation >k€ 50	76.1									
Total	76.1									
Grand total	155.0		139.3		139.3		139.3		69.4	

(All figures in k€)

3.7.3 Requested funding for staff

	Se- quen- tial no.	Name, academic degree, position	Field of research	Department of university or non-uni- versity insti- tution	Project commit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	McCord, Jeffrey, Prof. Dr.-Ing., Head of Research Group	Magnetic materials	IMS	4		Core support
	2.	Wulfinghoff, Stephan, Prof. Dr.-Ing. Head of Research Group	Model-ling	IMS	4		Core support
	3.	Dr. Kornel Richter	Magnetic materials	IMS	4		Core support
Non-research staff	4.	Robien, Sandra, Dipl.-Ing., Technician		IMS	2		Core support
Requested staff							
Research staff	5.	N.N., Doctoral Researcher	Magnetic materials	IMS		E13	
	6..	Marian Sielenkämper, Doctoral Researcher	Model-ling	IMS		E13	
Non-res. staff							

Job description of staff for the proposed funding period (supported through existing funds):

- Prof. Jeffrey McCord represents project A10 with regard to the magnetic domain investigation of the magnetostrictive films. He supervises the experimentally oriented doctoral researcher and supports planning and micromagnetic experiments, simulations, and the interpretation of the combined domain observation and noise characteristics results. He coordinates the cooperation with other projects of the CRC, in particular on specific magnetic layer deposition (**A1**) and model and sensor structure manufacturing (**A7**, **A9**). He co-coordinates the cooperation with projects that characterize the sensors.
- Prof. Stephan Wulfinghoff represents project A10 with regard to the modelling and simulation parts. He supervises the doctoral researcher carrying out the development of the numerical methods and simulation setups, the computational noise investigation of different model and sensor structures, and the survey of different sensor improvement strategies described in the working program. He coordinates

the cooperation with the modelling project **A8**. He co-coordinates the cooperation with the projects of the CRC that characterize the sensors and other relevant projects of the CRC.

3. Dr. Kornel Richter assists in the fields of high frequency MO imaging and data analysis.
4. Dipl.-Ing. Sandra Robien will contribute to the design of electronic components for the experiments.

Job description of staff for the proposed funding period (requested funds):

5. The doctoral researcher is responsible for the assembly of the mechanical and the time-resolved imaging setup (WP1), as well as the design of model structures (WP3). The researcher will conduct the MO imaging experiments on the model structures and on simple and real (WP3, WP4) sensor structures and will analyze the experimental results. He / she will conduct time-resolved domain imaging and noise measurements under the same conditions, correlate domain activity to ME response, will conduct basic micromagnetic simulations on special magnetic domain aspects, and will contribute to the selection of noise reduction strategies (WP5). The researcher will interact with the partner doctoral researcher.
6. M.Sc. Marian Sielenkämper already started to work as a researcher on the project. He significantly contributed to the preliminary work. He already possesses experience in the required modelling and simulation methods. He will be responsible for the implementation of the proposed computational strategies (WP2), the various model structure and sensor system models (WP3, WP4), and the sensor improvement strategies (WP5). The researcher will directly interact with the partner doctoral researcher.

3.7.4 Requested funding of direct costs

	2020/2	2021	2022	2023	2024/1
Existing funds from IMS	1.5	3.0	3.0	3.0	1.5
Sum of existing funds	1.5	3.0	3.0	3.0	3.0
Sum of requested funds	10.5	2.5	2.0	2.0	1.0

(All figures in k€)

Equipment up to k€ 10, software, consumables for financial year 2020/2

STANFORD RESEARCH SYSTEMS CG635 FOR LASER	5.00
The CG635 generates stable square wave clocks up to 2 GHz. It provides the frequency resolution, low jitter, and flexible output levels for the synchronization of electronics and laser.	
Mechanical and optical parts for feeding laser into the MO microscope, incl. despeckler units.	3.00
Consumables (electronics, microscope and optical parts)	2.50

Equipment up to k€ 10, software, consumables for financial year 2021

Consumables (electronics, microscope and optical parts)	2.50

Equipment up to k€ 10, software, consumables for financial year 2022

Consumables (electronics, microscope and optical parts)	2.00

Equipment up to k€ 10, software, consumables for financial year 2023

Consumables (electronics, microscope and optical parts)	2.00

Equipment up to k€ 10, software, consumables for financial year 2024/1

Consumables (electronics, microscope and optical parts)	1.00

Instrumentation for financial year 2020/2 in k€

ONEFIVE KATANA HP HIGH POWER PICOSECOND LASER	76.10
For the investigations of high frequency electrical modulated ME sensors, a laser that provides imaging capability in the (some) MHz regime and above is required. Most important, for the investigations of SAW devices, an imaging system that provides the possibility for matching the device operating frequency is needed. So far, only limited imaging experiments on SAW devices were possible. SAW devices with an operating frequency away from $N \times 50$ MHz are not accessible with our current system. A laser providing the capability for the investigation of both sensor types is required.	
The selected KATANA laser is a high power pulsed laser system in the visible range. It provides pulses of 35 ps duration and the standard pulse repetition rate can be varied from 100 kHz to 1 MHz, which is a prerequisite for SAW and electrical modulated ME sensor investigations. Continuous tuning of the repetition rate to adjust to the exact frequency of ME device operation is possible with the laser. All of these are essential requirements for the intended experiments.	

3.1 General information about Project B1

3.1.1 Project title: Sensor noise performance and analogue system design

3.1.2 Research areas:

408-01 Electronic Semiconductors, Components, Circuits, Systems

408-02 Communication, High Frequency and Network Technology, Theoretical Electrical Engineering

3.1.3 Project leader(s)

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M. Höft has a permanent position. Employment of A. Bahr will be guaranteed by state funds until 30.06.2024.

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

This project focusses on low-noise analogue signal processing and signal conditioning for maximizing the signal-to-noise ratio for the various magnetic field sensors that are being researched in the CRC. It therefore provides the essential link between sensor devices (**project area A**) and subsequent digital signal processing (**B2**). It also plays an important role in measurement system design, which is required for implementing the sensors on applications in biomagnetic diagnostics.

Thorough noise analysis for the various realizations of magnetoelectric and ΔE -effect sensors is a major area of work in order to conceive and build low-noise analogue front ends for signal acquisition. Therefore, all involved noise sources have to be investigated and appropriate descriptions, i.e. noise models, have to be developed. Generally, all noise sources can be categorized into sensor-intrinsic noise sources and noise of the readout electronics. In the interest of a minimum limit of detection, it is always required that the sensor itself contributes predominantly to the overall system noise. The noise of the sensor is therefore of particular research interest. However, to be able to characterize the sensor noise appropriately, and thus gain further insight into the underlying mechanisms, the electronics need to be designed very carefully. In particular, it is necessary to be able to quantify the noise of the measurement electronics and minimize its influence as far as possible. Research has shown that the noise behavior of the sensors is constantly improving, which in turn requires continuous adaptation of the electronics. In fact, the entire process of noise measurements, noise modeling, and adjustments of the sensor electronics can be understood as an iterative process which needs to be performed for every type of sensor system and change in sensor design. The process described has

already been performed for various types of sensor systems and will be expanded to include recently developed sensor concepts within the CRC, e.g. electrical frequency conversion with inductive readout.

In addition to well-established sensor concepts, novel readout methods will be investigated. Instead of utilizing piezoelectric materials for the conversion of a mechanical deflection into an electrical voltage, microwave resonators at approximately 3 GHz have proven to be suitable for the readout of magnetoelectric sensors. Also effect modulation concepts, e.g. based on flux modulation, promise to increase the signal-to-noise ratio (SNR). As a result, for each individual sensor concept the most suitable readout system with the highest possible SNR will be determined and the quantity limiting the performance will be known based on the developed noise models.

Based on noise investigations and readout system development, macroscopic setups emerge. To that end, highly optimized application-specific integrated circuits (ASICs) will be designed for those sensor types and applications, where off-the-shelf components are limiting the performance of the system. ASICs are electronics that are customized for a specific sensor type. In contrast, commercial off-the-shelf electronic circuits are rather aiming for a broader range of specifications and applications. As a result, in integrated circuit design the very specific requirements of the sensor can be taken into account. The electronics can be optimized for very specific requirements and thus the overall performance can be improved. Specific ASIC designs will include integrated electronics for ΔE -effect surface acoustic wave (SAW) sensors in the megahertz range as well as ultralow-noise amplifiers for the low frequency range (kilohertz).

3.3 Project progress to date

3.3.1 Report and current state of research

This project deals with research and development related to analogue signal conditioning and signal processing for single magnetic field sensors and small sensor arrays based on magnetoelectric sensor concepts. Bare sensors are combined with analogue front ends having the required low-noise electronics to form sensor systems. The CRC aims at biomagnetic applications that can be divided into two classes with regard to the technical requirements of the magnetic field sensor. On one hand, the detection of higher harmonics that arise due to the excitation with artificial signals in connection with the 3D-imaging of magnetically labeled cells (**B7**) and movement detection (**B9**) requires low-noise sensors in the frequency range around several kHz. Since typically only one higher harmonic has to be detected, the bandwidth of the sensor systems within this frequency range can be rather small ($BW < 5$ Hz). On the other hand, applications such as magnetocardiography (**B10**) and deep brain stimulation (**T1**) come with comparatively wide signal bands of interest with frequencies between DC and several kHz. All biomagnetic applications under investigation have the commonality that limits of detection (LOD) significantly below $1 \text{ pT/Hz}^{1/2}$ are required in the frequency ranges mentioned [St06].

In this project, various magnetic field sensor systems are investigated which combine resonant magnetoelectric (ME) cantilever sensors in passive mode (**Z1**) with magnetic frequency conversion (MFC, **A1**) and with electric frequency conversion (EFC, **A7**), as well as resonant ΔE -effect cantilever sensors (**A4**) and ΔE -effect surface acoustic wave (SAW) delay line sensors (**A9**).

In order to achieve low limits of detection, the design of appropriate readout electronics based on thorough noise analysis is necessary for each type of these sensor systems. In addition, however, it is just as important to understand the physical origins of intrinsic noise from the sensor both to improve a sensor further by appropriate design adaptations and to determine the fundamental noise limit.

Resonant cantilever magnetoelectric sensors in passive mode

A typical ME cantilever sensor in passive mode is operated with a low-noise preamplifier which is commonly designed as a charge amplifier. It was found that ME cantilevers based on magnetostrictive and piezoelectric films exhibit mainly two intrinsic noise sources: thermal-electrical noise of the dielectric material (the piezoelectric film) [Ja11] and thermal-mechanical noise due to the resonant character of the mechanical structure [B1-9]. Based on comprehensive noise modeling, not only these sensor-intrinsic noise sources can be determined but also the influence of the preamplifier on the overall noise floor can now be predicted. Fig. B1-1 shows the individual noise contributions compared to a noise measurement for a typical ME cantilever sensor with a resonance frequency of 850 Hz and a capacitance of 264 pF. Both the noise calculation and the measurement have been conducted with a standard charge amplifier based on a low-noise off-the-shelf operational amplifier (AD745) with a feedback network containing a capacitor (10 pF) in parallel to a resistor (5 G Ω). Obviously, the sensor-intrinsic thermal-mechanical noise ($E_{\text{co,ERmr}}$) is only dominant in a very narrow range

around the resonance frequency (f_{res}). Outside f_{res} either the voltage noise of the operational amplifier ($E_{\text{co,EnOP}}$ for $f > 400$ Hz) or its current noise ($E_{\text{co,InOP}}$ for $f < 400$ Hz) contributes the largest amount of noise. The level of the thermal-electrical noise ($E_{\text{co,ERME}}$) is never reached.

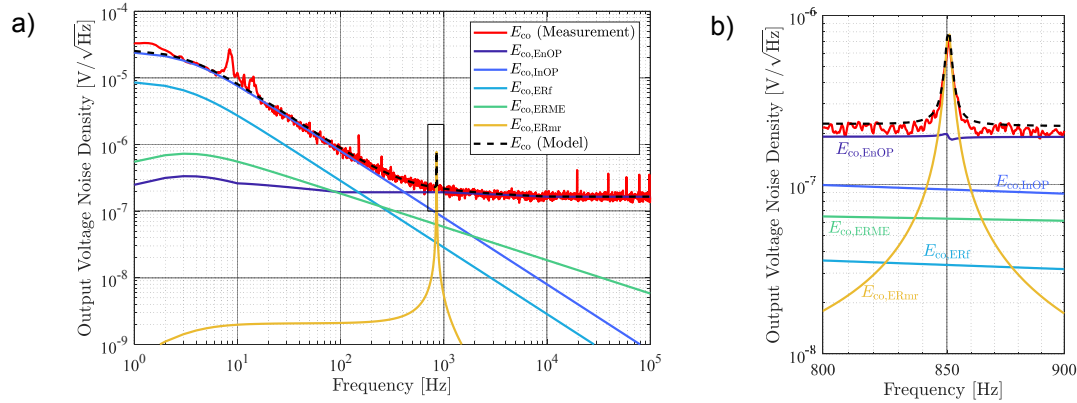


Figure B1-1: Calculated contributions of the individual noise sources of a typical ME cantilever sensor system in passive mode and in comparison to a noise measurement. When utilizing a standard charge amplifier, the sensor-intrinsic noise (thermal-mechanical noise, $E_{\text{co,ERmr}}$) is only dominant in a very narrow frequency range around the sensor's resonance frequency (here 850 Hz) [Du19,B1-9].

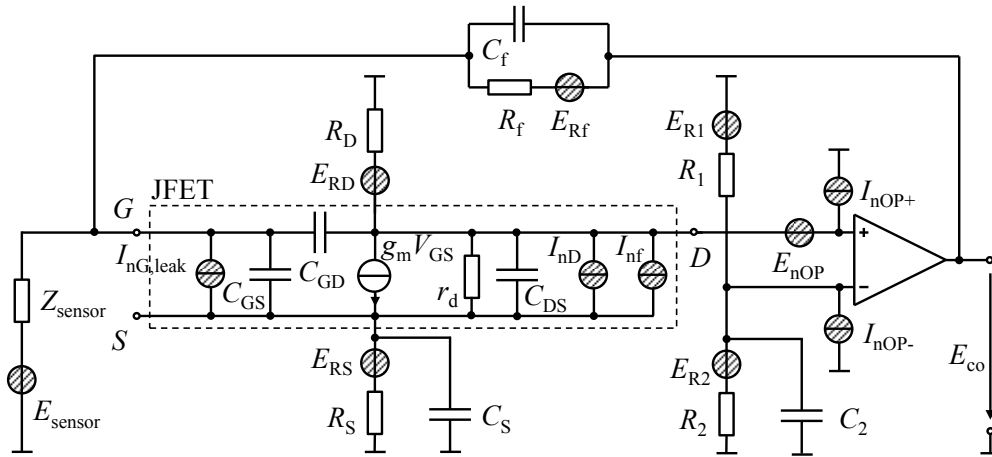


Figure B1-2: Noise equivalent circuit of a charge amplifier for piezoelectric sensors with reduced noise due to the utilization of a discrete low-noise junction field-effect transistor (JFET) at the amplifier's input stage [B1-7].

For the improvement of the overall noise behavior, one has to distinguish between low frequencies and the frequency range around the sensor's resonance frequency. Above several hundred Hz, the noise of the pre-amplifier can be distinctly reduced by including a discrete low-noise junction field-effect transistor (JFET) at the input of the charge amplifier. With the help of the developed noise equivalent circuit depicted in Fig. B1-2 and the analytical expressions for the various derived noise gains [B1-7], corresponding low-noise amplifiers can be designed. An example calculation of all the individual noise contributions for a cantilever sensor with a resonance frequency of 7450 Hz is shown in Fig. B1-3 (a). As intended, the sensor itself now has the largest impact on the overall noise floor at the amplifier's output and the calculated noise floor matches the measurement (red). The improvement can be seen particularly well in comparison to a classical charge amplifier (grey). Improving the low-frequency noise performance of such sensor systems to reach the noise level of the ME sensor especially requires ultralow input current noise that will be transformed into voltage noise by flowing through the high-resistance feedback resistor. For an example frequency of 10 Hz, Fig. B1-3 (b) depicts the requirements for the current and voltage noise of the operational amplifier and for the structure of a classic charge amplifier used so far (sensor's dielectric loss factor: 5×10^{-4}) [Du19]. Obviously, commercially available components suffer from higher voltage noise when optimized for ultralow input current noise (e.g. AD549L). In contrast, ultralow input voltage noise components like chopper amplifiers [Dr11] have high input current noise.

Even if the input current noise could be lowered under simultaneous retention of the input voltage noise (e.g. with the JFET charge amplifier structure), the voltage noise of the feedback resistor would still dominate. Its noise contribution could generally be decreased by choosing even higher values of resistance. However, this in turn would increase the noise due to the input current noise flowing through this resistor. Therefore, charge

amplifiers are generally not suited for low-frequency application with low-loss piezoelectric sensors. Instead, JFET-input voltage amplifiers could be used. An alternative solution is described below.

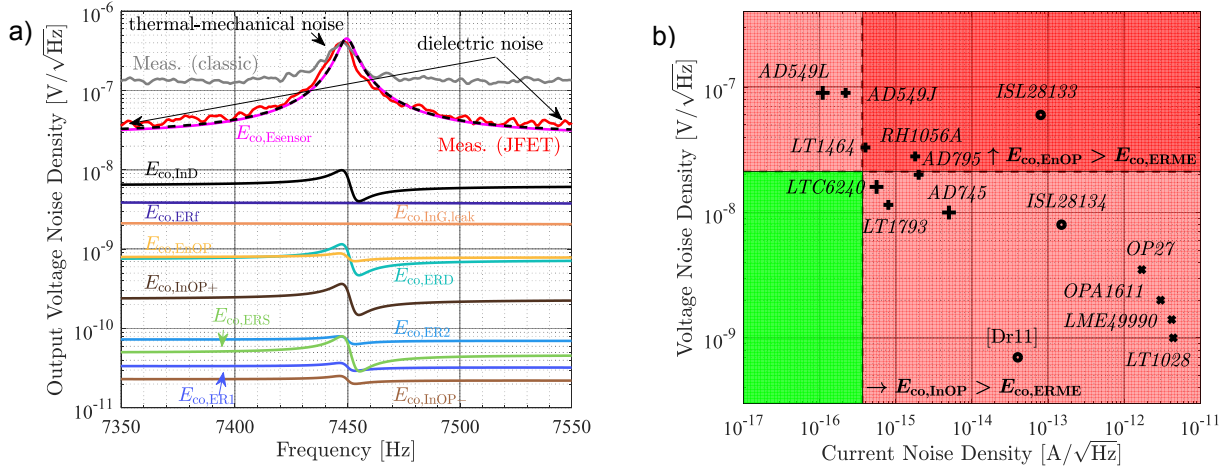


Figure B1-3: (a) Calculated contributions of the various noise sources of the low-noise JFET charge amplifier. A measurement with this amplifier shows a distinct lower noise floor compared to a measurement with a classic charge amplifier. (b) Requirements for the input current and voltage noise of the operational amplifier of a classic charge amplifier for a frequency of 10 Hz and a dielectric loss factor of the sensor of 5×10^{-4} . In the area highlighted green, the noise contribution of the operational amplifier is smaller than that of the sensor [Du19].

Readout of cantilever ME sensors with a microwave resonator

The principle of operation of a traditional ME cantilever is based on the conversion of a magnetically induced deflection into a proportional voltage across the electrodes of a piezoelectric material. As shown in Fig. B1-1 (a), the piezoelectric loss mechanisms lead to additional noise ($E_{co,ERME}$) which contributes far more to the overall system noise than the fundamental thermal-mechanical noise at low frequencies. In addition, the development of ultralow-noise amplifiers for piezoelectric sensors with very high output impedances is not trivial. To circumvent these problems, a novel readout principle has been conceived [B1-P2], the basic structure of which is depicted in Fig. B1-4 (a). In this structure, the cantilever is utilized as a magneto-mechanical transducer which behaves like a traditional ME cantilever, except for the missing piezoelectric layer [Sa18]. The cantilever acts as a transmission line microwave resonator with a resonance frequency given by its geometric dimensions, typically in the gigahertz range. In one possible realization, the cantilever is unilaterally clamped close above a ground plane, forming a quarter-wavelength resonator. Together with the ground plane, the cantilever forms a distributed capacitance $C_{\mu w}$ which can be adjusted by a tuning screw, and thus, changes the resonance frequency of the microwave resonator (cf. Fig. B1-4 (b)). A magnetically induced bending of the cantilever changes this capacitance ΔC , thus resulting in a microwave resonator exhibiting a magnetic field dependent resonance frequency. These frequency changes lead to both amplitude and phase modulation of the sensor's electric output signal which can be evaluated by classical readout systems [Sa18]. Preliminary measurements at the resonance frequency of the cantilever have shown comparable limits of detection restricted by the fundamental thermal-mechanical noise [B1-4, B1-9], after noise from the microwave excitation and readout circuit has been suppressed by appropriate circuitry. For the low-frequency range, improved limits of detection in comparison to piezoelectric cantilevers are expected.

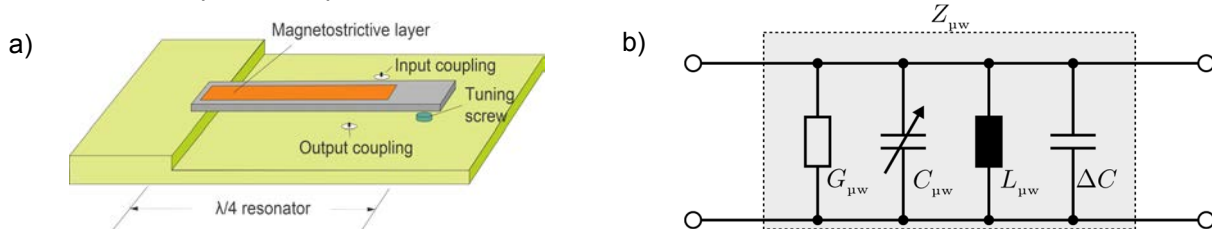


Figure B1-4: Possible realization of the microwave resonator (a) and the electrical equivalent circuit consisting of a parallel resonance circuit with a varying capacitor ΔC representing the change of capacitance induced by the cantilever bending (b). The arrow indicates a change due to a tuning screw [Sa18].

Resonant cantilever ME sensors with magnetic frequency conversion (MFC)

Magnetic frequency conversion (MFC) utilizes a magnetic pump signal to convert the signal of interest into the mechanical resonance frequency of an ME cantilever by utilizing the nonlinear characteristics of the magne-

tostriction [Ja12]. Noise that enters the system after the conversion process can be suppressed with this technique, lowering the LOD by more than one order of magnitude. A block diagram of magnetic frequency conversion is depicted in Fig. B1-5.

The pump signal is generated in a low-noise current source and applied via a dedicated pump coil. With a model of the transfer characteristic of the magnetic behavior, employing the sensor's magnetostriction curve and the elements of the block diagram, the system behavior of MFC can be predicted qualitatively depending on the applied magnetic excitation signal, bias field, and frequency [B1-6]. The model shows that the dynamic range is often limited by the high amplitude pump signal and that it can be enhanced with a small bias offset. This was proven experimentally [Du17] and further improved by additional cancellation techniques such as out-phasing [Sa19]. The operating point is determined with respect to maximum SNR, taking into account the noise increase depending on the excitation amplitude. This applies in particular to sensors with a single magnetostrictive layer, because such sensors exhibit significant magnetic noise when excited with a high amplitude signal [Sa17]. Recently however, sensors with antiparallel exchange bias magnetostrictive multilayer structures have been developed (A1) that in fact no longer exhibit magnetic noise [Jo19]. Thus, for these sensors either the thermal-mechanical noise or noise of the magnetic excitation limits the overall system performance with regard to the limit of detection, with recent values reaching $60 \text{ pT/Hz}^{1/2}$ at 10 Hz [B1-6].

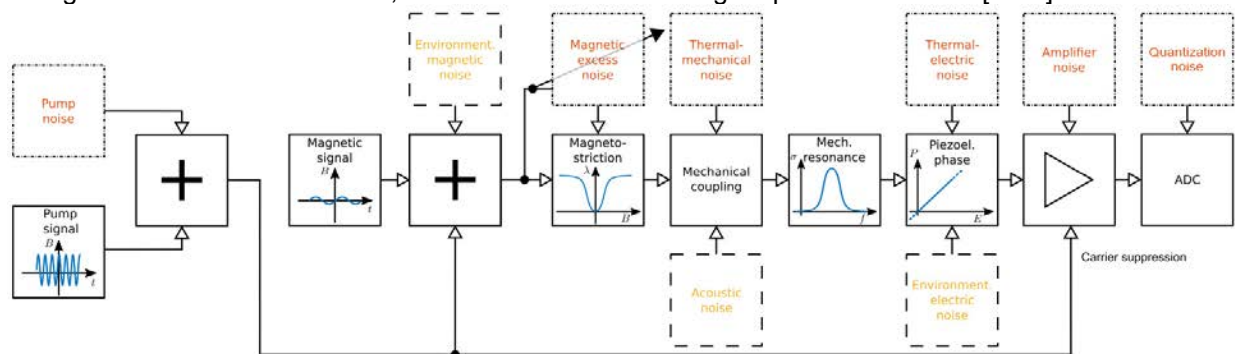


Figure B1-5: Block diagram of a resonant ME sensor system with magnetic frequency conversion [Sa18].

Resonant cantilever ME sensors with electric frequency conversion (EFC)

MFC yields low limits of detection in the range of tens of $\text{pT/Hz}^{1/2}$, but its practicability is limited due to the additional energy consumption for excitation of the magnetic pump field and its bandwidth limitation. This drawback can be avoided by replacing the magnetic pump signal with an electric excitation. Electrical frequency conversion (EFC, A7) utilizes strain modulation of a piezoelectric layer that is mechanically coupled to a magnetostrictive layer to convert the signal of interest into the mechanical resonance frequency where an effect enhancement takes place. As for MFC, the conversion process itself takes place in the nonlinear magnetostrictive material of the sensor. The excitation signal is applied directly to the piezoelectric layer.

So far, sensors with two piezoelectric layers were utilized for the excitation and for the readout [Ha16]. The output signal needs to be amplitude and/or phase demodulated. Noise sources involved are, amongst others, thermal-mechanical noise of the resonator, thermal-electrical noise of the piezoelectric layers, ferroelectric noise if a ferroelectric material (e.g. PZT) is utilized, and magnetic noise from the excited magnetostrictive material. For single layer magnetic materials, the magnetic noise, which is centered around the pump signal frequency, is the dominant noise source [Sa18]. Another recently developed readout method detects the stress-induced periodic magnetization change of the magnetostrictive phase of an ME composite which, in this case, acts as the magnetic core material of an additional pick-up coil [Ha18, B1-4]. For this method, a specific resonance at approximately 500 kHz is utilized. The induction coil can be tuned to the mechanical resonance frequency via an additional capacitor to further enhance the output signal. Advantages of this method are a low susceptibility to environmental interference, such as vibrations and acoustics, lower demands on low-noise signal processing, and higher bandwidth than conventional EFC and especially MFC. Since a second piezoelectric layer is not necessary, sensors with antiparallel exchange biased multilayers, originally developed for the application with MFC, could be applied in this readout scheme. A limit of detection of $70 \text{ pT/Hz}^{1/2}$ at a frequency of 10 Hz could be achieved [Ha19]. A noise model for determining the contribution of the individual noise sources (sensor intrinsic noise and the readout electronics) is required for further improvement of this kind of sensor system.

ΔE -effect sensors

Sensors based on the ΔE -effect lead to a magnetically induced change in the elastic modulus of a magnetostrictive material. To exploit this effect for sensor purposes, an electromechanical structure is required that reacts sensitively to changes of the elastic modulus.

A frequently used structure is a mechanical cantilever whose resonance frequency depends on the effective elastic modulus, and thus changes with the magnetic field. By application of an additional piezoelectric layer and an appropriate electrode structure, the change in resonance frequency can be detected utilizing an electric excitation signal. In fact, the sensor, i.e. the electromechanical resonator, can be interpreted as an electrical impedance which changes with the magnetic field. Therefore, a typical readout system contains a generator, followed by the sensor, and a charge or transimpedance amplifier for the detection of the current flowing through the sensor. Due to the high requirements for the low-noise implementation of the preamplifier, the JFET charge amplifier [B1-7] presented above is generally utilized. For cantilever-type sensors with resonance frequencies far below 100 kHz, the amplitude and/or phase demodulation of the modulated sensor signal is typically performed in the digital domain after further stages of amplification and high-resolution analogue-to-digital conversion. A possible realization of such electronics is shown in Fig. B1-6, which mainly consists of a digital-to-analogue converter for the generation of the excitation signal and an analogue-to-digital converter for reception. Both the digital signal processing, i.e. the signal generation and the demodulation, as well as the communication with a computer is performed by a microcontroller. Noise measurements and modeling of such a sensor system [B1-8] revealed that thermal-mechanical noise constitutes the fundamental noise limit of cantilever-type sensors. However, as one would expect, in comparison to passive-mode ME sensors additional noise sources come into play. As for magnetically (MFC) and electrically (EFC) excited ME composites, sensors based on single magnetostrictive layers exhibit significant magnetic noise when excited with a signal of large amplitude, limiting the limit of detection to approx. 100-200 pT/Hz^{1/2} at 10 Hz. It was found that the magnetic noise shows a 1/f frequency dependence after equalizing the frequency behavior of the narrowband resonator [Du19], indicating magnetic hysteresis losses as the origin for the increase in noise (see below). This assumption is supported by the fact that for operating points with high noise, the electrically measured losses of the resonator are also significantly greater. The same behavior has been observed for giant magnetoresistive sensors [Ha93].

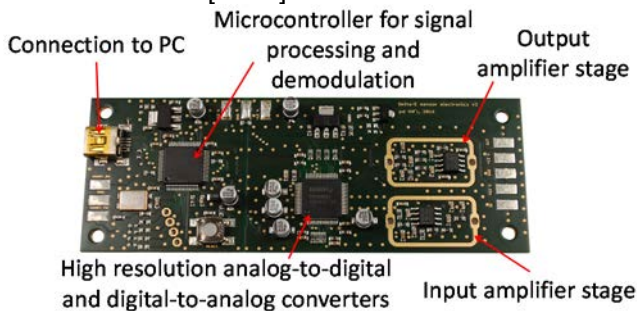


Figure B1-6: Photography of a printed circuit board containing the electronics for the readout of cantilever-type ΔE -effect sensors with resonance frequencies at approx. 7.5 kHz.

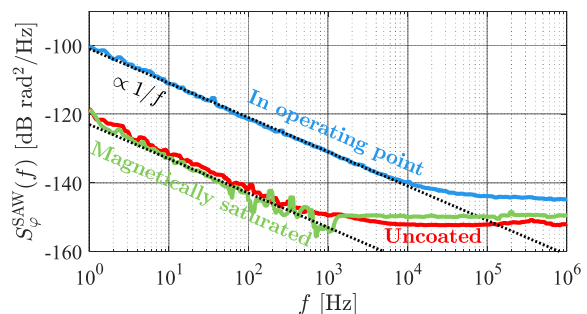


Figure B1-7: Phase noise of surface acoustic wave (SAW) delay line magnetic field sensors measured with a phase noise analyzer FSWP from Rohde & Schwarz [B1-2].

Another electromechanical platform appropriate for the detection of magnetically induced changes in the elastic modulus is the surface acoustic wave (SAW) delay line [Ki18] that offers bandwidths of several tens of kilohertz [B1-1]. Since the propagation velocity of a surface acoustic wave depends on the elastic modulus of the materials involved, the ΔE -effect leads to magnetically induced changes in the wave velocity when the sensor is coated with a film of magnetostrictive material. These changes in propagation velocity lead to phase changes, i.e. a phase modulation, of the injected sensor signal.

For the low-noise detection of the phase changes, two readout schemes have been proposed which comprise a closed-loop, i.e. self-oscillating, system and an open-loop system [B1-2]. The basic structure of the open-loop system is similar to the measurement principle utilized for ΔE -effect cantilever sensors. However, because of distinct phase noise of signal generators in the frequency range of the SAW sensor (approx. 150 MHz), a scheme for the suppression of this phase noise is necessary. By utilizing a heterodyne system structure, the local oscillator's phase noise could be inherently suppressed, despite the relatively large delay of the sensor (typically in the range of 1-2 μ s), which leads to a frequency dependent decorrelation of the phase noise in the sensor and the reference branch [B1-5]. The self-oscillating sensor system, in which the sensor is placed in the feedback branch of an amplifier and in which phase changes lead to a frequency modulation, has the advantage that a generator for the excitation of the sensor is not required. However, a frequency demodulator generally also requires a phase-stable frequency reference. For both readout structures, measurements and extensive phase noise modeling have been performed with the result that both systems, in principle, perform equally with regard to the minimum achievable limit of detection and that the sensor itself contributes the dominant noise to the overall system noise [B1-2, B1-3]. Fig. B1-7 shows an example measurement of the

sensor's intrinsic phase noise when operated in its magnetic operating point (blue), i.e. for a magnetic bias field for which a high magnetic sensitivity is achieved. When the same sensor is magnetically saturated by means of a strong permanent magnet, the phase noise decreases by approx. 20 dB (green) and reaches the same noise floor as a magnetostrictively uncoated delay line (red) [B1-2]. Since the increase in noise directly scales with additional insertion losses that, in turn, depend on the magnetic state of the sensor, a magnetic origin of this phase noise is strongly indicated [Du19]. This assumption is supported by the fact that the noise decreases with a slope of $1/f$, as previously observed for giant magnetoresistive sensors exhibiting magnetic noise due to magnetic hysteresis losses [Ha93, Ve97].

Application specific integrated circuit design for biomedical sensing

Biomedical signal processing with analogue electronic circuits requires the fulfillment of very demanding design requirements, especially regarding ultralow noise [Li10]. Figure B1-3 (b) exemplifies the input noise voltage and input noise current requirements for a charge amplifier. For the recording of brain signals in the electrical domain, an integrated circuit with very high noise specifications for implantable systems has been developed. The integrated circuit outperforms commercially available systems with respect to energy efficiency and enables a new type of brain signal recordings [B1-10, Ba16]. To enable the design of application specific integrated circuits (ASICs), a design environment with state-of-the-art industry design software (Cadence IC Design) and a high performance computing platform has been set up and brought into operation. The participation in the European-funded research program Europractice provides access to CMOS silicon foundry technology (electrical device models/design libraries and multi-project wafer (MPW) production services).

References

Below, the names of both past and future principal investigators of this project are printed in bold (in the following project phase, Prof. Bahr will take over the position as principal investigator from Prof. Knöchel).

- [Ba16] **A. Bahr**, L. A. Saleh, R. Hinsch, D. Schroeder, D. Isbrandt, W. H. Krautschneider, Small Area, Low Power Neural Recording Integrated Circuit in 130 nm CMOS Technology for Small Mammals, *International Conference on Microelectronics (ICM)*, 10.1109/ICM.2016.7847887 (2016).
- [Ch97] L. Chiesi, K. Haroud, J. A. Flanagan, R. S. Popovic, Chopping of a weak magnetic field by a saturable magnetic shield. *Sensors Actuators A Phys.* **60**, 5–9, 10.1016/S0924-4247(96)01410-0 (1997).
- [Dr11] D. Drung, J.-H. Storm, Ultralow-noise chopper amplifier with low input charge injection. *IEEE Trans. Instrum. Meas.* **60**, 2347–2352, 10.1109/TIM.2011.2114030 (2011).
- [Du17] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, J. McCord, D. Meyners, E. Quandt, G. Schmidt, **R. Knöchel**, **M. Höft**, Improved Magnetic Frequency Conversion Approach for Magnetoelectric Sensors. *IEEE Sensors Lett.* **1**, 1–4, 10.1109/LSSENS.2017.2699559 (2017).
- [Du19] P. Durdaut, Ausleseverfahren und Rauschmodellierung für magnetoelastische Sensorsysteme, (Diss., Kiel University, 2019).
- [Ha93] H. T. Hardner, M. B. Weissman, M. B. Salamon, S. S. P. Parkin, Fluctuation-dissipation relation for giant magnetoresistive $1/f$ noise. *Phys. Rev. B.* **48**, 16156–16159, 10.1103/PhysRevB.48.16156 (1993).
- [Ha16] P. Hayes, S. Salzer, J. Reermann, E. Yarar, V. Röbisch, A. Piorra, D. Meyners, **M. Höft**, **R. Knöchel**, G. Schmidt, E. Quandt, Electrically modulated magnetoelectric sensors. *Appl. Phys. Lett.* **108**, 182902, 10.1063/1.4948470 (2016).
- [Ha18] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yarar, A. Piorra, **R. Knöchel**, Y. K. Fetisov, E. Quandt, Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing. *J. Phys. D: Appl. Phys.* **51**, 0–18, 10.1088/1361-6463/aad456 (2018).
- [Ha19] P. Hayes, M. Jovičević Klug, S. D. Toxværd, P. Durdaut, V. Schell, A. Teplyuk, D. Burdin, A. Winkler, R. Weser, Y. Fetisov, **M. Höft**, **R. Knöchel**, J. McCord, E. Quandt, Converse Magnetoelectric Composite Resonator for Sensing Small Magnetic Fields. *Sci. Rep.* **9**, 16355, 10.1038/s41598-019-52657-w (2019).
- [He11] F. Hettstedt, Weichmagnetische Nanokomposite und deren Anwendungen in der Hochfrequenztechnik, (Diss., Kiel University, 2011).
- [Ja11] R. Jahns, H. Greve, E. Woltermann, E. Quandt, **R. Knöchel**, Noise performance of magnetometers with resonant thin-film magnetoelectric sensors. *IEEE Trans. Instrum. Meas.* **60**, 2995–3001, 10.1109/TIM.2011.2122410 (2011).
- [Ja12] R. Jahns, H. Greve, E. Woltermann, E. Quandt, **R. Knöchel**, Sensitivity enhancement of magnetoelectric sensors through frequency-conversion. *Sensors Actuators A Phys.* **183**, 16–21, 10.1016/j.sna.2012.05.049 (2012).
- [Jo19] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. D. Toxværd, **M. Höft**, **R. Knöchel**, E. Quandt, D. Meyners, J. McCord, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors. *Appl. Phys. Lett.* **114**, 192410, 10.1063/1.5092942 (2019).

- [Ki18] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, **M. Höft, R. Knöchel**, F. Faupel, E. Quandt, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Sci. Rep.* **8**, 278, 10.1038/s41598-017-18441-4 (2018).
- [Li10] Y. Li, C. C. Y. Poon, Y.-T. Zhang, Analog Integrated Circuits Design for Processing Physiological Signals. *IEEE Rev. Biomed. Eng.* **3**, 93–105, 10.1109/RBME.2010.2082521 (2010).
- [Pa12] M. Pan, J. Hu, W. Tian, D. Chen, J. Zhao, Magnetic flux vertical motion modulation for 1/f noise reduction of magnetic tunnel junctions. *Sensors Actuators A Phys.* **179**, 92–97, 10.1016/j.sna.2012.03.036 (2012).
- [Sa17] S. Salzer, P. Durdaut, V. Röbisch, D. Meyners, E. Quandt, **M. Höft, R. Knöchel**, Generalized Magnetic Frequency Conversion for Thin-Film Laminated Magnetolectric Sensors. *IEEE Sens. J.* **17**, 1373–1383, 10.1109/JSEN.2016.2645707 (2017).
- [Sa18] S. Salzer, Readout Methods for Magnetolectric Sensors, (Diss., Kiel University, 2018).
- [St06] K. Sternickel, A. I. Braginski, Biomagnetism using SQUIDS: status and perspectives. *Supercond. Sci. Technol.* **19**, S160–S171, 10.1088/0953-2048/19/3/024 (2006).
- [Ti16] W. Tian, J. Hu, M. Pan, D. Chen, J. Zhao, Magnetic Flux Vertical Motion Modulation for 1/f Noise Suppression in Magnetoresistance Field Sensors Using MEMS Device. *IEEE Trans. Magn.* **52**, 1–6, 10.1109/TMAG.2013.2264061 (2016).
- [Ve97] R. J. M. van de Veerdonk, P. J. L. Beliën, K. M. Schep, J. C. S. Kools, M. C. de Nooijer, M. A. M. Gijs, R. Coehoorn, W. J. M. de Jonge, 1/f noise in anisotropic and giant magnetoresistive elements. *J. Appl. Phys.* **82**, 6152–6164, 10.1063/1.366533 (1997).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications

- [B1-1] J. Labrenz, **A. Bahr**, P. Durdaut, **M. Höft**, A. Kittmann, V. Schell, E. Quandt, Frequency Response of SAW Delay Line Magnetic Field/Current Sensor. *IEEE Sensors Lett.* **3**, 1–4, 10.1109/LSENS.2019.2943129 (2019).
- [B1-2] P. Durdaut, A. Kittmann, E. Rubiola, J.-M. Friedt, E. Quandt, **R. Knöchel, M. Höft**, Noise Analysis and Comparison of Phase- and Frequency-Detecting Readout Systems: Application to SAW Delay Line Magnetic Field Sensor. *IEEE Sens. J.* **19**, 8000–8008, 10.1109/JSEN.2019.2914965 (2019).
- [B1-3] P. Durdaut, **M. Höft**, J.-M. Friedt, E. Rubiola, Equivalence of Open-Loop and Closed-Loop Operation of SAW Resonators and Delay Lines. *Sensors*. **19**, 185, 10.3390/s19010185 (2019).
- [B1-4] S. D. Salzer, C. Kirchhof, E. Quandt, **M. Höft, R. Knöchel**, Magnetolectric Microwave Magnetic Field Sensor at 3 GHz, *Asia-Pacific Microwave Conference (APMC)*, 10.23919/APMC.2018.8617346 (2018).
- [B1-5] P. Durdaut, A. Kittmann, **A. Bahr**, E. Quandt, **R. Knöchel, M. Höft**, Oscillator Phase Noise Suppression in Surface Acoustic Wave Sensor Systems. *IEEE Sens. J.* **18**, 4975–4980, 10.1109/JSEN.2018.2832289 (2018).
- [B1-6] S. Salzer, V. Röbisch, M. Klug, P. Durdaut, J. McCord, D. Meyners, J. Reermann, **M. Höft, R. Knöchel**, Noise Limits in Thin-Film Magnetolectric Sensors with Magnetic Frequency Conversion. *IEEE Sens. J.* **18**, 596–604, 10.1109/JSEN.2017.2776039 (2018).
- [B1-7] P. Durdaut, V. Penner, C. Kirchhof, E. Quandt, **R. Knöchel, M. Höft**, Noise of a JFET Charge Amplifier for Piezoelectric Sensors. *IEEE Sens. J.* **17**, 7364–7371, 10.1109/JSEN.2017.2759000 (2017).
- [B1-8] P. Durdaut, J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, F. Faupel, G. Schmidt, **R. Knöchel, M. Höft**, Modeling and Analysis of Noise Sources for Thin-Film Magnetolectric Sensors Based on the Delta-E Effect. *IEEE Trans. Instrum. Meas.* **66**, 2771–2779, 10.1109/TIM.2017.2709478 (2017).
- [B1-9] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, P. Hayes, A. Piorra, D. Meyners, E. Quandt, G. Schmidt, **R. Knöchel, M. Höft**, Thermal-Mechanical Noise in Resonant Thin-Film Magnetolectric Sensors. *IEEE Sens. J.* **17**, 2338–2348, 10.1109/JSEN.2017.2671442 (2017).
- [B1-10] **A. Bahr**, Aufnahme von Hirnsignalen mit extrem miniaturisierten elektronischen Systemen zur Untersuchung von lokalen neuronalen Vernetzungen, (Diss., Logos Verlag Berlin, 2017).

b) Other publications

None

c) Issued patents

- [B1-P1] Quandt, E.; Kittmann, A.; Zabel, S.; Yazar, E.; Faupel, F.; **Knöchel, R.; Höft, M.**; Durdaut, P.: Senso-relement für Magnetfelder mit hoher Frequenzbandbreite, DE102016123274B4.
- [B1-P2] Salzer, S.; **Knöchel, R.**; Quandt, E.; Thormählen, L.: Mikrowellenresonator-Magnetfeldmessvorrichtung sowie Magnetfeldmessverfahren, DE102018110511.

d) Pending patents

[B1-P3] Hayes, P.; Toxværd, S.; **Knöchel, R.**; Quandt, E.: Messvorrichtung für schwache, langsam veränderliche Magnetfelder, insbesondere für biomagnetische Felder, DE102019116779.5.

3.4 Project plan

Objectives

The essential goal of this project is to research the various thin-film magnetic field sensors with regard to the achievement of sensor systems with the highest possible signal-to-noise ratio (SNR) which corresponds with the lowest limit of detection (LOD). This is done by completing the bare sensors (project area A) with adequate analogue electronic circuits to provide analogue signal processing and conditioning. The SNR of the analogue output signal always has to be high enough such that subsequently introduced noise by analogue-to-digital conversion can be neglected and optimal digital signal processing (**B2**) is possible. Such analogue systems will be developed for ME cantilever sensors in passive mode (**Z1**), ME cantilever sensors with EFC (**A7**), ΔE -effect cantilever sensors (**A4**), and ΔE -effect SAW delay lines (**A9**).

The working hypotheses are as follows:

1. A comprehensive understanding of the sensor intrinsic noise sources will lead to an enhancement of the sensor systems.
2. Individualization of the electronics leads to sensor systems with the lowest LOD.
3. Sophisticated analogue signal conditioning and embedding of the sensitive element into the system will further improve the LOD.
4. Monolithically integrated low-noise electronics will further reduce the system noise; additionally, it enables the design of compact sensor systems with digital outputs.
5. Complete integration of low-noise electronics and sensor elements will enable sensor system front ends for biomedical applications, performed with individual sensors and arrays.

The time schedule for the various work packages is given in the following chart

(Main work done by: **blue**: H. Wolframm / Prof. Höft, **green**: N. N. / Prof. Bahr, **purple**: both):

No.	Work package	2020		2021				2022				2023				2024	
		III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP1	Experimental and theoretical analysis of sensor noise performance																
WP2	Sensor system electronics with maximum signal-to-noise ratio																
WP3	New sensor system approaches																
WP4	Monolithic integrated circuit design for maximizing signal-to-noise ratio																
WP5	System front ends for biomedical applications																

Intended research methods

For all noise investigations, the sensors are operated experimentally in an electrically, magnetically, and acoustically shielded environment. The electrical shielding consists of a copper fleece and prevents distortions through low- and high-frequency electrical fields (e.g. power lines, radio stations, or mobile phones). Acoustical shielding against air-borne sound is achieved with acoustical absorbers within the measurement box. Structure-borne sound is absorbed through elastic suspension of the box. The sensors themselves are situated within the box in a μ -metal cylinder, which provides magnetic shielding. If the shielding of the test box is not sufficient, a magnetically shielded room can be utilized (compare **Z2**), which also has electrical screening and may be lined with acoustical absorbers. Within the μ -metal cylinder, calibrated solenoids serve the generation of all kinds of magnetic fields. For this purpose, DC power current sources (KEPCO BOP20-10ML and Keysight B2962A) and several low-noise AC current sources (Keithley Instruments 6221) are available. In addition, an ultralow-noise DC current source based on a battery and a step motor-driven potentiometer has been developed. The analogue signal processing and conditioning circuits are also situated in the box, together with the sensors featuring their own electrical shielding. They are equipped with battery power supplies. For signal analysis, various devices are available. For frequencies below 100 kHz, an FFT signal analyzer (SRS SR785) and two lock-in amplifiers (SRS SR830) are frequently used. For the analysis and further processing of time domain signals, various high-resolution digital acquisition devices (e.g. USB-4431 from National Instruments) are available. For the operation of sensors with higher frequencies (several hundred kHz up to some GHz), various signal generators (e.g. R&S SMBV100A), spectrum analyzers (e.g. R&S FSV), an ultra-high frequency

lock-in amplifier (UHFLI from Zurich Instruments), and a noise measurement setup with an integrated signal source for two-port measurements (R&S FSWP) are available. Electrical characterizations of sensors are commonly performed with an impedance analyzer (ST2819A from Sourcetric) or with vector network analyzers (e.g. Agilent E8361A) with up to 4 ports (Rohde & Schwarz ZVA24). The design of ASICs is performed on the dedicated IC design environment (computing server, Cadence IC design software, Europractice).

Work plan

The various work packages derived from the goals previously presented will now be described in detail, together with the analytical methods and new technological approaches to be applied. Many work sub-packages overlap to a certain degree because results from one area of work can be used at least partly in another. The work program presented here is divided into analysis of the bare sensors, investigation and improvement of sensor systems, and the investigation and design of appropriate integrated sensor system electronics. It includes a detailed breakdown into sub-work packages.

WP 1: Experimental and theoretical analysis of sensor noise performance

In the continuing course of the project, it is expected that the inherent noise of the sensors will be further reduced. This applies in particular to magnetic noise, the reduction of which has already been demonstrated [Jo19]. These special layer systems so far exist only for macroscopic cantilever sensors, but are also to be transferred to the other sensor concepts (**A1**). Accordingly, the goal of this work package is to investigate the noise behavior of the advanced sensors, i.e. electrically modulated sensors, ΔE -effect cantilevers, and SAW delay lines. These results are analyzed in close cooperation with **A10**. Presuming that the noise performance of the analogue readout electronics can be always kept better than the sensor noise performance, the noise specifications for the readout electronics are obtained simultaneously. In addition, the sensor noise behavior must be re-determined if changes are made to the system, e.g. in the case of additional flux modulation.

WP 1a: Fundamental noise limits of piezoelectric cantilever sensors

Cantilever sensors can be used both passively (**B7**, **B9**, fabrication in **Z1**) and as resonators utilizing the ΔE -effect (**A4**) or as ME resonators for EFC (**A7**). As shown above, thermal-mechanical noise is the fundamental limit of these resonant sensors. If utilizing a piezoelectric cantilever, thermal-electrical noise also occurs due to dissipation in the piezoelectric material. The goal of this work package is to determine the fundamental noise limits for the cantilevers, which are mainly manufactured in **Z1**, but especially also in **A4** and **A7**. To achieve this, the noise behavior has to be measured and verified by comparison with calculations based on the existing noise models. The existing models have to be adapted or extended if, for example, special shear modes instead of simple bending modes are used. The results of this work package yield the specifications with regard to the respective preamplifiers (WP 2a).

WP 1b: Noise analysis of excited sensors

Sensors that are actively excited by means of a large signal (ΔE -effect cantilevers (**A4**), ME cantilevers for EFC (**A7**) and ΔE -effect SAW delay lines (**A9**)) in operation lead to magnetically induced changes in the amplitude (amplitude modulation) and/or to changes in the phase (phase modulation) of the output signal. Therefore, the amplitude and/or phase noise at the output of the sensor (depending on the sensor concept) must first be determined using the readout systems developed in WP 2 or using commercial noise measurement equipment. The various sensor concepts shall be compared on the basis of the respective equivalent magnetic noise or the frequency-dependent limit of detection. Since the limit of detection is defined by the ratio of noise and sensitivity, the sensitivity in the respective operating mode must also be determined for each sensor system. Both the sensitivity and the noise depend on the operating point of the sensor, which requires that all measurements be performed as functions of the magnetic bias field and the input power/amplitude of the sensor. Based on this data, the optimum operating point can then be determined for each sensor system with regard to a minimum limit of detection. Thus, the results obtained for the ΔE -effect SAW delay lines will later be compared to corresponding measurements with the integrated circuits developed in WP 4 at the optimum operating point of an example sensor.

WP 1c: Investigation of magnetic noise in thin-films

Sensor concepts in which the magnetic layer is periodically excited by a large signal (ME bending beams for EFC, ΔE -effect cantilevers and SAW delay lines) generally exhibit additional noise which is generated directly in the magnetic layer and always corresponds to related loss mechanisms. For sensors with simple magnetic layers that exhibit particularly high noise, it has been possible so far to characterize the magnetic noise directly. Due to the use of novel antiparallel exchange bias layer systems, whose noise is significantly lower [Jo19], characterizations of the magnetic noise in the sensor itself is often no longer possible, since it is superimposed by other noise sources of the sensor (e.g. thermal-mechanical noise of a cantilever). Therefore, in close cooperation with **A1**, a permeameter shall be developed (e.g. based on a coplanar line), which allows a broadband measurement of the complex permeability of soft magnetic thin film composites in dynamic operation.

Knowledge of this complex-valued permeability is necessary to compare results from noise measurements with calculations based on the fluctuation-dissipation theorem, and thus to be able to deduce the physical cause of the loss and noise processes. After the development of a broadband permeameter, magnetic single layers as well as various samples of exchange bias layer systems will be investigated with respect to their loss mechanisms. The permeameter has to be designed for broadband operation to be able to perform investigations both in the few hundred kilohertz range (EFC) as well as up to the gigahertz range (SAW).

WP 2: Sensor system electronics with maximum signal-to-noise ratio

In the course of the present project, both readout systems and associated noise models have already been developed. These serve as a basis for the projects in this work package. Since it can be assumed that the noise of the various sensors will be further reduced, the readout systems also have to be continuously improved and the associated noise models extended or adapted if necessary. For the following sensor concepts, low-noise readout systems are to be developed and analyzed, which are initially to be set up in macroscopic form. This refers to systems consisting of printed circuit boards and using commercial integrated circuits. The development of these systems should always take place against the background of a later miniaturization of the same functionality in a customized integrated circuit.

WP 2a: Preamplifiers for piezoelectric cantilevers

Analysis of the noise of the various piezoelectric cantilevers to be performed in WP 1a directly determines the requirements for permissible preamplifier noise. In this work package, low-noise charge and voltage amplifiers are constructed and further developed to this end. The suitability of the developed custom amplifier topologies with regard to noise is verified by measurement prior to the realization of corresponding integrated circuits. A further aspect concerns the behavior of the amplifiers in large signal operation. In contrast to passively operated sensors, it must be ensured for the operation of ΔE -effect cantilevers that the amplifier exhibits amplitude linearity over more than 6 decades and that the amplification factor does not fluctuate over time in order to prevent occurrence of significant parametric amplitude and phase noise. With regard to the use of the amplifiers in wearable applications (B9), energy efficiency is another important criterion.

WP 2b: Magnetoelectric cantilevers with EFC

As already discussed in the description of preliminary work, ME cantilevers using electrical frequency conversion have been investigated for some time. However, so far sensors with two piezoelectric layers have commonly been used, with one layer for excitation and another for readout. In the present time, sensors are used which have only one piezoelectric layer for excitation being read out inductively with the sensor acting as the core of an induction coil. This method significantly reduces the requirements for the preamplifier, since the coil is not only operated at resonance, but also represents a low-source impedance in contrast to high-impedance piezoelectric sensors. As with ΔE -effect sensor systems, however, high demands are placed on the noise of the electrical excitation signal and on the detector circuit. In the case of sensors with comparatively low resonance frequencies below 10 kHz, so far low-noise sensor systems were possible based on high-resolution D/A and A/D converter. However, if higher modes with typical frequencies in the 500 kHz range are used, D/A or A/D converters with correspondingly high sampling rates are required, for which the resolution decreases or the noise increases. Therefore, a synchronous analogue system must be designed in this work package that is capable of intrinsically suppressing the noise of the excitation generator sufficiently. First, it has to be determined whether a detection of amplitude or phase changes is more advantageous and whether a homodyne or a heterodyne structure is suited better. In addition, a dedicated noise model has to be developed and verified, taking into account the sensor with its magnetic and piezoelectric layers, the induction coil, and all components of analogue signal processing. The goal is to ensure that the total noise at the output of the sensor system will be dominated by the sensor or its fundamental thermal-mechanical noise.

WP 2c: ΔE -effect cantilevers

ΔE -effect cantilevers are mainly implemented in A4 where both the cantilevers as well as the readout electronics are integrated on a chip. As for electrically modulated ME cantilevers, the existing readout electronics are currently based on high-resolution A/D and D/A converters. Due to the low current operation and limited space requirements, this approach is no longer appropriate if arrays of ΔE -effect cantilevers are to be realized. For this reason, in this work package and in close cooperation with A4, purely analogue readout methods are developed which are constructed and verified here as systems assembled by discrete hybrid electronics (macroscopic systems) before custom monolithically integrated circuits are developed. Preliminary work has shown that an evaluation of phase changes compared to amplitude changes in ΔE -effect sensors leads to improved limits of detection. Therefore, the structure of a homodyne sensor system using an analogue and tunable phase shifter in combination with a mixer for phase demodulation is expected to be effective. Such a system can provide an analogue and demodulated output signal directly and, at the same time, suppress the phase noise of the exciting generator. In the course of the verification of the macroscopic system developed in this

work package, a corresponding noise model must also be developed to quantify the influence of the individual noise sources (generator, sensor, preamplifier, mixer, output amplifier) on the output signal.

WP 2d: ΔE -effect SAW delay lines

For ΔE -effect SAW delay lines in the frequency range around 150 MHz, various readout systems and corresponding noise models have already been researched [B1-2, B1-3]. It could be shown that these systems have sufficiently low noise. However, these systems have so far been built as hybrid integrated circuits using commercial components. These components also include mixers containing impedance and symmetry transformers. With regard to a realization in monolithic integrated circuit technology, such components or the entire system must be adapted so that an integration in CMOS technology will be possible. In addition, it must first be analyzed which structure of readout system is best suited for integration. There are essentially three structures: Open-loop systems can be built both as homodyne and heterodyne circuits in order to detect magnetically induced phase changes; Closed-loop systems, on the other hand, do not require a generator to excite the sensor, because the sensor is located in the feedback branch of an amplifier, which causes the system to oscillate autonomously and convert phase changes into frequency changes. However, a stable frequency reference is also generally required for the demodulation. The aim of this work package is to set up and verify a suitable readout system based on components that will also be available for later CMOS integration.

WP 3: New sensor system approaches

The development of sensor systems in WP 2 is based on predominantly classical concepts with the primary goal of creating a basis for corresponding CMOS integration (WP 4). The goal of this work package is to investigate new and advanced methods on the long-term improvement of the sensor systems. This goal is investigated by two methods, aimed at improving different aspects of the sensor systems: The ME microwave resonator presents the possibility of reading out cantilever sensors without the need of a piezoelectric layer. This offers advantages not only in terms of noise, but also in terms of process technology. Effect modulation is expected to improve the sensor system by suppression of $1/f$ noise.

WP 3a: ME microwave resonator

The strong advantage of the ME microwave resonator is its design without a piezoelectric layer and readout without low-frequency electronics. If magnetic noise is successfully suppressed (e.g. by utilization of antiparallel exchange bias multilayer systems from A1 [Jo19]), further improvement of the LOD can be achieved by utilization of a microwave resonator which does not exhibit any piezoelectric noise sources. Besides the implemented realization, other resonator designs such as waveguide resonators detuned by a cantilever and a thorough investigation of the microwave losses will increase the resonator's quality factor. As a by-product, the resiliency to low-noise environmental interferences will be improved by design. The tuning capabilities can be modified by the resonator design in order to, for example, adjust the microwave resonance frequency to other system components, adapting available theory from filter design. Passive non-contacting wireless readout will be implemented by, e.g., patch antennas with a pulsed microwave signal allowing for application in critical or enclosed environments. The concept is not restricted to passive mode or MFC readout and can also be adapted to ΔE -effect sensors and other sensor geometries. The concept allows for direct DC measurement of the sensor via measurement of the DC magnetic field induced bending of the cantilever and can thus also be used to measure magnetostriction curves of the sensor assembly. Disturbing effects such as temperature dependence or magnetic drift will be diminished by compensation approaches, e.g., with two similar assemblies measuring simultaneously or automatized pre-measurement calibration. A priori knowledge, for example, about the form of the resonator curve, will be exploited by model-based readout. The sensor construction will be done either micromechanically or with an appropriate macroscopic setup.

WP 3b: Effect modulation

Magnetic noise, which typically occurs in excited sensors, generally decreases with a slope of 10 dB/frequency decade (Fig. B1-7). The limit of detection can be significantly improved by frequency up-conversion of the signal to be measured using effect modulation. The effect modulation can be achieved in analogy to the concept of electrical chopper amplifiers: an already established method for flux modulation is the utilization of a piezoelectric cantilever, at the tip of which a soft magnetic material is attached. Using two additional flux concentrators, a periodic deflection of the beam by an electrical excitation leads to a periodic change of the magnetic flux through the sensor, if the cantilever is placed directly above the sensor. In conjunction with magnetoresistive sensors, it has already been shown that this method can lead to improvements of the detection limit by factors from 37.5 to 553 [Pa12, Ti16]. In another concept, the sensor is surrounded by a magnetically shielding material whose permeability is modulated by a current through an additional coil, thus leading to a frequency conversion of the flux density of the desired signal [Ch97]. Both methods are to be investigated theoretically and experimentally with regard to the conversion loss, and in particular, with respect to the potential improvement of the limit of detection for wideband ΔE -effect SAW delay line sensors (A9).

WP 4: Monolithic Integrated circuit design for maximizing signal-to-noise ratio

As the performance of the sensor element increases in terms of better noise performance and lower limits of detection, the requirements for the analogue amplifiers and signal conditioning circuits are also expected to increase. To keep the noise performance of the analogue integrated circuits below the noise level of the sensor elements, advanced electronic circuitry is required and investigated. The proposed method to tackle this challenge is the design of application specific monolithically integrated circuits. These circuits will be customized for the specific requirements of the individual sensors and thus will lead to an improved sensor system performance. The specifications of these circuits will be derived from the experimental results from WP 2. Additionally, the design of integrated circuits allows the integration of the complete amplifier including, e.g., high resistance feedback circuitry and capacitors into a single die. This reduces the parasitic effects of the interconnects and the individual passive components. In such reduced and compact systems, it has to be ensured that the magnetic fields of the power supply of the amplifier do not deteriorate the performance of the sensor system. This effect will be investigated. Since the dominant power supply currents of the amplifier are DC currents and even with discrete amplifiers no deterioration has been observed so far, it is expected that this effect will be very small and acceptable. By integration of the complete readout electronics, it will be possible to produce compact sensor systems with digital outputs that can be used to build sensor arrays.

WP 4a: Ultralow-noise preamplifiers for piezoelectric cantilevers

Sensors based on ME cantilevers require ultralow-noise preamplifiers that work in the sub-kHz range down to the Hz range. In this work package, it will be investigated how an ultralow-noise preamplifier can be designed in integrated circuit technique that fulfills the requirements of the most advanced ME cantilevers. The design includes simulation of the integrated circuit, layout of the design, and post layout simulation. Based on results of WP 2a, the specification for the charge and transimpedance amplifiers for the sensor elements with the highest performance will be derived. The low-noise integrated circuits will be designed in a 350 nm CMOS technology. From the electronic point of view, two major sources of noise are present in the low frequency regime: flicker noise and thermal noise. The flicker noise will be addressed in the integrated circuit design by using JFET input stages; the thermal noise can be addressed by using appropriate bias currents and operating points of the transistors. Fabrication of the ASICs will be done in a CMOS technology foundry through Europractice and takes approximately six months. After production, the ASICs will be characterized and verified.

WP 4b: Integrated circuits for ΔE -effect SAW delay lines

In WP 2d, electronic readout circuits for ΔE -effect SAW delay lines are investigated. These sensors work in the MHz frequency range. Different approaches for readout systems (open/closed-loop, homodyne/heterodyne) as well as noise models have been developed [B1-2, B1-3] and the equivalence of these systems has been theoretically shown. Since the SAW delay line sensors work in a high frequency regime, parasitic effects from the electronic components and its interconnects are very critical. Reducing these effects by integration of the complete first stage electronics into a single ASIC allows one to drastically reduce the parasitic effects of interconnects and components. In this work package, a fully integrated first stage readout circuit will be investigated. Among others, this includes a high frequency low-noise amplifier working at more than 150 MHz. The specifications and topology will be derived from WP 2d. Based on the requirements, a suitable CMOS technology will be chosen. The ASICs will be designed, fabricated, and verified as described in WP 4a.

WP 5: System front ends for biomedical applications

Based on the advanced sensor elements with highly improved limits of detection developed in project area A and on the advanced electronic readout circuits developed in WP4, complete system front ends for biomedical applications will be researched in this work package. The proposed method includes mainly system design aspects: sensor element and ASIC have to be integrated into a system. Special care has to be taken that the system setup, packaging, and interconnection do not lead to degradation of the complete system performance. The system front ends will be designed and fabricated. The systems will be individually characterized in the characterization setup that is also used in WP 1 and WP 2.

WP 5a: System front ends for biomedical applications with individual sensors

In this work package, a system front end for biomedical applications will be investigated that is optimized for measurements with individual sensors. Two versions will be designed: the first front end includes an ME cantilever sensor and the readout electronics developed in WP 4a. The second front end includes a SAW delay line sensor and the ASIC developed in WP 4b. After characterization, the systems will be used in biomedical applications of **B7**, **B9**, **B10**, and **T1**.

WP 5b: System front ends for biomedical applications with sensor arrays

Goal of this work package is the design of a system front end for biomedical applications that enables high spatial resolution measurements with sensor arrays. Based on the results of WP 5a and on simulations analyzing the mutual influence of sensors in arrays, the most suitable system front end will be selected for setting

up a sensor array. A system design will be created. Special care has to be taken in this design with regard to specific requirements of the biomedical experiment, the mutual influence of the sensor front ends, and the influence of the array on the magnetic field itself. After characterization, the sensor array will be used for high spatial resolution recordings in projects **B7**, **B10**, and **T1**.

Prospects

Research in this project is closely dependent on the sensor outcome of **project area A**, where bare sensors are researched. Such magnetic field sensors always have to be completed with dedicated and sophisticated analogue and digital signal processing to arrive at highly sensitive biomagnetic systems. Thus, on one hand this project will pursue conception, design, and improvement of highly sensitive front ends for those kinds of sensors which qualify for the applications mentioned. On the other hand, the type of applied sensors has immediate consequences on system design. The analogue part of system design will be closely linked with digital signal processing (**B2**), and is heavily dependent on the requirements which will be defined in the biomedical applications. With increasing grade of sophistication, arrays with growing number of sensors and more complicated sub-arrays will be required. This will be a further field of activity in this second funding period.

Research in the third funding period will focus on the customization and differentiation of the individual sensors and sensor arrays for the various biomedical applications in **project area B**. With increasing performance of the sensor systems, the demands from biological applications will differentiate. To illustrate this: high resolution heart rate characterization will have different spatial requirements than high resolution cell imaging. These demands will feed back into the design of sensor systems and sensor arrays. These, from biological application-derived system design specifications, will be the guideline for the third generation of sensor systems. Additionally, the sensor arrays will be extended to massive MIMO systems with a large number (>256) of individual sensors. While **B2** will explore the digital signal processing aspects of these systems, like parallel communication bus systems and real time aspects, **B1** will investigate the analogue aspects of such massive parallel systems like mutual influences and crosstalk from mutual inductance, self-inductance, skin effects, and other performance degradation. Another question will be how the magnetic fields of the communication bus system influence the performance of the sensors of a MIMO system and how this can be compensated for. The integrated circuits will be customized to provide the appropriate digital bus interfaces and enable bidirectional communication. By integration of logic and memory into the individual sensor systems, it will be able to individually calibrate the sensor elements and communicate in a massive MIMO system with each sensor individually, for example to tune different sets of sensor elements to different frequencies. In a real time closed-loop system, it might be a good idea to only activate a certain set of sensor elements that are closest to the point of interest and tune the activity and amplifications of the individual sensor elements for the biomedical application, for example in a motion compensation approach.

3.5 Role within the Collaborative Research Centre

As can be deduced from the working program, this project provides analogue signal processing and conditioning as the sole project. It complements the hardware of the various kinds of thin-film magnetic field sensors under investigation with the required electronic circuits in order to facilitate their practical application. It therefore provides the indispensable link between bare sensor hardware and subsequent digital signal processing. It also deals with an important part in measurement system design, required for bringing the sensors to application in biomagnetic diagnostics. In particular, the following collaborations with other projects are planned:

- A1: Investigation and characterization of magnetic noise in single and multilayer magnetic thin films.
- A2: Provision of low-noise preamplifiers and support on determination of sensor noise performance.
- A4: Collaboration on readout system development for ΔE -effect cantilever sensors.
- A7: Development of readout electronics and the noise model for ME cantilevers with electrical frequency conversion (EFC) and inductive readout.
- A8: Transfer of noise models to be integrated into the more general multiscale numerical modeling. Collaboration on cantilever-based flux modulator for SAW delay line sensor.
- A9: Feedback of measurement results in order to arrive at highly detective ΔE -effect SAW delay line sensors and collaboration on research of flux modulation techniques.
- A10: Investigation and characterization of magnetic noise in soft magnetic thin films.
- B2: Definition of the optimal interface between analogue and digital processing.
- B7: Sensor front ends for advanced localization of magnetic particle distributions (resonant ME cantilever sensors in passive mode).
- B9: Low-noise and low-energy preamplifiers for wearable sensor systems.
- B10: Sensor front ends for cardiologic applications (ΔE -effect SAW delay line sensors).
- T1: Sensor front ends for individualized deep brain stimulation (ΔE -effect SAW delay line sensors).

- Z1: Reception of ME cantilever sensors for noise investigations.
 Z2: Transfer of research results with respect to sensor system electronics and low-noise preamplifiers.
 Close cooperation on the development of sensor system front ends for biomedical applications.

This project will participate in the focus groups Comparison of Sensor Concepts, Magnetolectric Sensors, and Concepts based on ΔE -effect.

3.6 Differentiation from other funded projects

None

3.7 Project funding

3.7.1 Previous funding

Funding of this project within the Collaborative Research Centre started in 07/2016.

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum
Doctoral researcher, 100%	2	66.30	2	132.60	2	132.60	2	132.60	2	66.30
Total		66.30		132.60		132.60		132.60		66.30
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables	6.00		14.00		23.00		31.00		6.00	
Total	6.00		14.00		23.00		31.00		6.00	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation up to k€ 50	0		0		0		0		0	
Total	0		0		0		0		0	
Grand total	72.30		146.60		155.60		163.60		72.30	

(All figures in k€)

3.7.3 Requested funding for staff for the new funding period

	No	Name, academic degree, position	Field of research	Department of university or non-univ. institution	Commitment in hours/ week	Category	Funding source
Existing staff							
Research staff	1.	Höft, Michael, Prof. Dr.-Ing., Professor	Microwave Engineering	EIE	4		Core support
	2.	Bahr, Andreas, Prof. Dr.-Ing., Professor	Sensor System Electronics	EIE	4		Core Support
Non-research staff	3.	Taute, Wolfgang, Dipl.-Ing., Technician		EIE	4		Core support
Requested staff							
Research staff	4.	Wolfram, Henrik, M. Sc., Doctoral Researcher	Microwave Engineering	EIE		E13	
	5.	N. N., M. Sc., Doctoral Researcher	Sensor System Electronics	EIE		E13	

Job description of staff (supported through available funds):

1. Prof. Dr.-Ing. Michael Höft is responsible for the coordination and scientific management of B1 in agreement with Prof. Bahr. He advises the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of analogue system design, low-noise techniques, signal conditioning and processing, analogue filter technology, and related measurement setups. In particular, he will be the advisor of scientist 1 (Henrik Wolfram).
2. Prof. Dr.-Ing. Andreas Bahr is also responsible for the coordination and scientific management of project B1 in agreement with Prof. Höft. He advises the scientific employees with regard to planning, execution, and evaluation of the tasks, in particular with respect to monolithic integrated circuit design. In particular, he will be the advisor of scientist 2 (N. N.).
3. Dipl.-Ing. Wolfgang Taute supports the development of analogue circuits and measurement setups.

Job description of staff requested:

Two scientists are required to process the working program presented.

4. M. Sc. Henrik Wolfram will focus on the sensor noise performance and the development of sensor systems for ME cantilevers with EFC and ΔE -effect SAW delay lines. This includes both the development of macroscopic sensor system electronics as well as the appropriate integrated circuit design and evaluation. In addition, H. Wolfram will investigate the magnetic noise in thin films and ME microwave resonators.
5. N. N. will focus on the noise performance of ME cantilever sensors and the development of ultralow-noise preamplifiers for piezoelectric cantilevers. These preamplifiers will also be subject of integrated circuit design and evaluation. In addition, N. N. will investigate the effect modulation as a possibility to improve the overall limit of detection.

3.7.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/1
Existing funds from EIE	2.00	4.00	4.00	4.00	2.00
Sum of requested funds	6.00	14.00	23.00	31.00	6.00

(All figures in k€)

Funds available are used for acquisition of raw materials (aluminum, brass, copper, etc.), small mechanical parts, and the manufacturing of mechanical components required for laboratory setups of experiments in the central mechanical workshop of the department. Required consumables and small appliances are globally described and justified in the following sections: the planned work requires a great variety of individual parts, many of which are quite common and include special solders, conducting adhesives, passive electronic parts (SMD resistors, capacitors, inductors), active electronic circuits (op-amps, FETs, miscellaneous ICs, etc.), substrate materials, exposure masks, printed circuit boards (milling cutters for rapid prototyping and chemicals for etching and electroplating). More specific parts for the project are active electronic circuits such as high resolution ADCs, high resolution DACs, precision connectors, and cables. Especially ASICs have to be manufactured externally, which requires a large amount of the requested funds. All parts will be used for the development and manufacturing of the required analogue electronics for completion of the sensors, for building stand-alone interfaces to the digital world and interfaces for (re-)configuring the analogue measurement systems built in-house. The electronic systems also include small appliances like support material for experimental setups, power supplies, batteries, single-board processors, displays. Self-assembly of those parts is inefficient. The parts will be integrated into the in-house manufactured electronics.

Equipment up to k€ 10, software, consumables for		2020/2	2021	2022	2023	2024/1
Electronic consumables and materials	k€	4.00	8.00	7.00	7.00	2.00
Printed circuit board manufacturing	k€	1.00	4.00	3.00	3.00	1.00
Small appliances and support materials	k€	1.00	2.00	2.00	2.00	3.00
Fabrication of ASIC (WP 4a / WP 4b)	k€			11.00	19.00	

3.7.5 Requested funding for instrumentation for the new funding period

None

3.1 General information about Project B2

3.1.1 Project title: Digital signal processing

3.1.2 Research areas:

408-02 Communications, High-Frequency and Network Technology, Theoretical Electrical Engineering

3.1.3 Project leader

Schmidt, Gerhard, Prof. Dr.-Ing.
23.11.1971, German

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Do any of the above mentioned persons hold fixed-term positions? No

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	No
2.	clinical trials.	No
3.	experiments involving vertebrates.	No
4.	experiments involving recombinant DNA.	No
5.	research involving human embryonic stem cells.	No
6.	research concerning the Convention on Biological Diversity.	No
7.	investigations involving dual use research of concern.	No

3.2 Summary

This project focuses on digital signal processing approaches for enhanced readout of magnetoelectric sensors. The algorithms will be implemented for real-time applications to be prepared for closed-loop operation of entire sensor/actuator systems. The aim is to connect the sensor development and the biomedical analyses by digitally enhancing the sensor signals and providing additional information needed by the biomedical projects.

It starts with extending the existing noise cancellation and noise suppression techniques implemented so far by means of developing non-linear filter structures to resist the non-linear behavior of the ME sensors arising at high signal amplitudes (created by disturbing fields). Furthermore, we will focus on blind source separation techniques for multichannel measurements as well as empirical mode decomposition for single channel measurements to enhance the signal of the sensor. Moreover, the blind source separation approaches can be used in the "classical sense" for the separation of mixed signals.

In addition to the enhanced sensor signals, further information about the sensor is of great interest. Especially the exact position and orientation of the sensor are essential for the solution of inverse problems during medical analyses. Therefore, the sensor will be localized using additional coils transmitting orthogonal signals simultaneous to the biomagnetic measurement.

Moreover, the algorithms developed during the first funding period will be adapted to the new and improved sensor principles developed during the runtime of the Collaborative Research Centre and will be extended

towards multichannel measurements with respect to the cross-channel sensitivity between adjacent ME sensors.

This project is closely related to **B1** due to the hardware-close digital signal processing approaches. In cooperation, an optimal sensor system can be provided for the biomedical application projects. This indicates a strong cooperation with virtually all biomedical application projects (**B7**, **B9**, **B10**, and **T1**). In addition, strong cooperation is planned with the sensor-producing projects (especially with **A4**, **A7**, and **A9**) due to the adjustment of the digital signal processing algorithms and sensor read-out schemes to the individual sensor principles. The project **A8** provides further information about the sensor transfer functions for a more precise simulation of the sensor. The central project **Z2** supports this project by means of hardware development and passing the real-time system to the medical projects.

3.3 Project progress to date

3.3.1 Report and current state of research

The magnetoelectric (ME) sensors developed in this Collaborative Research Center (CRC) are based on a coupling of magnetostrictive and piezoelectric layers and are built as a cantilever (in the simplest version) [Ja13]. Due to the cantilever structure, resonance effects can be utilized for measurements with a high sensitivity. Various ME sensor principles have been investigated in the last few years and, in most of them, the resonance frequency and thus the area of highest sensitivity is in the kHz range. The frequency range of biomedical signals is rather low (a few hundred Hz) and thus the biomedical signals cannot be measured directly by the sensor. However, various measurement principles have been investigated in the last years, e.g. systems based on the so-called frequency conversion technique [Ja13; B2-5], ΔE -effect sensors [Za15], or SAW sensors [B2-4]. With these measurement principles, it is possible to measure magnetic signals with a low LOD.

Unfortunately, the cross sensitivity to acoustical and mechanical disturbances is rather high due to the mechanical structure of most of the ME sensors. Additionally, undesired magnetic fields, e.g. the earth's magnetic field, affect the sensor and thus superimpose on the biomagnetic signal. The aim of project B2 within the first funding period of the CRC 1261 has been to improve the measured signals of the ME sensors using various signal processing approaches. Concretely, the work plan for project B2 contained various adaptive filtering techniques for improving the individual measurement principles and was divided into four work packages:

1. Adaptive schemes for mode and read-out combination,
2. Adaptive control for the DA and AD frontends,
3. Digital cancellation and suppression of disturbing signal components, and
4. Active cancellation of exogenous magnetic fields.

An overall system overview including most approaches investigated in the work packages WP1 – WP4 is presented in [B2-2] and [Re17]. The algorithms investigated during the first funding period were developed for real-time applications. This was achieved by implementing the algorithms in the subband domain, a mixture of frequency and time domain. As a result, an appropriate frequency and time resolution as well as a low computational complexity of the system is achieved. In the following, the four work packages are shortly described and the progress of the last four years is explained.

WP 1 – Adaptive schemes for mode and read-out combination

As explained before, the ME sensors are read out in resonance to gain high sensitivity and thus a low LOD. Therefore, the ME sensors have to be excited magnetically or electrically by a carrier signal to convert the magnetic signal into higher frequency ranges. Thus the signal can be obtained from the sensor output signal by amplitude demodulation as well as by phase demodulation. Demodulating the sensor signal using a phase demodulation and an amplitude modulation in parallel and combining the output signals leads to a multi-demodulation read-out scheme. Additionally, the sensor can be excited in different modes. Exciting the sensor in multiple modes in parallel and combining these output signals leads to a multimode readout and is possible for all ME sensors occupying multiple modes. As shown in preliminary studies using ΔE -effect sensors, a multi-demodulation and multimode readout scheme improves the output signal in terms of signal-to-noise ratio (SNR) enhancement by about 4.5 dB [Re15].

Additional to the multi-demodulation and multimode read-out schemes, a multicarrier approach was investigated. This approach exploits that the bandwidth of the ME sensors increases using higher bending modes. If the bandwidth is high enough (higher than the bandwidth of the desired biomagnetic signal) the sensor can be excited by multiple carrier signals (as shown in Fig. B2-1). The combination of these output signals further enhances the overall output signal in terms of SNR.

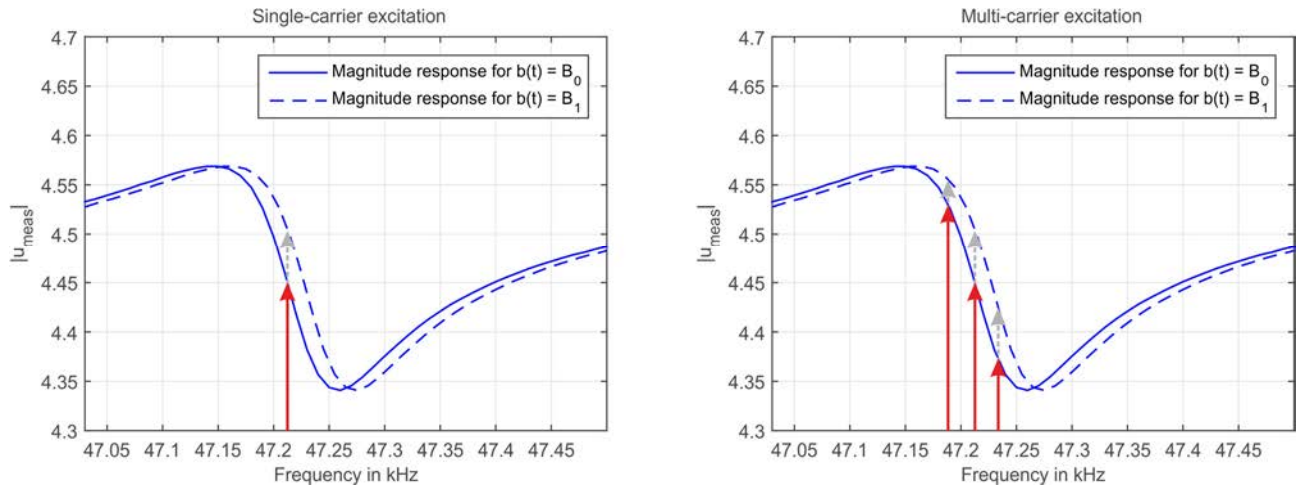


Figure B2-1: Magnitude response of the second mode of an ME sensor based on the ΔE -effect. In the left picture, only one carrier signal (at 47.22 kHz) is used, while in the second picture three carrier signals in parallel are used. Even if the carrier at 47.22 kHz leads to the largest effect, the two neighbouring ones can further improve the SNR. It has to be taken into account that the distance between two neighbouring carrier signals has to be at least twice the bandwidth of the measuring signal.

There are different ways for combining the signals extracted by the multicarrier and multimode approaches. Three different combination techniques have been implemented and compared: the minimum-variance-distortionless-response (MVDR) combination, the maximum-ratio (MR) combination, and the equal-gain (EQ) combination. The MVDR and MR combination approaches show the best results in terms of SNR enhancement [Re15; Re17]. The first mode of the sensor was excited once and the second mode of the sensor was excited with three carriers. The three carriers have an adequate distance regarding their frequencies. In Fig. B2-2 the magnitude spectral density of the amplitude demodulated signals of the four carrier signals is shown. The subband combination leads to a better SNR than the full band combination of the signals. An optimal weighting of the output signals generated by the multicarrier as well as by the multimode approach led to an SNR enhancement of about 6 dB [B2-7; Re17].

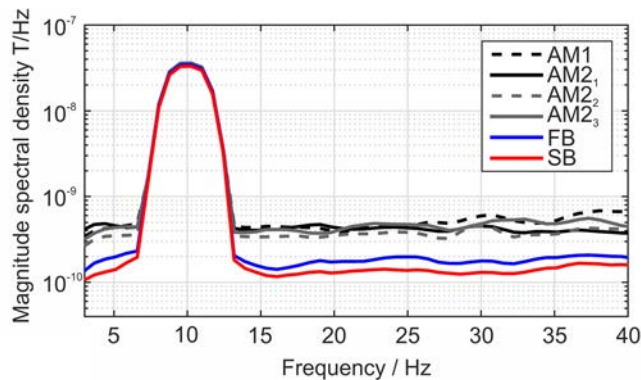


Figure B2-2: Amplitude demodulated (AM) signals of the first (AM1) and second (AM2_i) bending mode of the sensor. The second mode was excited by three carriers. The sensor received a sine signal with a frequency of 10 Hz. Obviously, the subband domain approach (SB) outperforms the full band domain (FB) approach. Due to the nearly similar SNR of all single signals, the improvement of the combination is quite high [B2-7; Re17].

The multicarrier as well as the multimode approach can also be used for sensors based on the magnetic frequency conversion technique. Unfortunately, increased restrictions regarding the carrier placements occur due to the high nonlinearities of this approach [Re17]. Nevertheless, an improvement of more than 2 dB can be achieved in comparison to a single mode and single carrier approach. Taken as a whole, the dynamic behavior of the adaptive mode and read-out combination presents a huge advantage. For instance, distortions in certain frequency ranges can be compensated by an adaptation of the weighting of the output signals. Additionally, additional electrodes (optimized for higher modes) led to a further improvement in terms of better SNR [B2-8]. Prior to the signal combination, linear and nonlinear equalization structures were applied to reduce the effects of the mechanical resonance (linear) of the sensor as well as the effects stemming from the magnetostriction curve (nonlinear).

WP 2 – Adaptive control for the AD and DA frontends

As mentioned earlier, the ME sensors have to be excited by a magnetic or electric carrier signal to modulate the magnetic signal into higher frequency ranges to measure biomagnetic signals with low frequencies [Ja12; Za15]. The carrier signal needs to be large in amplitude and causes a large dynamical range of the ME sensor signal and thus a weak resolution of the (bio-)magnetic signal due to the limited resolution of the AD (analog-to-digital) converter. An analog compensation of the carrier signal can reduce the dynamical range of the sensor output signal as shown in prior tests. During these tests, tuning by hand was necessary. Thus, an adaptive control for the AD and DA frontends as well as an analog performed and digital controlled carrier cancellation approach for a better resolution of the signal was investigated. A cancellation signal that matches the carrier signal of the sensor output in amplitude and phase has to be generated. Thus, an adaptive and automatic adjustment of the carrier signal amplitude and phase is necessary. The adaptation was investigated by two different algorithms, a gradient-based method and an algorithm searching successively for the minimum of a cost function. Both algorithms have been compared and approximately give the same results with respect to accuracy and time [Re17]. The effect of an active and a non-active carrier compensation is depicted in Fig. B2-3 for a sensor based on the magnetic frequency conversion approach as well as for a ΔE -effect sensor. A reduction of the carrier signal and thus of the signal dynamic of about 50 dB can be achieved.

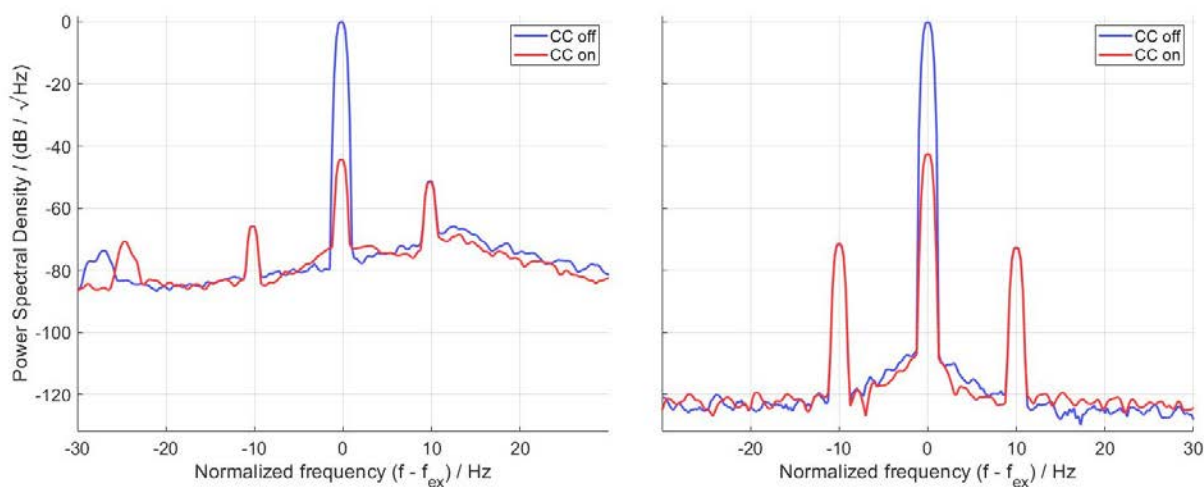


Figure B2-3: Comparison of the amplitude spectral densities of the ME sensor signals with and without compensation of the carrier signal (CC). The carrier signal can be compensated by up to 50 dB for the magnetic frequency conversion technique as well as for the ΔE -effect. Additionally, the noise floor of the sensor operating with the magnetic frequency conversion is enhanced at least slightly [Re17].

WP 3 – Digital cancellation and suppression of disturbing signal components

As described before, some of the ME sensors are highly cross sensitive towards mechanical and acoustical distortions. Additionally, undesired magnetic fields affect the sensor. Thus, the (bio-)magnetic signal will be superimposed by distortions and will be hard to measure. Therefore, preliminary studies have investigated first noise cancellation attempts using adaptive filter structures, which showed good results [Re15a]. The SNR improvement achieved so far was extended in the last funding period by combining noise cancellation and noise suppression approaches as well as by using multiple reference sensors.

Microphones, acceleration sensors, as well as magnetoelectric and piezoelectric (PE) sensors with different resonance frequencies were connected to the system simultaneously. PE sensors are produced similar to ME sensors but without the magnetostrictive layer. Thus, the PE sensors have the same cross-sensitivity to vibrations and acoustic distortions but cannot measure magnetic fields. A sensor array with four different PE sensors is shown in Fig. B2-4. The acceleration sensors as well as the microphones are not affected by the magnetic signals but are able to measure the acoustical and mechanical distortions. Only the additional ME sensors are able to measure the magnetic and non-magnetic distortions. To measure the distortions but not the biomedical signal, the ME reference sensors either have to be less sensitive or have to be placed at a sufficient distance to the source.

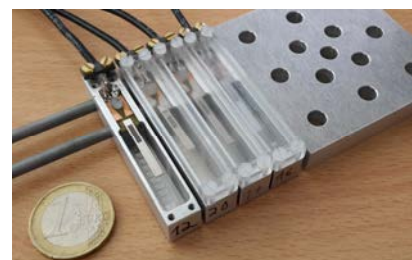


Figure B2-4: Sensor array of four PE sensors with different resonance frequencies [Re17].

A comparison of different reference sensors for ME sensors has been published in [B2-6]. In Fig. B2-5 the SNR gain for different sensors as reference sensors are presented. The results show that PE sensors are most suitable as reference sensors for the cancellation of vibrations and acoustical distortions, because they show the same behaviour as the ME sensors, especially if the resonance frequency of the PE sensors is close to the resonance frequency of the ME sensor. Microphones are slightly poorer with respect to vibrations but are also suitable for the cancellation of acoustical distortions.

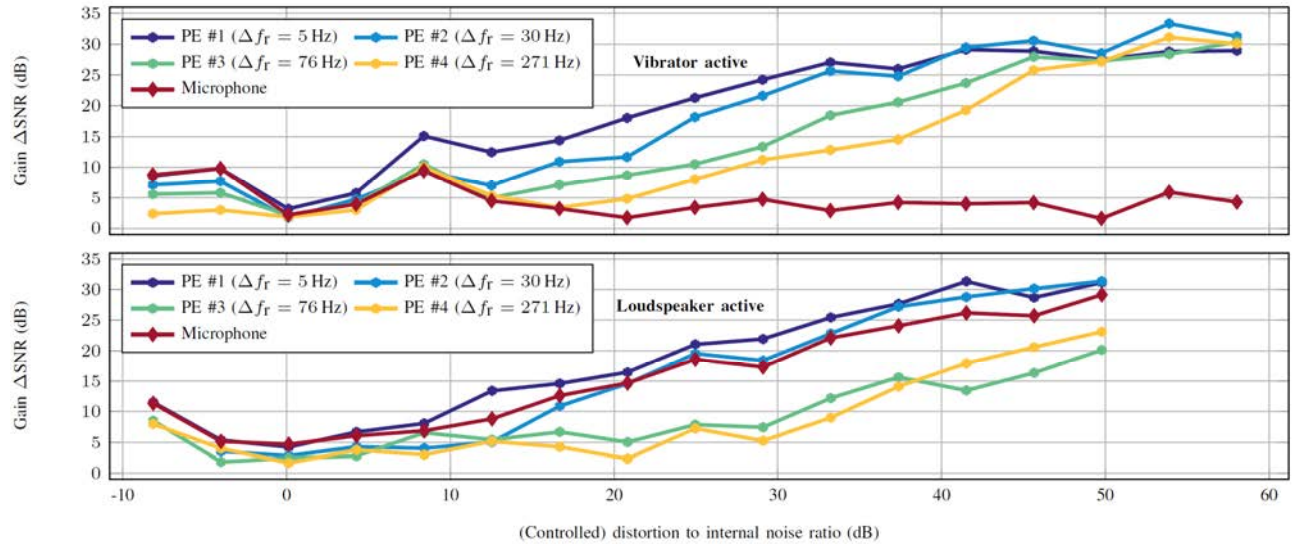


Figure B2-5: Comparison of the SNR gain after applying an adaptive filter using different reference sensors. The piezoelectric (PE) sensors are similar to the ME sensors, but without the magnetostrictive layer. Various PE sensors with different resonance frequencies were used so that the difference of the resonance frequencies Δf_r of the PE sensors and the ME sensor was varying. The sensors were excited once acoustically by a loudspeaker and once mechanically by a vibrator. The PE sensors show better results in terms of SNR gain if the resonance frequency is close to the resonance frequency of the ME sensor. The PE sensors are superior to a microphone as a reference sensor, especially if the distortions are vibrations [B2-6].

Because different reference sensors can be used for different distortions (e.g. magnetic, acoustic), a single-channel compensation is not efficient if different noise sources affect the sensor. Therefore, a multichannel compensation approach was investigated in addition to the single-channel compensation approach. Using different reference sensors in parallel, different distortions can be cancelled out efficiently [Re17]. All adaptive filter structures have been investigated in real-time by implementing the structures in the subband domain.

Additionally, the combination of noise cancellation and noise suppression approaches allowed obtaining a suppression of distortions (dominated by 50 Hz components) of 70 dB in comparison to 50 dB with approaches involving only noise cancellation [B2-2].

Furthermore, different adaptive averaging techniques were used for the SNR enhancement of (pseudo)periodic signals. Thus, a first measurement of a human r-wave using ME sensors could be performed and was published in [B2-3].

WP 4 – Active cancellation of exogenous magnetic fields

Besides the digital enhancement of the ME sensor output signal as described in the work packages WP1 and WP3, a mixed digital and analogue preprocessing of the signals can be advantageous. For instance, high noise amplitudes can cause a large dynamical range of the signal and thus a suboptimal usage of the amplifier and AD converter as described in the work package WP2. Exogenous magnetic fields, stemming e.g. from the magnetic field of the earth or from disturbing hardware, can be cancelled besides or additional to the methods proposed before by so-called active cancellation. For this, a coil generates a magnetic signal that adds destructively to the disturbing exogenous fields. Methods already known from active noise control [Ku99; Ku06], e.g. the filtered-xLMS algorithms, were tested. In a first step, one sensor measuring one direction and one coil for generating the anti-field were used. A first-order infinite impulse response (IIR) filter was applied for measuring the mean of the sensor signal. This signal was used as cost function for adjusting the anti-field signal generated by the coil. Thus, at least the earth's magnetic field can be actively cancelled. First results were published in [B2-2] using fluxgate magnetometers but can easily be transferred to ME sensors.

Additional magnetic sensors (e.g. ME sensors with a lower LOD) have to be placed at a sufficient distance to the biomedical source to make sure that they only measure the undesired magnetic fields and not the desired ones. The aim is to establish a multi-coil system created in a so-called Helmholtz setup. Finally, system identification schemes realized as adaptive filter structures should be implemented to drive the coils and thus create the magnetic anti-fields. The 3D-Helmholtz coil setup is depicted in Fig. B2-6.

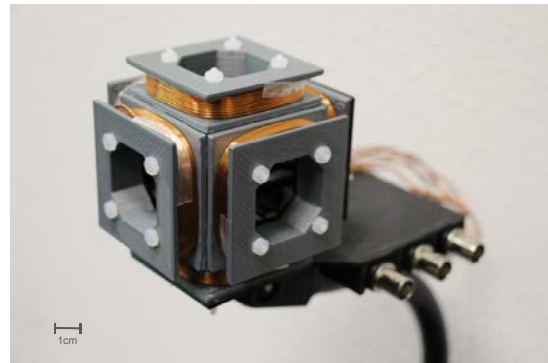


Figure B2-6: Helmholtz coil setup for the active cancellation of disturbing magnetic fields.

System overview

Altogether, a system operating in real-time was built consisting of the algorithms and methods proposed in the four work packages described above. The graphical user interface (GUI) of the system is shown in Fig. B2-7. The upper part of the GUI shows the single modules which are cascaded or processed parallel and can be switched on and off during runtime. The processing of the algorithms is done in the subband domain to keep the computational complexity low.

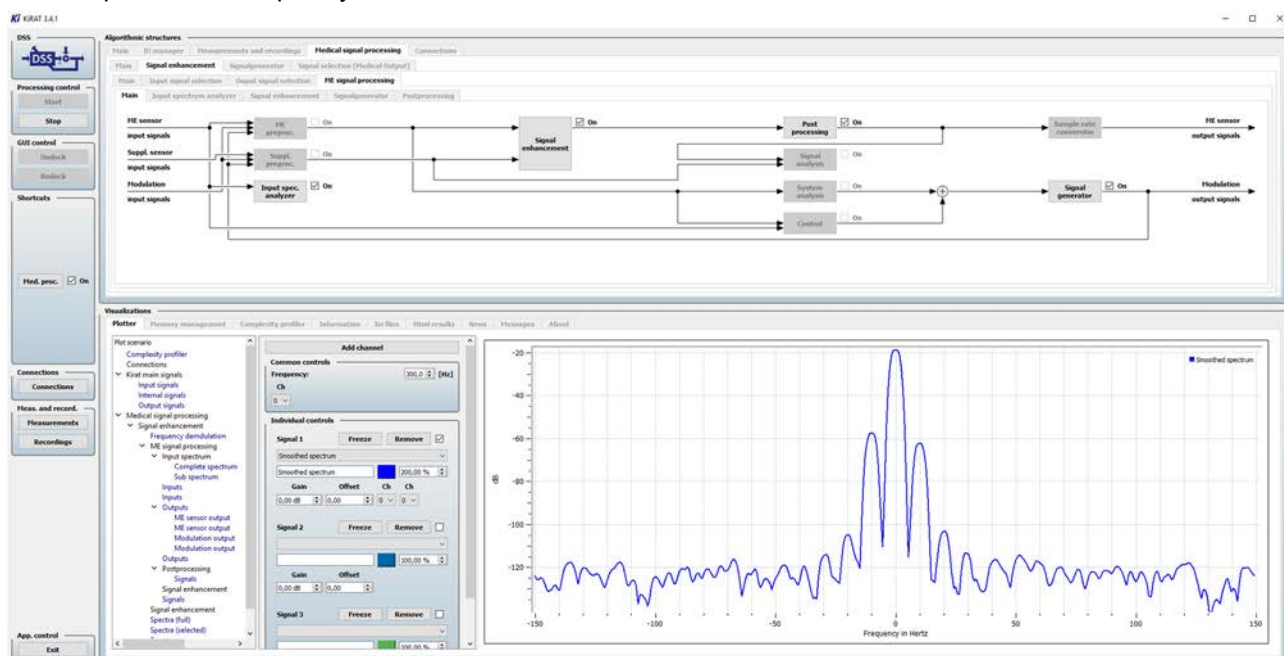


Figure B2-7: Graphical user interface of the closed-loop real-time system consisting of the algorithms investigated in the first funding period. Single modules can be connected, processed parallel or switched on and off during runtime.

References

- [Ba01] S. Baillet, J. C. Mosher, R. M. Leahy, Electromagnetic Brain Mapping. *IEEE Signal Processing Magazine*, (2001).
- [Be05] J. Benesty, S. Makino, J. Chen, *Speech Enhancement* (Springer, 2005).
- [Bi06] C. M. Bishop, *Pattern Recognition and Machine Learning* (Springer Science + Business Media, 2006).
- [Go16] I. Goodfellow, Y. Bengio, A. Courville, *Deep Learning*, (Adaptive computation and machine learning series, 2016).
- [Ha84] M. S. Hämäläinen, R. J. Ilmoniemi, Interpreting Measured Magnetic Fields of the Brain: Estimates of Current Distributions. *Report TKK-F-A559*, (1984).
- [Hy99] A. Hyvärinen, Fast and robust fixed-point algorithms for independent component analysis. *IEEE Transactions on Neural Networks* **10**, 626-634 (1999).
- [Hy01] A. Hyvärinen, J. Karhunen, E. Oja, *Independent Component Analysis* (John Wiley & Sons, Inc., 2001).
- [Ja12] R. Jahns, H. Greve, E. Woltermann, E. Quandt, R. Knöchel, Sensitivity enhancement of magnetoelectric sensors through frequency conversion, *Sens. Actuators A, Phys.* **183**, 16-21 (2012).

- [Ja13] R. Jahns, A. Piorra, E. Lage, C. Kirchhof, D. Meyners, J. L. Gugat, M. Krantz, M. Gerken, R. Knöchel, E. Quandt, Giant Magnetoelectric Effect in Thin-Film Composites, *Journal of the American Ceramic Society* **96**, 1673 (2013).
- [Ka60] R. E. Kalman, A New Approach to Linear Filtering and Prediction Problems, *Transactions of the ASME, Journal of Basic Engineering*, 35-45 (1960).
- [Ka04] J. Karvanen, T. Tanaka, Temporal Decorrelation as Preprocessing for Linear and Postlinear ICA (ICA 2004, LNCS 3195, Springer-Verlag, Berlin Heidelberg, 2004), pp. 774-781.
- [Ku99] S. M. Kuo, D. R. Morgan, Active noise control: a tutorial review, in *Proceedings of the IEEE* **87**, 943 (1999).
- [Ku06] S. M. Kuo, S. Mitra, G. Woon-Seng, Active noise control system for headphone applications. in *Control Systems Technology, IEEE Transactions* **14**, 331 (2006).
- [Ku06a] F. KÜch, W. Kellermann, "Nonlinear Acoustic Echo Cancellation" in *Topics in Acoustic Echo and Noise Control*, C. A. Hänsler, G. Schmidt, Eds. (Springer, 2006), pp. 205-261.
- [Le98] T. Lee, A. Ziehe, R. Orglmeister, T. Sejnowski, Combining Time-Delayed Decorrelation and ICA – Towards Solving the Cocktail Party Problem. *Acoustics, Speech and Signal Processing, Proceedings of the 1998 IEEE International Conference*, (1998).
- [Mi10] B. Mijovic, M. De Vos, I. Gligorijevic, J. Taelman, S. Van Huffel, Source separation from Single-Channel Recordings by Combining Empirical-Mode Decomposition and Independent Component Analysis. *IEEE Transactions on Biomedical Engineering* **57**, (2010).
- [Na97] K. Na, S.-I. Chae, Single-Sensor Active Noise Cancellation Using Recurrent Neural Network Predictors. *Proceedings of International Conference on Neural Networks (ICNN'97)*, (1997).
- [Re15] J. Reermann, G. Schmidt, S. Zabel, F. Faupel, Adaptive Multi-mode Combination for Magnetoelectric Sensors Based on the delta-E Effect. *Procedia Engineering, Eurosensors 2015* **120**, 536-539 (2015).
- [Re15a] J. Reermann, G. Schmidt, I. Teliban, S. Salzer, M. Höft, R. Knöchel, A. Piorra, E. Quandt, Adaptive Acoustic Noise Cancellation for Magnetoelectric Sensors. *IEEE Sensors Journal* **15**, 5804-5812 (2015).
- [Re17] J. Reermann, Signalverarbeitung für magnetoelktrische Sensorsysteme. *Dissertation*, (2017).
- [Ri03] G. Rilling, P. Flandrin, P. Goncalves, On Empirical Mode Decomposition and its Algorithms. *Proceedings 6th IEEE-EURASIP Workshop on Nonlinear Signal and Image Processing (NSIP)*, (2003).
- [Sa07] T. H. Sander, M. Burghoff, P. Van Leeuwen, L. Trahms, Application of decorrelation-independent component analysis to biomagnetic multi-channel measurements. *Biomedizinische Technik* **52**, 130-136 (2007).
- [St06] M. Stella, D. Begustic, M. Russo, Adaptive Noise Cancellation Based on Neural Networks. *2006 International Conference on Software in Telecommunications and Computer Networks*, (2006).
- [Za15] S. Zabel, C. Kirchhof, E. Yarar, D. Meyners, E. Quandt, F. Faupel, Phase modulated magnetoelectric ΔE effect sensor for sub-nano tesla magnetic fields. *Applied Physics Letters* **107**, (2015).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [B2-1] J. Sautter, F. Faubel, M. Buck, **G. Schmidt**, Artificial Bandwidth Extension Using a Conditional Generative Adversarial Network with Discriminative Training. *2019 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 7005-7009 (2019).
- [B2-2] J. Reermann, E. Elzenheimer, **G. Schmidt**, Real-time Biomagnetic Signal Processing for Uncooled Magnetometers in Cardiology. *IEEE Sensors Journal* **15**, 4237-4249 (2019).
- [B2-3] J. Reermann, P. Durdaut, S. Salzer, T. Demming, A. Piorra, E. Quandt, N. Frey, M. Höft, **G. Schmidt**, Evaluation of Magnetoelectric Sensor Systems for Cardiologic Applications. *Measurement (Elsevier)* **116**, 230-238 (2018).
- [B2-4] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, **G. Schmidt**, M. Höft, R. Knöchel, F. Faupel, E. Quandt, Wide Band Low Noise Love Wave Magnetic Field Sensor System. *Scientific Reports* **8**, (2018).
- [B2-5] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, J. McCord, D. Meyners, E. Quandt, **G. Schmidt**, M. Höft, Improved Magnetic Frequency Conversion Approach for Magnetoelectric Sensors. *IEEE Sensors Letters* **1**, 1-4 (2017).
- [B2-6] J. Reermann, C. Bald, S. Salzer, P. Durdaut, A. Piorra, D. Meyners, E. Quandt, M. Höft, **G. Schmidt**, Comparison of Reference Sensors for Noise Cancellation of Magnetoelectric Sensors. *2016 IEEE Sensors*, 1-3 (2016).
- [B2-7] J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, F. Faupel, **G. Schmidt**, Adaptive Readout Schemes for Thin-Film Magnetoelectric Sensors Based on the delta-E Effect. *IEEE Sensors Journal* **16**, 4891-4900 (2016).

- [B2-8] S. Zabel, J. Reermann, S. Fichtner, C. Kirchhof, E. Quandt, B. Wagner, **G. Schmidt**, F. Faupel, Multimode Delta-E Effect Magnetic Field Sensors with Adapted Electrodes. *Applied Physics Letter* **108** (2016).
- [B2-9] P. Hayes, S. Salzer, J. Reermann, E. Yarar, V. Röbisch, A. Piorra, D. Meyners, M. Höft, R. Knöchel, **G. Schmidt**, E. Quandt, Electrically Modulated Magnetoelectric Sensors. *Applied Physics Letters* **108**, (2016)
- [B2-10] A. Santillán Guzmán, M. Fischer, U. Heute, **G. Schmidt**, Real-time Empirical Mode Decomposition for EEG Signal Enhancement. *Proc. EUSIPCO 2013*, (2013).

3.4 Project plan

Objectives

ME sensors still suffer from cross-sensitivities to mechanical and acoustical distortions and are additionally affected by magnetic distortions. In the first funding period, research on various adaptive filter structures has been conducted for the enhancement of the ME sensor output signals. Especially linear filter structures have been investigated, but the ME sensors show a high nonlinearity operating in high magnetic fields, even if they originate from environmental distortions. Thus, research on non-linear filter techniques has to be done. Moreover, the robustness of the ME sensor measurements has to be increased for operation in clinical routines by using robust signal processing algorithms and providing additional information about the ME sensor (signal). Additionally, there is cross-sensitivity between (adjacent) ME sensors, which should be taken into account and can finally be taken advantage of.

The aim of this research project is the SNR enhancement of the ME sensor output signals, as well as the improvement of the robustness of the entire sensor system. We expect that these goals will be reached by consideration of the cross-channel-sensitivities as well as the non-linearity of the ME sensors. Thus, an enhancement of the entire sensor system frontend should be achieved.

The research on the ME sensor system will be realized with a combination of four work packages. All four work packages are based on close cooperation with the sensor producing projects, such as **A4**, **A7**, **A9**, and **Z1**, as well as the medical application projects, such as **B7**, **B9**, **B10**, and **T1**. Additionally, the strong collaboration between the analog signal processing project **B1** and the central project **Z2** is of great importance. All attempts proposed in the four work packages are oriented towards real-time multichannel ME sensor processing and the work packages are described briefly in the following:

1. Extension of the read-out schemes for multichannel analysis

As described in the previous chapter, different read-out schemes for the ME sensors have been investigated in the last few years. These attempts have to be extended and redesigned for the new and enhanced sensor concepts that will be developed in the CRC. Additionally, the read-out schemes have to be redesigned for multichannel measurements. Initially, the read-out schemes applied to one sensor should not disturb surrounding sensors. Moreover, the multichannel read-out of the sensor should automatically select the best sensor or an optimal mixture of sensors to ensure the best overall SNR for the biomedical analyses of interest.

2. Determination of the position and orientation of the sensor

For the solution of the inverse problem that has to be solved in various medical applications, the exact position and orientation of the measuring sensor have to be known. Therefore, orthogonal signals will be sent by multiple coils placed around the place of measurement. The inverse solution will lead to the exact position and orientation of the sensor. The localization of the sensor will be done simultaneously with the measurement of the desired biomagnetic signal.

3. Implementation of blind source separation techniques

The signals measured by the ME sensors are usually mixtures of various biomagnetic signals and different noise sources. The signals can be separated by blind source separation techniques, for instance, by independent component analysis (ICA). Additionally, the blind source separation techniques can be used for removing the superimposed noise and thus extracting the desired biomagnetic signal(s) out of the ME sensor signals.

4. Non-linear noise cancellation approaches

The ME sensors show non-linear behavior, especially if they are operated at high signal amplitudes. Thus, the linear adaptive filter techniques proposed in the first funding period should be extended towards non-linear filter structures. Volterra filters are a prominent example for modeling and thus for noise cancellation of non-linear systems. Moreover, neural networks can be used for (non-linear) noise cancellation.

Proposed research methods

All proposed methods are oriented towards multichannel ME sensor processing. Multichannel AD- and DA-converter cards with 24-bit resolution are already installed. The ME sensors, as well as coils and reference sensors, will be connected to the investigated real-time framework. This framework will be extended towards the proposed multichannel signal processing approaches and thus should provide the basis for SNR optimized measurements with the ME sensors developed in this CRC. The system is constructed as a closed-loop system, so the delay of the system has to be rather small. The delay of the whole processing chain, consisting of input hardware, AD and DA converters as well as the digital signal processing unit has a rather small delay of between 5.4 ms as a minimum and about 1 s as the maximum delay.

Work plan

The four work packages of this proposal described at the beginning of this section will now be described in more detail. The three work packages WP 1, WP 3, and WP 4 pursue the objective to further enhance the ME sensor signals as already started in the first funding period of this CRC. The two work packages WP 1 and WP 3 focus on multichannel measurements and the handling of the cross-channel-sensitivity of the ME sensors. The last work package WP 4 focuses on the non-linear behavior of the ME sensors. The work package WP 2 should provide further information additional to the enhanced ME sensor signals. The first work package WP 1 is the extension of the already proposed read-out schemes for multichannel analysis. Since the ME sensors are improved continuously over the funding period, the classical read-out schemes have to be adapted to these sensors, and thus the multichannel read-out schemes have to be adjusted continuously over the funding period, too. Thus, this work package is spread over the entire funding period, but it is only necessary to work on that topic full time in the first year. Afterwards, that work package will only be worked on intermittently. Hence, the other three work packages will be interrupted accordingly. In the following table the time schedule for the following funding period is illustrated.

Table B2-1: Work schedule

Work packages	2020		2021				2022				2023				2024	
	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP 1: Extension of read-out schemes towards multichannel analysis																
WP 2: Localization of the sensor																
WP 3: Implementation of blind source separation techniques																
WP 4: Non-linear noise cancellation approaches																

The four work packages will be described in the following in more detail. The risks of the approaches will be pointed out and alternative strategies will be presented if the proposed methods do not lead to the expected results. Moreover, an overview of the entire real-time system and prospects for the third funding period will be presented next, since all work packages will be realized using this system.

Overview of the resulting closed-loop system

Project **B2** is embedded in the signal chain starting with the measurement of the ME sensors and finishing with the analyses of the measured biomagnetic signals. Project **B2** measures the signals of the ME sensors amplified by low-noise amplifiers (investigated in Project **B1**) and digitally enhance the signals to forward them

to the medical application projects. For this, a closed-loop real-time system was developed during the first funding period, which will be extended during the second funding period for the optimal processing of the ME sensor signals.

In Fig. B2-8, an overview of the system resulting from the attempts worked on in the first and second funding period of project **B2** is shown. Summarized, multiple ME sensors as well as multiple reference sensors (e.g. microphones or additional ME sensors) are connected to the system. Noise cancellation approaches, for instance adaptive filters, are applied and the signals of the ME sensors are enhanced by blind source separation techniques and noise suppression approaches.

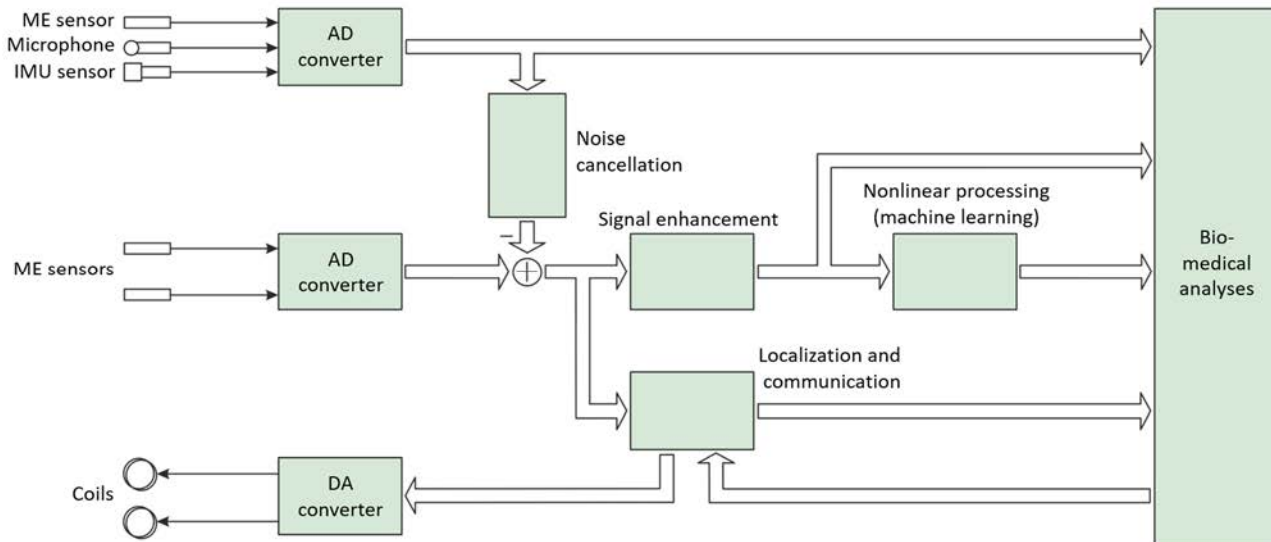


Figure B2-8: System overview of the closed-loop real-time system developed in this project. Multiple ME sensors as well as various reference sensors and coils are connected to the system. The noise is removed from the signal by different approaches, for instance noise cancellation and noise suppression approaches, and the signal is further enhanced by blind source separation approaches. Feature extraction schemes as well as the localization of the sensors provide further information about the measurement setup for the subsequent bio-medical analysis.

The enhanced signals can be forwarded directly to the biomedical analysis projects, and in addition feature extraction and pattern recognition approaches are exerted for further enhancement and/or extraction of additional information out of the ME sensor signals. Furthermore, coils are connected to the system for the transmission of artificial magnetic signals. These signals can be used for the localization of the sensors and thus for providing additional information of the sensor to the biomedical analysis. Altogether, a closed-loop system is formed for the enhanced readout of the ME sensor signals with additional provision of information. Thus, the sensors are optimally connected to the biomedical analysis projects, working with the pure biomagnetic signals.

WP 1 – Extension of the read-out schemes towards multichannel analysis

In this work package, the read-out schemes developed will be extended towards multichannel analysis of the ME sensors. The read-out schemes announced so far have in common that the sensor is excited by a multitude of carrier signals. Unfortunately, these carrier signals can cause cross talk between adjacent ME sensors, for instance when measuring with ΔE -effect sensors. Previous work on multichannel measurements did not take such cross-channel sensitivity into account. Thus, the read-out schemes have to be redesigned for measurements with multiple sensors. For instance, a compromise between carrier frequency and frequency-dependent sensitivity of the sensor has to be made.

Additionally, an SNR-based combination of the sensor signals can be applied. As in the single sensor case, the combination techniques minimum-variance distortionless-response (MVDR) combination, maximum-ratio (MR) combination, and so-called equal-gain (EQ) approaches should be tested first. In Fig. B2-9 a system overview of the extended read-out scheme is shown.

Moreover, an appropriate positioning – especially among themselves – of the sensors is of great interest for the optimal read-out of the ME sensor signals. Thus, the distance and orientation of the sensors to each other should be investigated and an SNR optimal positioning should be applied. Furthermore, the ability for three-dimensional measurements should be determined.

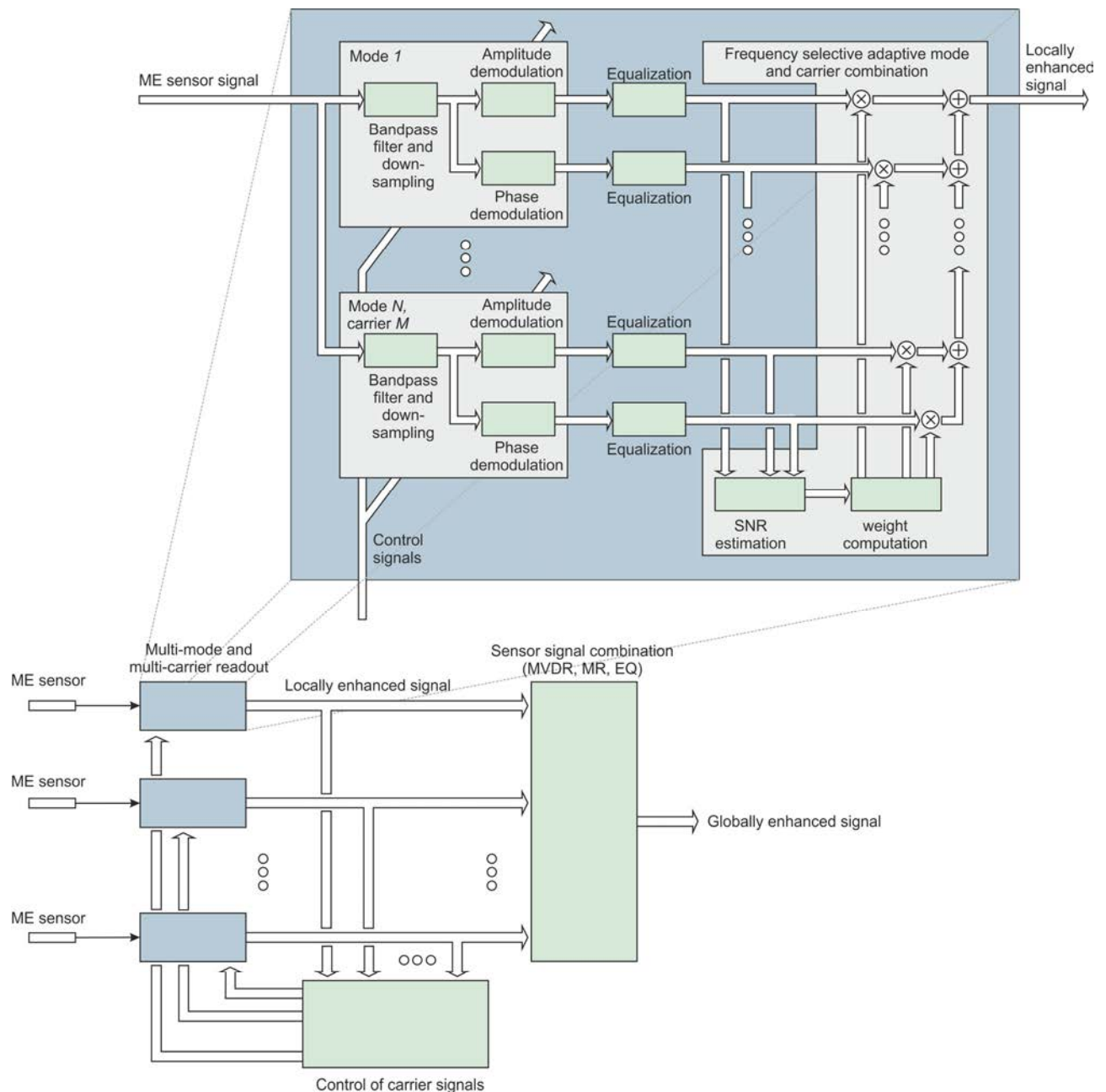


Figure B2-9: Overview of the proposed extension of the read-out schemes to multichannel measurements. In addition to the combination of various modes and demodulation schemes, the sensors are combined in an optimal fashion. Moreover, the carrier signals for all ME sensors are controlled centrally. Thus, it is ensured that the cross talk due to interfering carrier signals is minimized.

Furthermore, the CRC research on various ME sensor principles and new concepts are developed continuously over the funding period. Thus, new read-out schemes, for instance for the SAW sensors [B2-4] in project **A9** or the electrically modulated sensors [B2-9] in project **A7**, have to be developed that are adapted to the individual sensor properties.

WP 2 – Determination of the position and orientation of the sensor

Due to the flexible handling of magnetic measurements, the exact position and orientation of the sensors used is mostly not known during the measurement. But if an inverse problem is to be solved, for instance determining sources in the heart or the brain, the position and orientation of the sensors have to be known. This can be achieved by placing various coils with fixed (a priori known) positions next to the sensors transmitting orthogonal signals. For some applications, it might be beneficial to move the ME sensors during the measurement. Additionally, it is important to know the exact position and orientation of the sensor at all times of the measurement. Thus, the aim is to measure the desired signals and localize the measuring sensors simultaneously.

This can be achieved by using different modes for the localization and for the measurement. As a consequence, one mode has to be used to receive the signals sent out by the coils – the signals of the coils can be adjusted to the sensor properties – and the other mode(s) can be used for the measurement of the desired magnetic signal. First attempts in collaboration with project A4 have shown that it is suitable to use the first mode in direct detection (so without modulation of the signal) for the measurements of the coil signals and to use the second mode using the ΔE -effect for the desired measurement.

The signals transmitted through the coils are received by the ME sensor. Depending on the distance and angle of the ME sensor with respect to the transmitting coil, the amplitude received by the ME sensor differs. Due to the fixed position and orientation of the coils, the position and orientation of the sensor can be determined by the amplitudes of the signals measured by the sensor. This is called an inverse problem, which can be solved by various algorithms, for instance a minimum norm algorithm [Ha84] or a linear constraint minimum variance (LMCV) beamformer [Ba01].

The signals transmitted through the coils are received by the ME sensor. To separate the signals after measurement, the transmitted signals have to be orthogonal. This can be achieved by a separation in frequency. The signals are transmitted simultaneously through all coils but consist of different frequency components. This can be realized by transmitting, for instance, chirps, micro-chirps, or Kasami sequences. If a generation of signals orthogonal in frequency is not possible, for instance because of the limited bandwidth of the ME sensors, the signals can be separated in time. This would lead to a lower time resolution but to a stable solution. The individual signal components of the coils can be separated by a matched filter approach.

In Fig. B2-10 the system overview for the localization of multiple ME sensors is shown. The signal measured by the ME sensor has to be separated into the individual coil signals first, so the signals have to be orthogonal in time or in frequency. Afterwards, the ratios of the coil signals have to be determined and an inverse solution has to be computed. Afterwards, the estimated position and orientation can be smoothed by a Kalman filter, for instance [Ka60]. Thus, a robust localization of the sensor should be guaranteed. We are targeting a position accuracy in the sub-millimeter range.

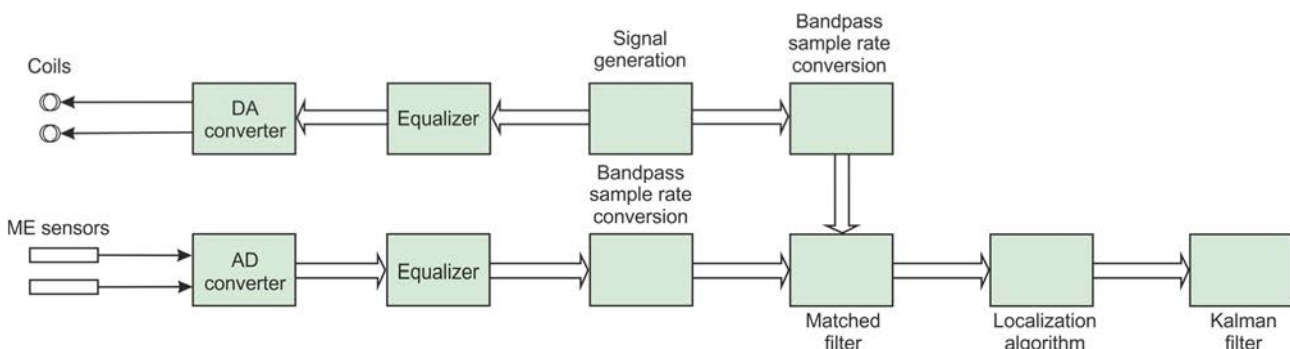


Figure B2-10: System overview of the localization approach for the ME sensors. Through coils positioned next to the ME sensor, artificial, orthogonal signals can be transmitted. These signals vary with distance and orientation with respect to the ME sensor. For reduction of the computational complexity, the signals can be converted into lower frequencies and down sampled by a band pass sample rate conversion. Due to the fact that the signal received by the ME sensors is a mixture of the individual coil signals, a matched filter has to be computed to separate the signal components again. Finally, an inverse solution can be computed and the position and orientation of the sensors can be estimated. A Kalman filter in series ensures a stable estimation of the position and orientation of the sensors.

First simulations showed good results in terms of localization accuracy. A minimum norm algorithm calculates the inverse solution and thus estimates the position and orientation of the sensor using a discrete searching grid. Thus, only discrete positions can be estimated by the algorithm, but these values are smoothed using a Kalman filter approach. A reduction of the grid resolution leads to better localization results on the one hand but causes higher computational costs on the other hand. Fig. B2-11 shows the results for a sensor moving from one corner of the grid to the other. The estimated and the real position of the sensor are depicted as well as the estimation error. The estimation error lies in the range of the grid resolution, but the localization accuracy can still be improved. This will be worked on in the first part of the work package. Afterwards, the localization accuracy during real measurements will be investigated. Therefore, as a first step, fixed-positioned sensors and, as a second step, moving sensors will be measured and localized.

For the solution of the inverse problem, a proper forward solution must be generated. Therefore, also the sensor properties, like the transfer function of the sensor, have to be taken into account. Initially, the sensor will be modeled as a point source. For further improvements of the solution, an enhanced model of the transfer function of the sensor will be provided by **A8**.

WP 3 – Implementation of blind source separation techniques

The signals measured by the ME sensors are mixtures of different magnetic and non-magnetic signal sources. Desired biomagnetic signals are superimposed by surrounding magnetic and acoustic noise sources. The signals as well as the transmission channel (mixing matrix) between the sources and sensors are unknown. Blind source separation (BSS) techniques can help to separate the individual signals and thus remove the disturbances from the biomagnetic signals or separate individual desired biomagnetic signals. The BSS solution is using the spatial diversity of the measuring sensors and is thus only possible with a multitude of ME sensors. The general mixing model is based on a number of N independent signals and M observations (typically stemming from M different sensors).

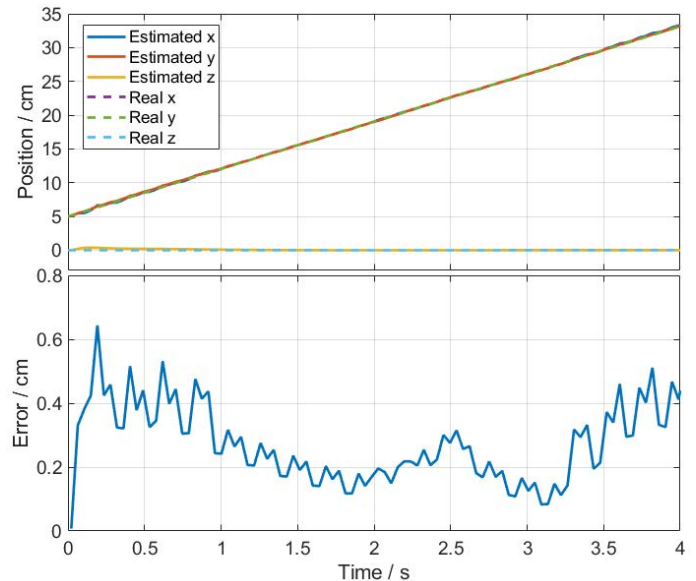


Figure B2-11: Real and estimated positions of a simulated moving sensor. The sensor position was estimated by a minimum norm algorithm and the grid resolution was 0.5 cm. The lower plot shows the error between the estimated and real position of the sensor. The mean error is lower than the grid resolution. Decreasing the resolution results in better localization results but also leads to a higher computational complexity.

The BSS problem can be solved by various attempts, such as independent component analysis (ICA). The ICA is based on the assumption that the measured signal is a combination of statistical independent signal components. The choice of algorithm is dependent on the problem to be solved. Various ICA algorithms have been investigated and used for biomagnetic analysis so far, like the time-delayed decorrelation (TDD) algorithm [Sa07]. A first comparison of different ICA algorithms has been investigated with respect to the implementation in real-time and the usage for biomedical analysis. The best compromise of computation time and separation accuracy is achieved by the so-called Fast ICA algorithm [Hy99; Hy01]. In Fig. B2-12 the separation of two sine signals of 10 Hz and 30 Hz is shown. The signals have been transmitted by two different coils ($N = 2$) and the mixture has been measured by two ME sensors ($M = 2$).

Dependent on the algorithm used, several assumptions have to be fulfilled by the signals. Thus, different algorithms must be used for different problems to obtain individually optimized separation performance. Additionally, a combination of multiple algorithms should be investigated for an optimal separation, as stated in [Le98; Ka04]. With the BSS technique, the cross-channel sensitivities of the ME sensors can be exploited and an enhanced signal denoising is possible.

Additionally, empirical mode decomposition (EMD) can be applied to single channel ME sensor signals. The EMD separates the signal in so-called intrinsic mode functions – signal components fulfilling a certain type of criteria [Ri03]. Thus, the noise contained in the sensor signal can be separated from the desired magnetic signal. Using adaptive kernels (EMD) instead of fixed ones, for instance using a Fourier transform, will lead to a better separation of the noise from the signal. First attempts of EMD have been already investigated in [B2-10]. These approaches have to be adapted to ME sensor signals first. Afterwards, a combination of EMD and ICA is possible for the enhanced analysis of single-channel measurements [Mi10].

If the noise cancellation approaches using ICA, EMD, or a combination of both algorithms do not lead to success, classical multichannel Wiener Filter approaches [Be05] will be implemented to make use of the multichannel measurements and cross-sensitivities of the ME sensors.

WP 4 – Non-linear noise cancellation approaches

The ME sensors show a highly non-linear behavior, especially when they are operating at high signal amplitudes. Due to this, linear filter structures for the cancellation of magnetic and non-magnetic noise are limited in precision. The last funding period showed quite good results in terms of SNR enhancement of the ME sensor

output signals, but we are confident further improvements to these results can be made using non-linear filter structures.

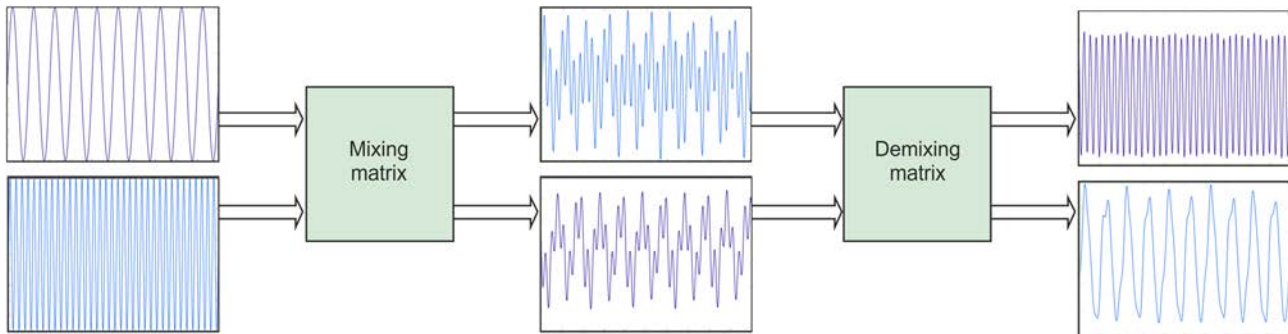


Figure B2-12: First BSS attempts for the ME sensors. On the left, two sine signals with a frequency of 10 Hz and 30 Hz transmitted by two different coils are shown. Both signals are measured by the two ME sensors and thus a mixture of both sine signals (and noise) is measured by each ME sensor individually. The signals in the middle of the figure show the demodulated signals of the two ME sensors measuring through the ΔE principle. Using a Fast-ICA algorithm (denoted as demixing matrix), the sine signals are separated again without observing the correct order (permutation problem of ICA) and amplitudes of the individual signals.

The most prominent non-linear filter structure is the Volterra filter [Sch80; Av10]. Volterra filters are used for the system identification of non-linear systems and have linear behavior between the system output and the filter coefficients [Av10]. To reduce the computational complexity, the Volterra filter will be implemented in the subband domain. Dependent on the problem and precision of the filter, quadratic, cubic, or even higher order filter coefficients are used [Ku06a]. Thus, Volterra filters possess a high computational complexity due to the high amount of filter coefficients, even if used in the subband domain. The usability of Volterra filters for the noise cancellation of ME sensors will be investigated during the second funding period.

Volterra filters are only one example for non-linear filter structures. To reduce computational complexity and for calculating a quite robust non-linear estimation of the ME sensor system, neural networks can also be used [B2-1]. Neural networks can be operated in various ways, but in this work package only regression approaches which generate a continuous output should be investigated [Bi06]. In this form, neural networks can be used for the active noise cancellation of the ME sensor signals. Here, the neural networks model adaptive filters for the cancellation of noise sources [St06; Na97]. This should be applied to the ME sensor signals to further enhance the ME sensor output signals. Neural network structures can model non-linear filter structures and thus can be used for the non-linear noise cancellation of the ME sensors.

Prospects

In the third funding period, the multichannel approaches should be extended to so-called *massive MIMO systems* with more sensors (e.g. 256 and more) and more coils (magnetic “senders”). The sensors should be placed and operated partly organized (e.g. as line or grid arrays) and partly distributed (e.g. at different parts of the body). Due to the huge amount of sensors and coils, the processing load will increase dramatically. Thus, parallel processing approaches have to be investigated to ensure the real-time ability. While **B2** focusses on the digital signal processing aspects, **B1** will investigate the analog aspects of the massive MIMO systems. The close cooperation of **B1** and **B2** will provide a digital bus interface for a bidirectional communication. Thus, further functionality can be integrated into the sensor, for instance the communication of the massive MIMO system with each sensor individually. The real-time closed-loop system will provide the ability to activate only a certain set of sensor elements that are closest to the point of interest and tune the activity and amplifications of the individual sensor elements for the biomedical application.

As a second extension, closed-loop operation of the entire system should be investigated in more detail with focus on biomedical applications. Right now the systems are already prepared for low-delay detection and classification approaches. The results of these detections, however, are not yet used immediately by the medical applications. The parameters of deep brain stimulation might be controlled, e.g., by the detected physical state of patients. This leads to demands of the entire loop delays of only a few tens of milliseconds.

Furthermore, the project **B2** will support the transition from single-system applications, like “pure” cardiologic applications, to multi-application approaches, e.g. combined cardiologic and neurologic measurements that are combined with movement analysis.

3.5 Role within the Collaborative Research Centre

The project **B2** serves together with the project **B1** as the connection between the sensor development projects (e.g. **A4**) and the medical application projects (e.g. **B9** or **B10**) and is thus strongly linked to several projects within the CRC 1261. The following table shows details about the planned cooperation of the project **B2**:

A2, A3, A4, A7:	Setup of specifically tailored read-out schemes for the sensor principles investigated in these projects.
A9:	
A8:	The sensor models that are investigated in A8 will be incorporated in the forward models used in the project (WP 4). A first sensor model version available in 2021 will be replaced with extended versions in 2023.
B1:	This project will cooperate strongly with B1 in terms of improving the ME sensor frontends.
B9, B10:	Cooperation in the design and implementation of the real-time framework for medical applications (heart and movement jacket)
B7, B9, B10, T1:	Utilization of the closed-loop real-time framework for measurement purposes.
Z1:	Production of ME sensors, feedback regarding sensor performance.
Z2:	Passing the real-time system to this project for enhanced measurements.

The project B2 will participate in the focus groups FB "Biomedical Applications" and FG "Comparison of Sensor Concepts" in terms of the following topics:

FB:	Sensor fusion and selection of the SNR optimal sensor signal, as well as real-time preprocessing and supply of additional information for signal analyses.
FG:	Real-time signal processing aspects for improved sensor read-out schemes.

3.6 Differentiation from other funded projects

Gerhard Schmidt has no conflicting funding in the area of digital signal processing for ME sensor systems. A request for funding of this project has not been submitted to any other addressee.

3.7 Project funding

3.7.1 Previous funding

Funding of this project within the Collaborative Research Centre started in 07/2016. Previously, it was funded under a different DFG programme from 01/2015 to 06/2016 (reference number SCHM 1507/9-1).

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral researcher, 100 %	1	34.2	1	68.4	1	68.4	1	68.4	1	34.2
Total		34.2		68.4		68.4		68.4		34.2
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables	14.0		4.0		4.0		4.0		2.0	
Total	14.0		4.0		4.0		4.0		2.0	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation up to k€ 50	0.0		0.0		0.0		0.0		0.0	
Total	0.0		0.0		0.0		0.0		0.0	
Grand total	48.2		72.4		72.4		72.4		36.2	

(All figures in k€)

3.7.3 Requested funding for staff for the new funding period

	No.	Name, academic degree, position	Field of research	Department of university or non-university institution	Project commitment in hours per week	Category	Funding source
Existing staff							
Research staff	1.	Schmidt, Gerhard, Prof. Dr.-Ing., Professor	System Theory	EIE	4		Core support
Non-research staff	2.	Prehn, Kevin, Lab Engineer		EIE	4		Core support
Requested staff							
Research staff	3.	Bald, Christin, M.Sc., Doctoral Researcher	Digital signal processing	EIE		E13	

Job descriptions of staff for the proposed funding period (supported through existing funds):

1. Prof. Dr.-Ing. Gerhard Schmidt is responsible for the coordination and scientific management of project B2. He advises the scientific employee with respect to planning, execution and evaluation of the tasks, in particular in matters of digital system theory and machine learning approaches.
2. Kevin Prehn will support the development and programming for the described work packages.

Job descriptions of staff for the proposed funding period (requested funds):

3. M.Sc. Christin Bald, doctoral researcher (Ph.D. candidate), who investigates the research ideas proposed in this document (working on project **B2** since end of 2017).

3.7.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/1
Existing funds	1.5	3.0	3.0	3.0	1.5
Sum of requested funds	14.0	4.0	4.0	4.0	2.0

(All figures in k€)

Available funds are used for acquisition of small mechanical parts, electric circuits, cables, shielding, and damping material and the manufacturing of mechanical components required for laboratory setups of experiments in the central mechanical workshop of the department. In total this requires about 4000 Euro per year (in addition to 3000 Euros being paid by University accounts). This number stems from experience from the last funding period.

Equipment up to k€ 10, software, consumables for financial year 2020/2

Electronic consumables, small appliances, and support materials	k€	2.0
High-precision AD-converter card extension	k€	7.0
Multichannel current source (DC and AC in parallel)	k€	5.0

Equipment up to k€ 10, software, consumables for financial year 2021

Electronic consumables, small appliances, and support materials	k€	4.0

Equipment up to k€ 10, software, consumables for financial year 2022

Electronic consumables, small appliances, and support materials	k€	4.0

Equipment up to k€ 10, software, consumables for financial year 2023

Electronic consumables, small appliances, and support materials	k€	4.0

Equipment up to k€ 10, software, consumables for financial year 2024/2

Electronic consumables, small appliances, and support materials	k€	2.0

3.1 General information about Project B3(E)

3.1.1 Project title: Inverse solutions for localization of biomagnetic activity in heart and brain

3.1.2 Project leader(s)

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3.2 Project history

3.2.1 Report

Current density reconstruction for heart and brain requires the solution of an underdetermined inverse problem. In order to obtain a unique solution, additional constraints need to be imposed on the problem. Temporal information in surface M/EEG as well as in M/ECG may be used to improve current density reconstruction. This can be performed via state-space models and Kalman filters. A state-space model consists of two equations that describe the system dynamics and the measurement, respectively. Since the aforementioned inverse problems are high dimensional, modified versions of the standard Kalman filter are used to solve the state estimation problem. In this project we use a linear transformation, spatial whitening, to transform the fully coupled state-space model into a weakly-coupled one where only neighbor coupling is preserved. This allows for a Kalman filter to be defined at each point in the source space. After sequential state estimation, the linear transformation is reversed to obtain the final current density distribution. Additionally, maximum likelihood estimation is used to obtain the parameter matrices of the state-space model. To the best of our knowledge, this approach, the spatiotemporal Kalman filter (STKF) [Ga04], is unique to our group and it had not been applied to M/ECG data before this project. In M/EEG source imaging, we applied this approach to M/EEG data from patients with epilepsy. The doctoral work of Laith Hamid was successfully finished within the framework of this CRC and the algorithmic developments of the STKF and its regional form in addition to their applications in epileptology were described in the dissertation that was published in [B3-1].

In WP1 we recorded simultaneous MCG-ECG with two kinds of MCG systems, namely superconducting quantum interference devices (SQUID) and optically-pumped magnetometers (OPM) (Figure B3-1a). We performed these measurements for three volunteers in the *Physikalisch-Technische Bundesanstalt* (PTB) in Berlin. As our goal was to perform realistic and accurate forward and inverse analyses, we also recorded Magnetic Resonance Images (MRI) in Kiel for the same three volunteers. The active sensors were around 200 SQUID sensors (we used only the first layer of 53 sensors for the analysis), 10 OPM sensors (superimposed to 20 positions) and 32 ECG electrodes. We did not need to suppress the artifacts because the signal-to-noise ratio (SNR) was high for the sensor types that we used.

As our group has experience in solving the inverse problem for the brain, it was the task of this work package to construct a pipeline for the forward and inverse analyses for the heart. We used the MRI to segment the torso via semi-manual methods using two software packages, Insight Segmentation and Registration Toolkit (ITK) (available at <http://www.itk.org>) and Seg3D (available at <http://www.sci.utah.edu/cibc-software/seg3d.html>). From this segmentation we then constructed a finite element model (FEM) for the torso and other tissues using the SimBio-Vgrid mesh generator (available at <http://vgrid.simbio.de>). The torso model was segmented as realistically as possible and was constructed from 9 regions, namely lungs, spleen, kidney, bones, heart, liver, stomach, esophagus and torso/fat (Figure B3-1b). Then we calculated the Leadfield Matrix

(LFM) using SimBio. We used the LFM to solve the inverse problem via STKF, low-resolution brain electromagnetic tomography (LORETA) [Pa94] and Minimum Norm Estimation (MNE) [Hä84] algorithms. The block diagram for the pipeline is depicted in (Figure B3-1c) and was published in [B3-5]. From the comparison between the localization results of LORETA and STKF, we can see that the Kalman filter could localize the P-point, which has a lower SNR compared with the R-point, better than LORETA. It also described the transition from the Sinoatrial (SA) node to the Atrioventricular (AV) node better (Figure B3-1d). Adaptive STKF with state-space generalized autoregressive conditional heteroscedasticity (GARCH) model was applied to the data and it showed a slight improvement over the standard STK.

Additionally, we simulated datasets for different sensor distributions, numbers, and locations to study the effect of these factors on the source imaging results and find the optimal distribution, number, and location for the array of ME sensors. First, the array from the back side gave the weakest results. Second, we observed that the increase in the number of sensors by combining multiple layers does not necessarily improve the localization. The last result was that the orientation of the source dipole plays an important role in the distribution of the sensors, since the orientation of the magnetic sensors should be orthogonal to that of the dipole.

The evaluation of the simulated datasets was performed via the Euclidean distance between the simulated location and the reconstructed source location on the source grid. The validation of the real datasets from the volunteer's measurement in PTB Berlin was discussed and determined with the help of the Department of Cardiology in the UKSH (Prof. Norbert Frey) in Kiel. Additionally, we gave feedback to the other groups about the optimal number, distribution, and orientation for constructing the optimal array of ME sensors.

The details and the plan of this work package were changed from the proposal because of the reasons mentioned below. First, the cardiological project **B4** was not funded and we had planned close cooperation with **B4**. Even though the Department of Cardiology was supportive by validating our results through visual inspection, they could not dedicate enough time and personal resources to the research project anymore. Second, the sensitivity of the ME sensors was not enough to perform MCG without averaging. So instead, we used data from simulations, SQUID, and OPM sensors for our analyses. Third, the torso phantom was not available, since the torso phantom from the previous funding period, which was constructed by the Engineering Faculty of the University of Kiel (during CRC 855 and PAK 902), was too simplistic and the CRC 1261 did not plan to build a new and more realistic torso phantom.

In WP2 we apply dynamical inverse methods based on state-space modeling and Kalman filtering to solve the inverse problem in electrophysiological brain imaging. In CRC 855 we tested our STKF on epileptic spikes [Ha15a] and focal seizures [Ha15b]. Additionally, we investigated the effects of the definition of the 3D volumetric grid and the Laplacian operator on the accuracy of source imaging [Ha15a]. For CRC 1261 we introduced dimensionality reduction to the STKF pipeline to remove redundancy and reduce the computational time [B3-2]. Additionally, we showed that STKF outperformed standard source imaging methods in the case of a small number of electrodes or sensors [B3-3]. We also implemented and tested adaptive forms of STKF to improve the accuracy and spatial resolution of source imaging. The first algorithm, the regional STKF (RSTKF), allowed for region-specific state-space dynamical noise variances. Compared to standard STKF, the new approach improved the accuracy and spatial resolution of source imaging in an epilepsy patient with hippocampal sclerosis [B3-4]. Additionally, RSTKF successfully localized deep thalamic activity from simulated data (paper will be submitted at the end of January 2020). The second algorithm, array square-root STKF with state-space generalized autoregressive conditional heteroscedasticity (ASR-STKF-ssGARCH), used the array square-root form of the Kalman filter to improve the numerical stability of STKF-ssGARCH (manuscript is in preparation and will be submitted at the end of January 2020). The use of state-space GARCH allows for better modelling of non-stationary recordings. The application of STKF-ssGARCH as well as ASR-STKF-ssGARCH resulted in improved accuracy and spatial resolution compared to STKF (Figure 1e). Additionally, the array square-root form improved the reconstruction of brain dynamics due to the improved numerical stability [B3-4] (Figure B3-1f).

Head phantoms are used for sensor characterization, testing of sensor arrays as well as evaluation of source imaging algorithms. Instead of the single-source wet MEG phantom from CRC 855, we cooperated with **Z2** to construct a dry MEG phantom with 8-24 sources. The coils were placed inside a head phantom in order to simulate sources with different locations, extents, and depths. To use the phantom for source imaging, we performed a CT scan of the head phantom at the Department of Neuroradiology of the UKSH in Kiel. The CT image was then segmented via the software CURRY7 (Compumedics Neuroscan, Dresden, Germany, <https://compumedicsneuroscan.com>) and we obtained the head geometry and the coil positions. We have used the phantom to perform MEG measurements via fluxgate sensors (Technical Faculty, CAU Kiel) and a CTF SQUID system (Institute for Biomagnetism and Biosignalanalysis, University of Münster) and performed MEG source imaging via standard source imaging approaches (Figure B3-1g). Additionally, the head phantom

is available at the Technical Faculty in Kiel for use by other projects in the CRC 1261 for sensor characterization.

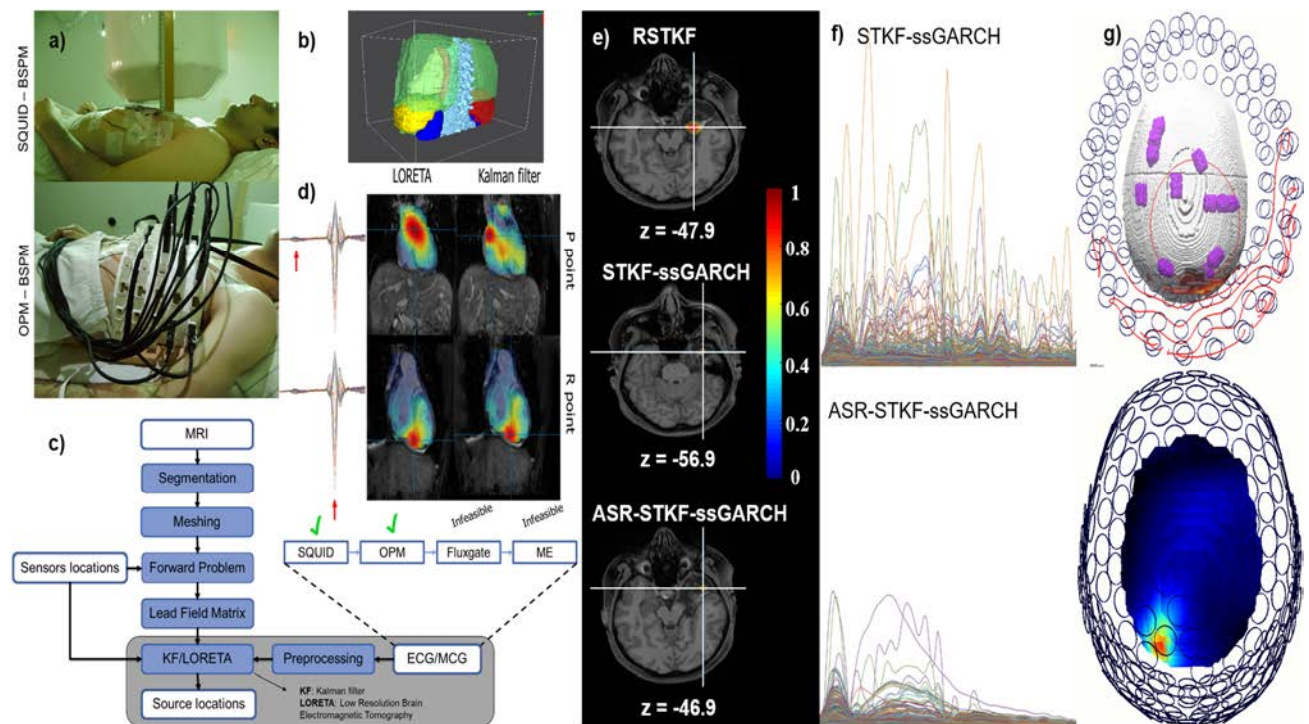


Figure B3-1: a) Pipeline for the forward and inverse problems for the heart. b) The measurement setup in PTB Berlin. c) Comparison of source imaging from LORETA and STKF. d) Nine-region torso model. e) Localization of the epileptogenic zone via regional STKF (top), STKF-ssGARCH (middle) and ASR-STKF-ssGARCH (bottom). f) Reconstruction of dipole time series via STKF-ssGARCH (top) and ASR-STKF-ssGARCH (bottom). g) Source imaging from phantom recordings via fluxgates (top) and SQUID MEG (bottom).

Since no recordings with real patients with implanted deep brain stimulation (DBS) electrodes were performed within the CRC 1261 by project **B5**, we decided to concentrate on simulations, phantom recordings, and EEG data to test our algorithms. Additionally, the time slot that was assigned to DBS data was reassigned to phantom and simulated data.

In WP3 we started the project with prior experience in EEG-MEG fusion within the framework of source imaging via STKF [Ha13]. We wanted to apply this approach on simultaneously recorded ECG-MCG. Additionally, we wanted to use STKF to fuse data from different sensor types, such as gradiometers and magnetometers. We implemented an algorithm for fusion of magnetic measurements from magnetometers and gradiometers. This approach is based on the extension of the measurement equation of the state-space model to accommodate the different forward solutions, measurement noises, and scaling factors of the sensor types, respectively. We are currently testing the algorithm using recordings from the Elekta phantom that were recorded by K. Taylor and J. Mosher (Epilepsy Center, Cleveland Clinic Neurological Institute, Cleveland, OH USA). The data were made available through Brainstorm [Ta11], which is documented and freely available for download online under the GNU general public license (<http://neuroimage.usc.edu/brainstorm>). We expect the results to be ready by the middle of February 2020. To the best of our knowledge, we are the only group that is performing MEG-EEG as well as MCG-ECG fusion via state-space modelling and Kalman filtering.

Additionally, since there is a lack of publications about MCG-ECG fusion, we decided to apply the fusion model published in [Ha13] on the data recorded in PTB Berlin from the **WP1**. This part will be finished by the end of February 2020. Similarly to [Ko11], we intend to make the MCG-ECG recordings in addition to the MR images and the leadfield matrices publicly available around the end of the first funding period as reference datasets to evaluate heart models and source imaging methods.

In WP4 our project cooperated with **B7** to implement and test an inverse solution for 3D-imaging of magnetically labelled cells. The subspace Barzilai-Borwein non negative least-squares (SBB-NNLS) algorithm [Ki13] was implemented. It is a non-negative least-squares (NNLS) approach which we used to solve the inverse

problem of magnetic particle mapping. Here a gradient descent algorithm was used to solve the constrained optimization problem in an iterative fashion and ensure that the particle distribution remains non-negative. In order to improve the sensitivity of the inversion approach to noise, a regularization approach was used. The regularization parameter was chosen after visual inspection of several inversion results such as to avoid blurring or ripple-like structures in the reconstructed distributions. We started the cooperation from the beginning of the first funding period (not from the middle of 2018), and it led to the first successful application of ME-based magnetic particle mapping via the application of the abovementioned approach [B3-6].

Since our project will not apply for funding in the next funding period, we will offer our algorithmic results and knowledge to the new cardiological project **B10** for the purpose of knowledge transfer within the CRC 1261.

References

- [B3-1] **L. Hamid**, *M/EEG Source Imaging via the Spatiotemporal Kalman Filter and Its Applications in Epileptology* (Arbeiten über Digitale Signalverarbeitung, Shaker Verlag, Düren, Germany, 2019).
- [B3-2] **L. Hamid**, A. Al Farawn, I. Merlet, N. Japaridze, U. Heute, **U. Stephani**, **A. Galka**, F. Wendling, **M. Siniatchkin**, Spatial projection as a preprocessing step for EEG source reconstruction using spatiotemporal Kalman filtering. 39th Int. Conf. IEEE EMBS, Jeju Island, 2213-2217 (2017). DOI: 10.1109/EMBC.2017.8037294.
- [B3-3] **L. Hamid**, A. Al Farawn, I. Merlet, N. Japaridze, U. Heute, **U. Stephani**, **A. Galka**, F. Wendling, **M. Siniatchkin**, Source reconstruction via the spatiotemporal Kalman Filter and LORETA from EEG time series with 32 or fewer electrodes. 39th Int. Conf. IEEE EMBS, Jeju Island, 2218-2222 (2017). DOI: 10.1109/EMBC.2017.8037295
- [B3-4] P. Mégevand, **L. Hamid**, M. Dümpelmann, M. Heers, New horizons in clinical electric source imaging. *Z. Epileptol.* **32**, 187-193 (2019). <https://doi.org/10.1007/s10309-019-0258-6>
- [B3-5] **N. Habboush**, **L. Hamid**, **M. Siniatchkin**, **U. Stephani**, **A. Galka**, Pipeline for Forward Modeling and Source Imaging of Magnetocardiographic Recordings via Spatiotemporal Kalman Filtering. 40th Int. Conf. IEEE EMBS, Honolulu, 199-202 (2018). DOI: 10.1109/EMBC.2018.8512188
- [B3-6] R. M. Friedrich, S. Zabel, **A. Galka**, N. Lukat, J. M. Wagner, C. Kirchhof, E. Quandt, J. McCord, C. Selhuber-Unkel, **M. Siniatchkin**, F. Faupel, Magnetic particles mapping using magnetoelectric sensors as an imaging modality. *Scientific Reports* **9**, 2086 (2019).
- [Ga04] **A. Galka**, O. Yamashita, T. Ozaki, R. Biscay, P. Valdés-Sosa, A solution to the dynamical inverse problem of EEG generation using spatiotemporal Kalman filtering. *NeuroImage* **23**, 435-453 (2004).
- [Hä84] M. Hämäläinen, "Interpreting measured magnetic fields of the brain: estimates of current distributions" (Tech. Rep. TKK-F-A559, Helsinki Univ., 1984).
- [Ha15a] **N. Habboush**, **L. Hamid**, N. Japaridze, G. Wiegand, U. Heute, **U. Stephani**, **A. Galka**, **M. Siniatchkin**, The choice of the source space and the Laplacian matrix in LORETA and the spatio-temporal Kalman filter EEG inverse methods. 37th Int. Conf. IEEE EMBS, Milan, 2745-2749 (2015). DOI: [10.1109/EMBC.2015.7318960](https://doi.org/10.1109/EMBC.2015.7318960)
- [Ha15b] **L. Hamid**, M. Sarabi, N. Japaridze, G. Wiegand, U. Heute, **U. Stephani**, **A. Galka**, **M. Siniatchkin**, The performance of the spatiotemporal Kalman filter and LORETA in seizure onset localization. 37th Int. Conf. IEEE EMBS, Milan, 2741-2744 (2015). DOI: [10.1109/EMBC.2015.7318959](https://doi.org/10.1109/EMBC.2015.7318959)
- [Ha13] **L. Hamid**, Ü. Aydın, C. Wolters, **U. Stephani**, **M. Siniatchkin**, **A. Galka**, MEG-EEG fusion by Kalman filtering within a source analysis framework. In 2013 35th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC) (pp. 4819-4822). DOI: [10.1109/EMBC.2013.6610626](https://doi.org/10.1109/EMBC.2013.6610626)
- [Ki13] D. Kim, S. Sra, I. S. Dhillon, A non-monotonic method for large-scale non-negative least squares. *Optimization Methods and Software* **28**, 1012-1039 (2013).
- [Ko11] H. Koch, R. D. Bousseljot, O. Kosch, C. Jahnke, I. Paetsch, E. Fleck, B. Schnackenburg, A reference dataset for verifying numerical electrophysiological heart models. *Biomedical engineering online* **10**, 11 (2011).
- [Pa94] R. D. Pascual-Marqui, C. M. Michel, D. Lehmann, Low resolution electromagnetic tomography: a new method for localizing electrical activity in the brain. *International Journal of psychophysiology* **18**, 49-65 (1994).
- [Ta11] F. Tadel, S. Baillet, J. C. Mosher, D. Pantazis, R. M. Leahy, Brainstorm: a user-friendly application for MEG/EEG analysis. *Computational intelligence and neuroscience* **2011**, 8 (2011).

3.2.2 Project-related publications by participating researchers

a) Peer-reviewed articles and books

[B3-1] **L. Hamid**, *M/EEG Source Imaging Via the Spatiotemporal Kalman Filter and Its Applications in Epileptology* (Arbeiten über Digitale Signalverarbeitung, Shaker Verlag, Düren, Germany, 2019).

[B3-2] **L. Hamid**, A. Al Farawn, I. Merlet, N. Japaridze, U. Heute, **U. Stephani**, **A. Galka**, F. Wendling, **M. Siniatchkin**, Spatial projection as a preprocessing step for EEG source reconstruction using spatiotemporal Kalman filtering. 39th Int. Conf. IEEE EMBS, Jeju Island, 2213-2217 (2017). doi: 10.1109/EMBC.2017.8037294.

[B3-3] **L. Hamid**, A. Al Farawn, I. Merlet, N. Japaridze, U. Heute, **U. Stephani**, **A. Galka**, F. Wendling, **M. Siniatchkin**, Source reconstruction via the spatiotemporal Kalman Filter and LORETA from EEG time series with 32 or fewer electrodes. 39th Int. Conf. IEEE EMBS, Jeju Island, 2218-2222 (2017). doi: 10.1109/EMBC.2017.8037295

[B3-4] P. Mégevand, **L. Hamid**, M. Dümpelmann, M. Heers, New horizons in clinical electric source imaging. *Z. Epileptol.* **32**, 187-193 (2019). <https://doi.org/10.1007/s10309-019-0258-6>

[B3-5] **N. Habboush**, **L. Hamid**, **M. Siniatchkin**, **U. Stephani**, **A. Galka**, Pipeline for Forward Modeling and Source Imaging of Magnetocardiographic Recordings via Spatiotemporal Kalman Filtering. 40th Int. Conf. IEEE EMBS, Honolulu, 199-202 (2018). doi: 10.1109/EMBC.2018.8512188

[B3-6] R. M. Friedrich, S. Zabel, **A. Galka**, N. Lukat, J. M. Wagner, C. Kirchhof, E. Quandt, J. McCord, C. Selhuber-Unkel, **M. Siniatchkin**, F. Faupel, Magnetic particles mapping using magnetoelectric sensors as an imaging modality. *Scientific Reports* **9**, 2086 (2019).

[B3-7] S. Moontaha, **A. Galka**, T. Meurer, **M. Siniatchkin**, Analysis of the Effects of Medication for the Treatment of Epilepsy by Ensemble Iterative Extended Kalman Filtering. 40th Int. Conf. IEEE EMBS, Honolulu, 187-190 (2018). doi: 10.1109/EMBC.2018.8512179.

[B3-8] S. Moontaha, **A. Galka**, **M. Siniatchkin**, S. Scharlach, S. von Spiczak, **U. Stephani**, T. May, T. Meurer, SVD Square-root Iterated Extended Kalman Filter for Modeling of Epileptic Seizure Count Time Series with External Inputs. 41st Int. Conf. IEEE EMBS, Berlin, (2019) (accepted)

b) Other publications

c) Patents

3.3 Funding

Funding of this project within the Collaborative Research Centre started in July 2016. The project will be completed by the end of the current funding period.

3.3.1 Project staff in the ending funding period

	Se- quen- tial no.	Name, aca- demic degree, position	Field of re- search	Department of uni- versity or non-uni- versity institution	Project com- mit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1	Siniatchkin, Michael, Prof.Dr.med., Professor	Medical signal pro- cessing	IMPS (until end of 2019), EVKB Bielefeld (since Jan. 2019)	4		Core support

	2	Stephani, Ulrich, Prof.Dr.med., Professor	Medical signal processing	Pedneuro, Deanery of Medical Faculty of CAU Kiel	4		Core support
	3	Galka, Andreas, Dr. phil., Senior Researcher	Medical signal processing	IMPS (until end of 2018)	4		Core support
Staff funded with approved grant money							
	4	Hamid, Laith, Dr.-Ing-, Post-doctoral Researcher	Digital signal processing	IMPS	40	E14	
	5	Habboush, Nawar, M.Sc., Doctoral Researcher	Digital signal processing	IMPS	40	E13	

Job descriptions of staff (supported through existing funds):

- 1) Prof. Dr. med. Michael Siniatchkin is responsible for the coordination and the scientific management of the project B3. He represents the project within the CRC and externally. He advises the scientific staff in the planning and execution of the data processing as well as in the interpretation of the results.
- 2) Prof. Dr. med. Ulrich Stephani is responsible first of all for clinical interpretation of results and coordination of data analysis.
- 3) Dr.rer.nat. Andreas Galka is responsible for coordination of algorithmic development of spatiotemporal Kalman filter (STKF) as well as for algorithms of fusion and adaptive KF. He supervises the work of post-docs and doctoral researchers from the algorithmic point of view. Dr. Galka is an experienced researcher who has successfully worked on STKF development in the last 15 years. He provided essential results for the current project. Dr. Galka cooperated with project B7 on WP 4.

Job descriptions of staff (funded with approved grant money):

- 4) Dr.-Ing. Laith Hamid (Post-doc) is an experienced researcher who contributed substantially to the development of STKF for the analysis of brain signals. He is familiar with the algorithmic developments and will be responsible for the planning, execution, and evaluation of WP 2 and WP 3. Mr. Hamid was first a PhD candidate and then finished his doctoral thesis in 2018.
- 5) M.Sc. Nawar Habboush (PhD candidate) worked as a PhD candidate in the subproject P7 of the PAK 902. He continued his work in the new CRC because he is familiar with methods which are scheduled to be used in the project. In his master thesis, he worked on the development of algorithms of fusion and regional STKF, and therefore he was prepared to start with the project immediately. Mr. Habboush works on WP 1 and WP 3.

3.1 General information about Project B5(E)

3.1.1 Project title: Individualized Deep Brain Stimulation

3.1.2 Project leader(s)

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3.2 Project history

3.2.1 Report

The central objective of **B5** within the first period of the CRC 1261 (2016/2 – 2020/1) was to develop a method using magnetoelectric (ME) sensors to measure the stimulated electrical field of a deep brain stimulation (DBS) electrode that is implanted into the brain of patients with Parkinson's disease [B5-3, B5-4, B5-6, B5-7]. Deep brain stimulation involves implanting an electrode into a certain, specific area deep in the brain that is attached to an implantable pacemaker that is placed under skin near the clavicle (see Fig. B5-1, left). This project represents an application which is of high clinical relevance and was less critical with regard to magnetic field

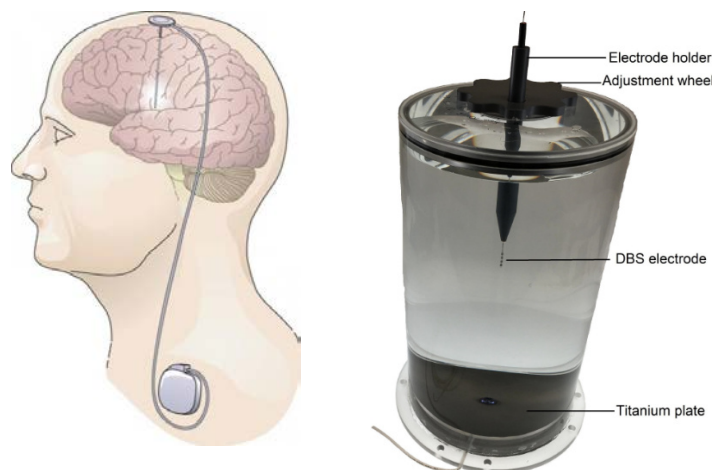


Figure B5-1: Deep brain stimulation system as a sketch (left, www.ninds.nih.gov) and the cylindrical phantom head filled with saline solution with an integrated fixed DBS electrode (Medtronic Model 3389) are shown.

strengths in comparison to the fields of real brain activity. However, it turned out that the bipolar electrode configuration of DBS had to be used for processing the work packages (instead of the monopolar mode) and we therefore have to deal with only weak magnetic fields. For this reason, the investigated magnetic field measurements were performed with a newly developed phantom head that was needed to work through the work packages 1 to 4 (see Fig. B5-1, right). This project will be finished at the end of this funding period, but its open objectives will be continued under the transfer project T1 in the second funding period. The company Boston Scientific (producer of DBS equipment) has shown interest and will contribute further to the transfer project. In the following, a summary of the individual work packages is given, in which the essential results are discussed.

For our analysis in this biomedical application, we tested in WP1 different, single magnetometers that are developed within the framework of the CRC such as the resonant ME sensor in passive mode [Sa16], electrically modulated resonant ME sensor [Ha18], and magneto-elastic surface acoustic wave (SAW) sensor [B5-5]. In addition, we used the fluxgate sensor (Fluxmaster, Stefan Mayer Instruments) as a reference sensor and achieved the following results, which we also discussed with the **A** projects: Resonant sensors that have a small bandwidth measure only one harmonic frequency of the whole DBS signal and ignore the rest of the

signal. Fig. B5-2 shows the normalized power spectrum of an example, measured DBS signal with a stimulation frequency of 160 Hz. The adjusted repetition frequency and its harmonics can be clearly seen. A curve with the cumulative sum of the power spectrum is also depicted. A single frequency component contains only about 3% of the signal power (black dot), whereas, e.g., the fluxgate sensor operating between 1 Hz and 1 kHz measures about 20% of the signal power. Thus, the SAW sensor was most promising for this application because it can measure the largest part of the signal power, i.e. ~95%. Since the noise level of the sensor decreases over the frequency [B5-2], the peaks from the third and higher harmonics can be seen in the frequency domain.

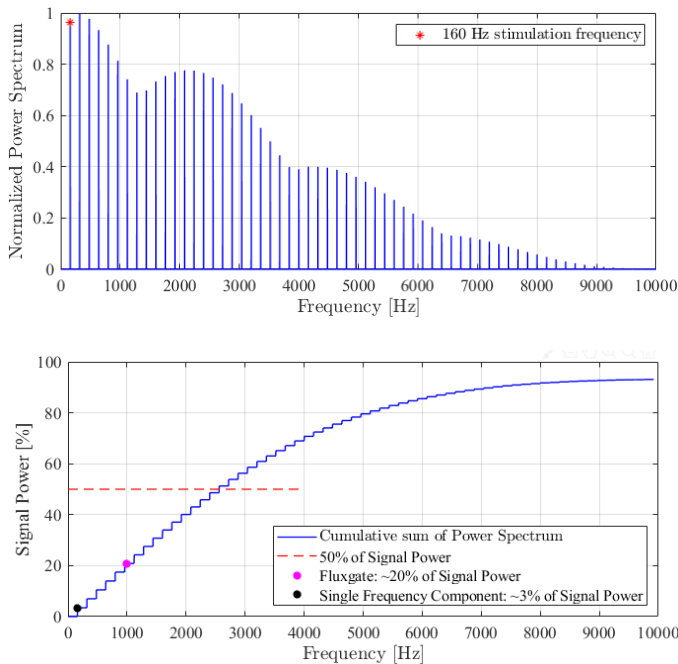


Figure B5-2: Normalized power spectrum of a measured DBS signal with a stimulation frequency of 160 Hz is shown (top figure). The repetition frequency and its harmonics can be seen clearly. A curve with the cumulative sum of the power spectrum is shown (bottom). The fluxgate sensor that operates between 1 Hz and 1 kHz measures about 20% of the signal power, whereas a single frequency component (ME sensor) contains about 3% of the power.

The magnetic properties of electrical pulses delivered by the DBS system were analyzed in detail with these sensors and have been published in [B5-1]. There are differences in the magnetic properties of both monopolar and bipolar electrode configurations: The magnetic flux densities are in the pT-range in the bipolar stimulation mode and decrease quadratically within a distance of 45 mm to 125 mm. In monopolar stimulation mode, we found the fields in the nT range with linear decrease over the measured distances. The bipolar stimulation mode generates a more focused spatial resolution of the magnetic field around the phantom surface, which is essential and better suited for electrode localization. This can subsequently be modelled as an electrical current dipole whose forward calculated fields using the Biot-Savart law for a current dipole [Mo92] can be fitted with the measured magnetic fields. We have shown in [B5-1] that the dipole fitting approach was able to detect the position of the electrode in the phantom head as a proof of concept that the behavior of the bipolar mode can be estimated by the model assumptions used. We concluded that although the monopolar stimulation mode provides a magnetic field 100 times larger, it is less suited to be used for electrode localization due to the corresponding broad field distribution. The reason is that the whole system including the electrode, the cable, and the pacemaker contribute to the overall magnetic field. It does not provide any information about the height of the electrode (z-coordinate), which substantially limits the possibilities for localization that was the main part of WP2.

In WP2 we developed a new method for non-invasive localization of the deep brain stimulation electrode with magnetic field measurements that adds a new possibility to conventional methods with neuroimaging approaches by visual inspection via metal artifacts in computed tomography (CT) or post-operative magnetic resonance imaging (MRI) or a combination of both. We investigated the localization accuracy for different electrode positions in the phantom. In order to validate the localization accuracy, the same measurement was performed five times at each considered electrode position at $a = 20, 25, 30, 35$ and 40 mm ending up with a total of 25 measurements. The real Cartesian coordinates of those electrode locations in the phantom head and the calculated Cartesian coordinates from the measured magnetic data (localization result) can be seen on the right side in Fig. B5-3. The following contents can be taken from the figure: The localization accuracy, which can be represented by the calculated Euclidean distances (error) between the real and calculated position, increases the closer the electrode is placed to the surface of the model. At the electrode position $a = 40$ mm, the Euclidean distance is even less than 1 mm between the real source and the calculated source. Positions at $a = 35$ mm and $a = 30$ mm show localization errors of about 1 mm, which increase to about 2 mm the

further the electrode is moved to the center of the phantom. The reason for those slight deviations of the result is that the distance of the electrode to the sensor points increases the deeper the electrode is placed in the model, and thus an even smaller amplitude of the magnetic field is measured due to the quadratic decrease of the field. Our findings showed that the electrode was localized with an accuracy of about 1.5 mm over all performed measurements [Ya19].

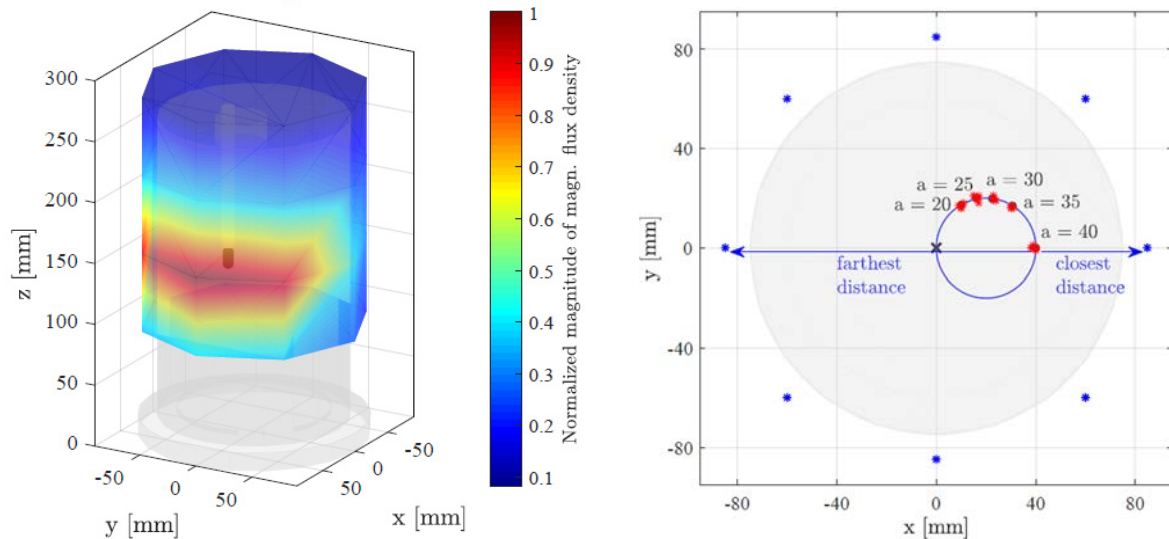


Figure B5-3: The measured magnetic field distribution of bipolar electrode configuration created by 32 measuring points is shown (left side). The magnitude of the magnetic flux density at each measuring point was calculated and interpolated between the points. The top view of the cylinder (grey circular area) is shown (right side). The electrode can be rotated along the inner circle (blue). The DBS electrode was placed at $a = 20, 25, 30, 35$, and 40 mm. The blue asterisk markers indicate the positions of the measuring points. The blue arrows indicate the closest (45 mm) and farthest (125 mm) measuring point to the example position $a = 40$. The red asterisk markers represent the results of electrode localization.

In collaboration with Prof. Schnitzler and his group in Düsseldorf, we assessed the phantom with the commercial DBS system inside the SQUID-MEG with a noise level of $3 \text{ fT/Hz}^{1/2}$ as shown on the left side in Fig. B5-5 for WP3. For typical physiological stimulation parameters (1.5 mA , $60 \mu\text{s}$, 130 Hz), we measured the maximum field strength at the fundamental frequency of $\sim 14 \text{ pT}$ for the monopolar and $\sim 140 \text{ fT}$ for the bipolar electrode configuration.

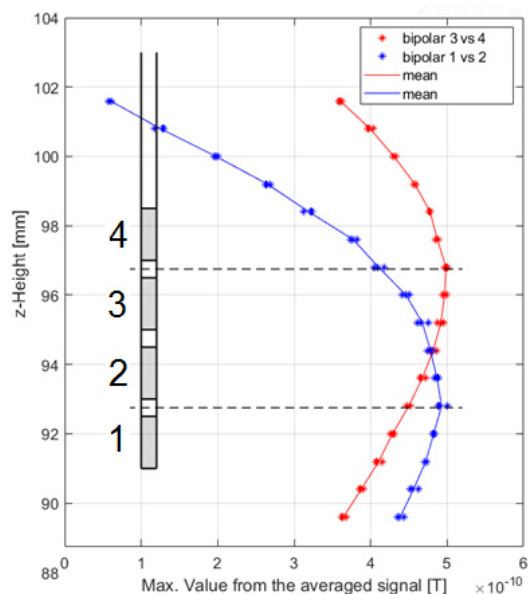


Figure B5-4: Vertical measured magnetic field of bipolar DBS mode with activated contacts 1 vs. 2 (blue) and 3 vs. 4 (red) with high resolution (0.8 mm steps).

This confirms once again that the fields in monopolar mode is approximately 100 times larger than the fields in the bipolar mode. We also confirm our findings for the magnetic properties of DBS. The middle and right part of the Fig. B5-5 show the measured and theoretically calculated magnetic field distribution for the bipolar DBS mode with an adjusted stimulation amplitude of about 11 mA . In the middle figure, we can see the round artefact near the top of the MEG helmet that is caused by the DBS connector, which connects the electrode with the pacemaker. The artefact that goes down from the left side is probably caused by the wire. We assumed that the magnetic field caused by the current in the conductor is not completely removed, since the current flowing through the conductor to the electrode flows back through the conductor but placed parallel and in close vicinity to the feeding conductor, so their contributions do not cancel out each other. Both symmetrical artefacts at the bottom of the MEG helmet are the desired DBS artefact caused by the DBS pulse. The theoretically calculated magnetic field distribution for the same electrode location considering the same SQUID sensor orientations can be seen on the right side in Fig. B5-5. Subsequently, an electrode localization could be performed with the dipole fitting approach, but there is an essential point that has to be considered: The phantom

positioning has been monitored at the beginning of each recording. Therefore, four small head position indicator (HPI) coils were placed in different positions on the phantom that should be localized in a three-dimensional space with respect to the MEG sensor array to bring the phantom and the sensors into the same Cartesian coordinate system. The HPI fitting already results in slight deviations of a few mm. Thus, the desired electrode localization with an accuracy of less than 1 mm cannot be achieved. In comparison, with our head scanner that is constructed in-house with non-ferromagnetic materials and is located in the magnetically shielded chamber of the Faculty of Engineering (Series Ak3B, Vaccumschmelze) for measurements, an optimized sensor trajectory of variable measuring points around the phantom head with a minimum step size of 0.8 mm can be programmed. Fig. B5-4 shows two example measurements for the bipolar electrode configurations with activated contacts 1 vs. 2 and 3 vs. 4 over the z-axis with the highest step resolution. The corresponding z-heights of the physical center of the activated contacts illustrate the maximum magnetic field strengths that were measured for both configurations. This enables a measuring accuracy of less than 1 mm.

The position of the electrode has been calculated based on these magnetic field recordings as described above in our phantom head with fluxgate, ME, SAW, or SQUID sensors. Afterwards, the detection of the stimulated area around the calculated position has been estimated in different views by advanced modelling approaches and simulations in WP4. The volume of tissue activated (VTA) that has been elaborated in particular by McIntyre and colleagues [Ma18] has been calculated by using the open-source toolbox Lead-DBS providing FEM-based VTA model for our simplified phantom head and for five Parkinsonian patients based upon the patient's stimulation parameters. Since we did not perform magnetic field measurements with patients, the process of reconstructing electrode placement was performed with pre- and postoperative CT using Lead-DBS toolbox. Between January and March 2020, M. Yalaz, the PhD-student of this project will visit Cameron McIntyre and his group in Cleveland, Ohio, who are leaders in the field of VTA calculation. This research stay will mainly be used to develop the calculation of the VTA by using a previously performed magnetic field measurement which was used to locate the physical center of the stimulation.

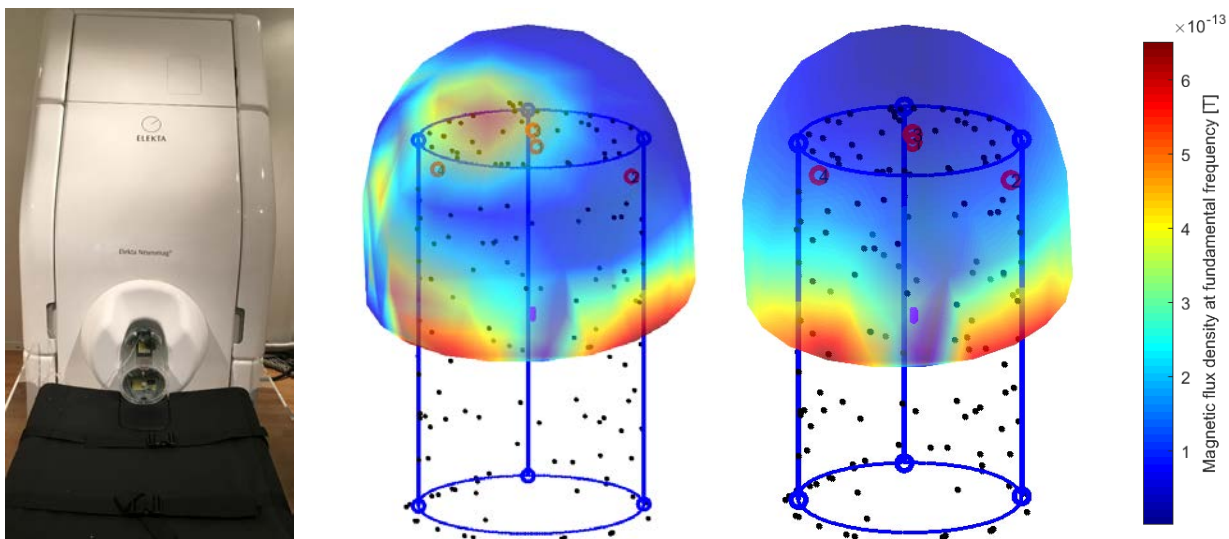


Figure B5-5: On the left side, the cylindrical phantom head in the MEG system (TRIUX, Elekta Neuromag®) can be seen. The Vercise PC stimulator from Boston Scientific is placed and fixed inside the model. The middle and right figure show an example measured and theoretically calculated magnetic field distribution for both bipolar electrode configurations with 102 MEG SQUIDs and with the adjusted stimulation parameters 11 mA of amplitude, 130 Hz of frequency, and 60 µs of pulse width.

In the following, we would like to report on the problems and limitation for performing work packages during this funding period. In order to arrive at a viable system for biomedical diagnostics, sensor arrays are needed to get completely rid of the head scanner. This would enable confident results from patients due to much faster measurement time. Sensor arrays could not be developed during this funding period due to the evaluations of several double tuning fork designs that have been investigated in collaboration with Z2. We expected that we will thereby get rid of strong influence of vibrational and acoustic interferences of ME sensors. The evaluation of the sensor assemblies showed that the double-fork concept did not solve the problem of interference compensation. Possible reasons are explained in Z2. In addition, no magnetic field measurements were performed on real DBS patients, as they were exposed to sensor arrays (faster measurement) on the one hand and suitable high sensitive sensors for the bipolar electrode configuration on the other hand. Therefore, side effect studies and gait disturbance and apathy study could not be carried out in WP5.

References

- [Ha18] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yarar, A. Piorra, R. Knöchel, Y. Fetisov, E. Quandt: Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing, *Journal of Physics D: Applied Physics* 51 (2018).
- [Mo92] J. C. Mosher, P. S. Lewis, R. M. Leahy: Multiple dipole modeling and localization from spatio-temporal meg data, *IEEE Trans on Bio Eng* 39(6) (1992), 541-557.
- [Ma18] N. Maling, S. F. Lempka, Z. Blumenfeld, H. Bronte-Stewart, C.C. McIntyre: Biophysical basis of subthalamic local field potentials recorded from deep brain stimulation electrodes, *J Neurophysiology* 120(4) (2018), 1932-1944.
- [Sa16] S. Salzer, R. Jahns, A. Piorra, I. Teliban, J. Reermann, **M. Höft**, E. Quandt, R. Knöchel: Tuning Fork for Noise Suppression in Magnetoelectric Sensors, *Sensors & Actuators: A. Phys* 237 (2016), 91-95.

3.2.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [B5-1] **M. Yalaz**, A. Teplyuk, M. Muthuraman, **G. Deuschl**, **M. Höft**: The Magnetic Properties of Electrical Pulses delivered by Deep Brain Stimulation Systems, *IEEE Trans on Instrumentation and Measurement*, doi:10.1109/TIM.2019.2945744 (2019).
- [B5-2] P. Durdaut, A. Kittmann, E. Rubiola, J.-M. Friedt, E. Quandt, R. Knöchel, **M. Höft**: Noise Analysis and Comparison of Phase- and Frequency-Detecting Readout Systems: Application to SAW Delay Line Magnetic Field Sensor, *IEEE Sensors Journal*, 19(2019), 8000-8008
- [B5-3] S. Paschen, J. Forstenpointner, J. Becktepe, S. Heinzel, H. Hellriegel, K. Witt, A.-K. Helmers, **G. Deuschl**: Long-term efficacy of deep brain stimulation for essential tremor: An observer-blinded study. *Neurology*. 19;92(12) (2019) e1378-e86.
- [B5-4] P. Krack, J. Volkmann, G. Tinkhauser, **G. Deuschl**: Deep brain stimulation in movement disorders: from experimental surgery to evidence-based therapy, *Movement Disorders*, in press (2019).
- [B5-5] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, **M. Höft**, R. Knöchel, F. Faupel, E. Quandt: Wide Band Low Noise Love Wave Magnetic Field Sensor System, *Scientific Reports*, 8, (2018), 278.
- [B5-6] M. Muthuraman, J. Raethjen, N. Koirala, A. R. Anwar, K. G. Mideksa, R. Elble, S. Groppa, **G. Deuschl**: Cerebello-cortical network fingerprints differ between essential, Parkinson's and mimicked tremors, *Brain*, (2018), 1770-1781.
- [B5-7] N. Koirala, V. Fleischer, M. Glaser, K. E. Zeuner, **G. Deuschl**, J. Volkmann, M. Muthuraman, S. Groppa: Frontal Lobe Connectivity and Network Community Characteristics are Associated with the Outcome of Subthalamic Nucleus Deep Brain Stimulation in Patients with Parkinson's Disease. *Brain Topogr*, (2018), 311-21

b) Other publications

- [Be19] J. S. Becktepe, F. Gövert, L. Kasiske, **M. Yalaz**, K. Witt, **G. Deuschl**: Pupillary response to light and tasks in early and late onset essential tremor patients, *Parkinsonism & Related Disorders* 66 (2019), 62-67.
- [Ya19] **M. Yalaz**, A. Teplyuk, **G. Deuschl**, **M. Höft**: Dipole Fit Localization of the Deep Brain Stimulation Electrode using 3D Magnetic Field Measurements, *IEEE Transactions on Biomedical Engineering*, submitted (2019).

c) Issued Patents: none

d) Pending Patents: none

3.3 Funding

Funding of this project within the Collaborative Research Centre started in 07/2016. The project focused on individualized deep brain stimulation will be completed by the end of the current funding period. The open objectives and further ideas will be continued under the transfer project T1 in the second funding period in cooperation with the company Boston Scientific and A.-K. Helmers as an additional project leader.

3.3.1 Project staff in the ending funding period

	Se- quen- tial no.	Name, academic degree, position	Field of re- search	Department of university or non-uni- versity institu- tion	Commit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	Deuschl, Günther, Prof. Dr. med., Professor	Neurology	UKSH neuro	10		UKSH/ Core support
	2.	Höft, Michael, Prof. Dr.-Ing., Professor	Microwave Engineering	EIE	4		Core support
Staff funded with approved grant money							
Research staff	3.	Mevlüt Yalaz, M.Sc., Researcher	Microwave Engineering	EIE		E13	
	4.	Jos Becktepe, Dr. med. Medical Doctor	Neurology	UKSH neuro		Ä1 (25%)	
	5.	Katrin Lange, Medical Labora- tory Assistant	Neurology	UKSH neuro		E9 (50%)	

Job descriptions of staff (supported through existing funds):

1. Prof. Dr. Günther Deuschl was responsible for the coordination and scientific management of the research project B5 in agreement with Michael Höft. He advised the scientific employees with respect to planning, execution and evaluation of the tasks, in particular in matters of actual data acquisition (DBS system, stimulation parameter), result interpretation, and ethics.
2. Prof. Dr.-Ing. Michael Höft was also responsible for the coordination and scientific management of the research project B5 in agreement with Günther Deuschl. He advised the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of system design, the involved signal processing applications, and in matters of the related measurement setups and procedures.

Job descriptions of staff (funded with approved grant money):

3. M.Sc. Mevlüt Yalaz worked since 12/2016 as a doctoral researcher (Ph.D. candidate) and handled the scientific tasks with a focus on engineering tasks in this project.
4. Dr. med. Jos Becktepe handled the scientific tasks concerned with patient-related and medical aspects of this project. Specifically, he oversaw patient recruitment and data handling together with Katrin Lange.
5. Katrin Lange was the technician who performed and organized extended assessments of patients and knows high-density EEG technology and all kinds of routine assessments in electrophysiology.

3.1 General information about Project B6

3.1.1 Project title: Multimodal Mapping of Nerve Pathology with Magneto-Electric Sensors

3.1.2 Project leader(s)

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3.2 Project history

3.2.1 Report

1) Introduction

The central objective of project B6 within the first funding period of the CRC 1261 (2016/2 – 2020/1) was the non-invasive mapping of nerve function and dysfunction (pathology) by a combination of magneto-electric (ME) sensor sampling with ultrasound or magnetic resonance (MR) imaging. Concretely the work plan for project B6 contained different steps for an establishment of the new multimodal nerve mapping and was divided into three specific work packages. In work package 1, the experimental setup with the measurement and analysis pipeline using a simple phantom should be established. In work package 2, the phantom-based measurements should be adapted to *in vivo* conditions (healthy human nerve), as shown in Fig. B6-1. Finally, in work package 3, patient cohorts with different types of nerve pathologies should be examined and the added value of the novel multimodal nerve mapping in comparison to established electrical nerve conduction studies should be evaluated. In the following, the progress of the first funding period is described.

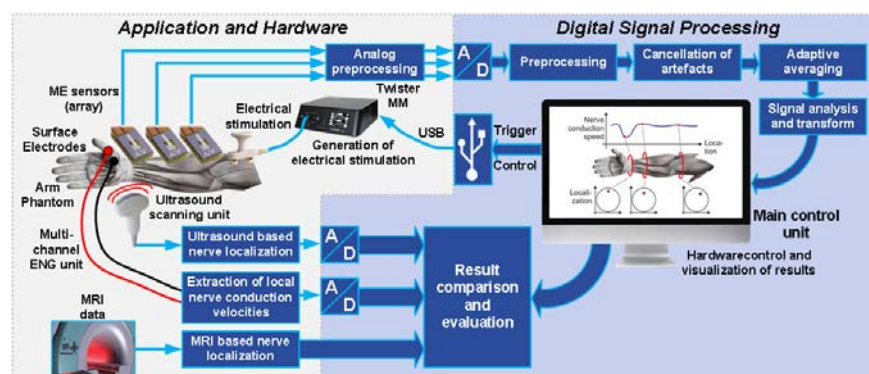


Figure B6-1: Overview of the ME sensor system for nerve measurements

In the first step, it was of interest to identify which signal strengths in the time domain and signal distribution in the frequency domain can be detected with Magnetoneurography (MNG) for experimental design and as a basis for simulations. In the literature, only very limited data is available on magnetic field properties of peripheral human nerves [Tr89, Ma04], mainly obtained with Superconducting Quantum Interference Devices (SQUIDs). The SQUID investigations applied a sensory stimulation of the median nerve (N. medianus) that resulted in nerve action potentials of low amplitude. Higher signal amplitudes are expected by a simultaneous electrical stimulation of afferent as well as efferent nerve fibers, which can be achieved via a “mixed nerve

stimulation" procedure [Bu99, B6-5]. Therefore, within the first funding period, we decided to perform *in vivo* MNG measurements on two subjects in collaboration with the PTB in Berlin, instead of the comparably less helpful arm phantom experiments originally planned in work package 1 - *Development and validation of electrical stimulation and ME and electrical sensor setup for measurements of electrically generated signals in a conductive agent surrounded by soft tissue (phantom)* (cf. Fig. B6-2 (a)).

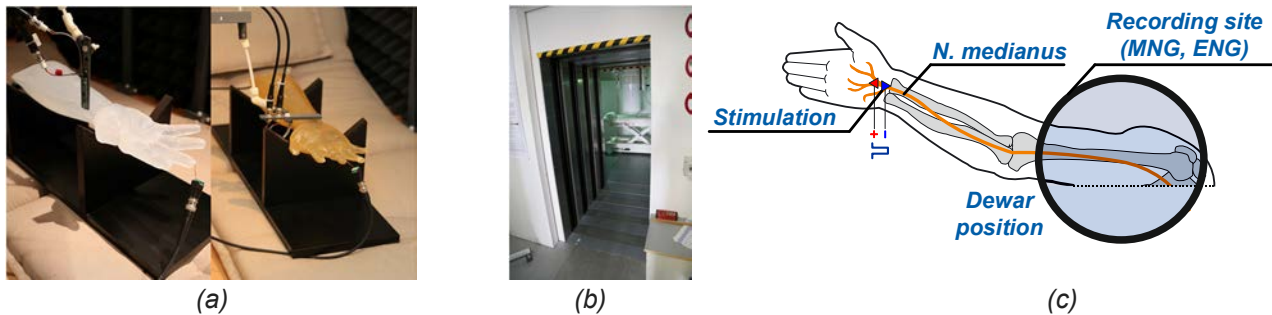


Figure B6-2: (a) Basic arm phantoms used for initial magnetic measurements (left - soap with copper wire; right - water, ballistic gel with copper wire). (b) 304-SQUID vector magnetometer system within the active and passive magnetically shielded chamber BMSR-2. (c) Illustration of stimulation and recording site for electrical (ENG) as well as magnetic (MNG) measurement [B6-2].

II) Magnetoneurography at the PTB in Berlin – Estimation of real nerve signal amplitudes

Methods: We used a 304-SQUID vector magnetometer system [Bu04] within the active and passive magnetically shielded chamber (BMSR-2) [Bo00]. The SQUID system, in combination with the magnetically shielded room (MSR), as shown in Fig. B6-2 (b), ensures a total noise level of about $2.3 \text{ fT}/\sqrt{\text{Hz}}$ at 1 kHz. Similar values are achieved within a frequency range of 100 Hz - 10 kHz [Bu04]. However, with this high sensor sensitivity, direct signal detection of the nerve impulses was not ensured, because in addition to sensor noise, biological interferences, e.g., from the heart and muscle magnetic fields generally occur.

Consequently, by means of unweighted averaging triggered by an electrical stimulation pulse, the signal-to-noise ratio (SNR) improved proportionally to the root of the number of averaging periods. The SQUID dewar was centered and aligned above but without direct skin contact to the upper arm (cf. Fig. B6-2 (c)). We positioned our subjects in a prone position on a non-magnetic patient bench, as shown in Fig. B6-3. The distance between nerve and skin was smaller than 1.54 cm for both subjects and were precisely estimated by using ultrasound. SQUID premeasurements have already demonstrated that a magnetic nerve signal detection by only stimulation of sensory fibers was not realizable. We used the identical custom-built stimulator of previous MNG publications and tried averaging methods. Thus, we decided to apply the mixed nerve stimulation by a unipolar rectangular pulse of 15 mA with a duration of 200 μs in the vicinity of the musculus abductor pollicis brevis (APB) with a stimulation rate of 8.547 Hz as indicated in Fig. B6-3, such that both motor and sensory fibers were excited simultaneously. In addition to and simultaneously with the MNG, electrical nerve measurements were performed using a custom-built amplifier by the PTB specifically for use in the magnetically shielded chamber.

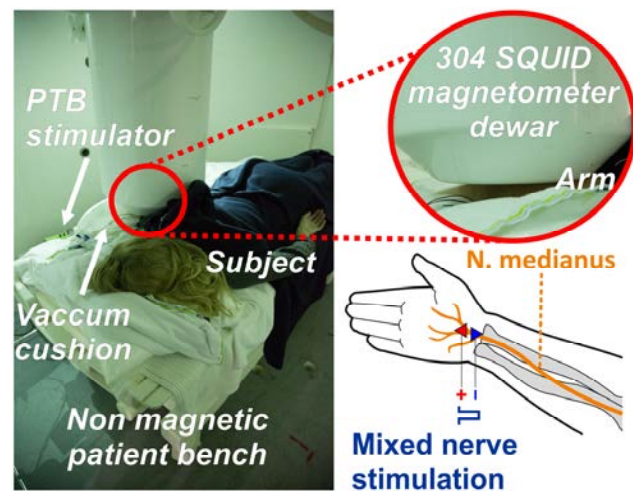


Figure B6-3: Measurement setup with subject positioned under SQUID system [B6-2].

such that both motor and sensory fibers were excited simultaneously. In addition to and simultaneously with the MNG, electrical nerve measurements were performed using a custom-built amplifier by the PTB specifically for use in the magnetically shielded chamber.

Results: The results for each subject are presented in Fig. B6-4; it is to be noted that the nerve conduction velocity (NCV) obtained in the electrical and the magnetic measurements are identical. The MNG amplitudes were subject-dependent and ranged from 17 fT to 60 fT in a frequency range from 100 Hz to 1 kHz. The spatial distribution of the magnetic field as a function of time was consistent with a propagating nerve impulse (not shown) and supports the interpretation of the magnetic peaks in Fig. B6-4 between 4-8 ms (subject 1) and between 6-10 ms (subject 2) as nerve signals.

Computer simulation results based on the recorded SQUID signals and their amplitudes have indicated that it will be unrealistic to achieve an SNR of 0 dB at the resonance frequency of a ME sensor (f_{res}) with an LOD of $1 \text{ pT}/\sqrt{\text{Hz}}$. More details about the successfully realized MNG measurement at the PTB in Berlin, including a proof-of-principle simulation for ME sensors, are presented in [B6-2], respectively.

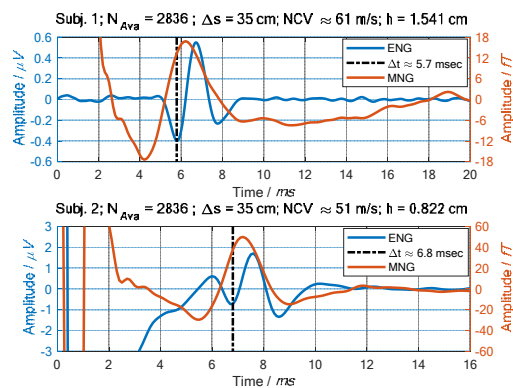


Figure B6-4: Results of the MNG measurements averaged over 2836 stimulations [B6-2].

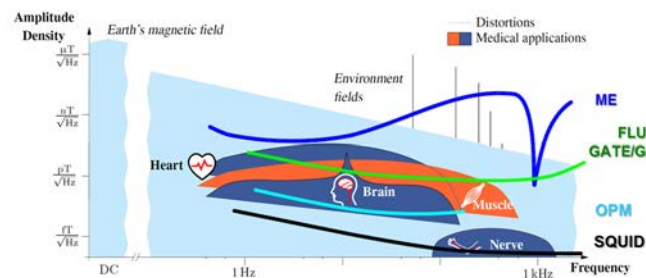


Figure B6-5: Representative biomagnetic fields generated by neuronal or muscular tissue and their amplitude densities in accordance with [Re93, St06, Cl06] including typical interferences from the environment.

III) Magnetoneurography with competitive room temperature sensor concepts

The executed SQUID MNG measurements at the PTB in Berlin makes an estimation of real nerve signal amplitudes feasible. However, the realistic biologic amplitude density of nerves is entirely too low ($\text{fT}/\sqrt{(\text{Hz})}$) for the CRC sensors with their available sensitivity ($\text{pT}/\sqrt{(\text{Hz})}$) at the current state-of-research. Additionally, nerve signals of humans are very fast, which requires a signal bandwidth in the kHz range to be detectable by competitive room temperature sensor concepts. This required bandwidth is currently also not available with Optically Pumped Magnetometers (OPMs). A detailed overview of different sensor concepts, possible medical applications and available distortions are presented in Figure B6-5. Finally, an overestimation of the available magnetic field amplitude and magnetic flux density has been done in this project proposal, which makes MNG with ME sensors and other room-temperature sensor concepts presently not achievable. The magnetic flux density available from nerves was unfortunately overestimated in the original proposal. In the project we determined a magnetic flux to be within the fT-range. These values mean that it is not currently feasible to use ME sensors for Magnetoneurography. Thus, the focus of the project has been changed to electrical signals recorded by electroneurography, which is usually performed in a patient with suspected polyneuropathy to refine the diagnosis.

IV) Improvement of the current gold standard

This diagnostic gold standard for the assessment of thickly myelinated peripheral nerves is of limited spatial resolution since it provides only average data (nerve conduction velocity, nerve or muscle action potential amplitude) on relatively large nerve segments. Accordingly, different distribution patterns of pathologies cannot be distinguished. But precise knowledge of the distribution and type of nerve damage is relevant to ensure correct diagnosis and therapy, which range from spontaneous recovery to highly sophisticated chronic treatment regimens, which are often expensive - both financially and in terms of burden for the patient. As a consequence, the content of work packages 2 and 3 were adapted due to the previous findings into the electrical domain. Instead of the ME sensor acquisition chains, we developed a finer-grained functional-spatial model consisting of a multichannel approach combined with ultrasound data and evaluated this with a patient cohort.

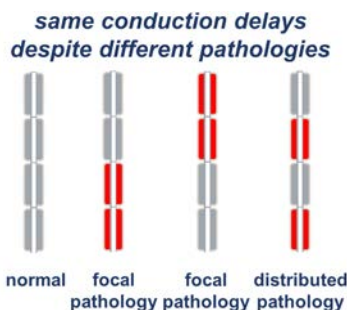


Figure B6-6: Different within-segment myelin pathologies cause same conduction delay.

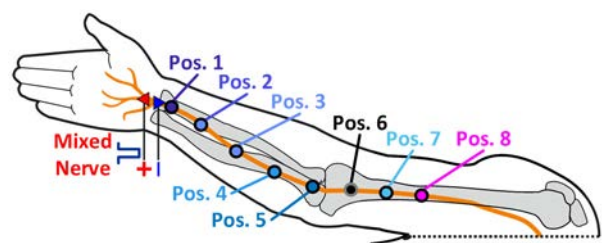


Figure B6-7: Surface projection of N. medianus. The stimulation site remains in the palm of the hand, the eight recording positions along the nerve are marked.

V) Development and validation of stimulation with electrical acquisition chains in vivo

Methods: Based on ultrasound, we positioned eight electrodes along the course of the median and ulnar nerves, and we recorded the nerve depth (distance to skin), as shown Fig. B6-7. Bipolar direct current stimulation was applied in the palm of the hand, resulting in the excitation of both motor and sensory nerve fibers

such that eight mixed nerve action potentials (MNAPs) could be recorded along the nerve. We used a patient cohort for evaluation and checked the added value of this method in comparison to established electrical nerve conduction studies. We performed measurements in ten healthy volunteers and twelve times in patients (4 CIDP, 2 MMN, 5 GBS, 1 CTS).

Results: Using the measurement setup described, we reliably obtained MNAPs and their latencies of two peripheral nerves (N. medianus / N. ulnaris) along their course with offline signal enhancement. We successfully observed a jump in nerve conduction velocity based on segmental demyelination.

Conclusion: Unfortunately, the measurement of diseased nerves with reduced MNAPs is more difficult and lead to limited signal amplitude. The signal detection is restricted by the depth of the nerve combined with a priori lower signal amplitude due to age and nerve abnormalities. More details including the individual signals and their neurophysiological quantities of the healthy volunteers and patients are presented in [B6-1] and [B6-5], respectively. Yet, this method is very time consuming and not very practical in clinical routine. A higher distribution power to differentiate various types of nerve abnormalities can be also performed by only analyzing the compound muscle action potentials (CMAP) at two different stimulation locations (distal/proximal). Each measured response reflects the proportion of healthy axons of the motor nerve and lies typically in mV-range (factor 1000 higher compared to stimulation-triggered nerve action potentials). These signals are also easy and time-efficient to record.

VI) Application of new analysis methods to compound muscle action potentials (CMAPs)

From CMAPs usually the amplitude, latency, and the nerve conduction velocity are automatically calculated. These values are used to determine the pathology of the nerve (axonal damage) or its sheath (myelin damage). CMAP abnormalities can be found when nerve fibers conduct at different velocities (temporal dispersion, TD) or when individual fibers have entirely lost their impulse transmission capabilities (conduction block, CB). In both conditions, TD and CB, the amplitude of a CMAP recorded after stimulation proximal to an affected nerve segment is lower than after stimulation distal to that segment. In CB this happens because nerve fibers that are blocked between the stimulation sites do not contribute to the CMAP upon distal stimulation. In TD this happens because only perfectly synchronous SMUPs sum up in a “constructive” manner by phase-aligned summation (in-phase addition) while asynchronously generated SMUPs as in TD sum up in a more or less “destructive” manner due to phase cancellation ($\pm 180^\circ$ phase shift or anything in-between). For the differential diagnosis of peripheral nerve disorders, it is important to distinguish between CB and TD, which both are expressions of various forms of demyelinating nerve disorders and may occur at the same time in the same nerve segment [Ki91] [Sc99]. This makes differential diagnosis quite challenging, as shown in the Example Fig. B6-8. In this Figure, an exemplary CMAP simulation, as in an acquired polyneuropathy is performed: non-uniform reduction of the conduction velocity of some but not all nerve fibers causes pronounced temporal dispersion with an abnormal decrease of the CMAP amplitude after proximal stimulation. A significant amplitude reduction by 6 mV ($\approx 71\%$ amplitude reduction of distal response) and signal broadening for the proximal compared to the distal stimulus response can be observed. A normal nerve conduction velocity of 49 m/s results. Note the clear difference in signal shape between distal and proximal response.

VII) Outlook

Presently, our project goal is to analyze and to differentiate various types of CB and TD abnormalities by applying advanced digital signal processing approaches including a nerve pathology classification for electro-neurography. Therefore, the CMAP signals (distal/proximal) and their signal composition will be analyzed in an advanced offline postprocessing step in the time-domain as well as in the frequency-domain. First, very promising results in this respect have already been indicated in electrophysiological studies with the help of the High Frequency Attenuation (HFA) [Sc06]. TD shifts the individual frequency components of the distal signal to lower frequencies for the proximal signal [Sc01], as presented in Fig. B6-9.

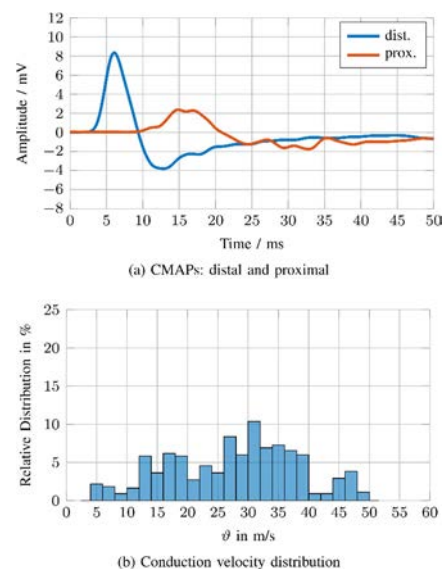


Figure B6-8: Simulation results based on a conduction velocity distribution influenced by chronic inflammatory demyelinating polyneuropathy

In conclusion, we have learned that – given the current state-of-research - MNG is not feasible with room-temperature sensor concepts (ME, Fluxgate, OPM). Besides that, through our work in the electrical domain we have identified the need for intelligent signal processing methods in order that the clinical gold standard can be advanced by extraction of further signal features with the goal of obtaining a prospective nerve disease classification. Subsequently, automated classification approaches (Gaussian mixture models (GMM), Hidden Markov models (HMMs) and artificial neural networks (ANN)) could help neurophysiologists to better distinguish between CB and TD in the future. As a consequence, we will apply for a separate DFG knowledge transfer project that helps us to continue this promising line of research and successfully transfer our findings into clinical routine. We see a better future for our line of research separate from the CRC1261, as our planned research will depend on sensitive electrical measurements. This project makes the foundation to focus our research on electrical signals of peripheral nerve signals, especially to work on quantitative electroneurography for polyneuropathy classification. Additionally, we have established excellent cooperation with an experienced clinical neurophysiologist (Prof. Dr. med. Wilhelm Schulte-Mattler), whose fundamental research emphasis is clinical neurophysiology.

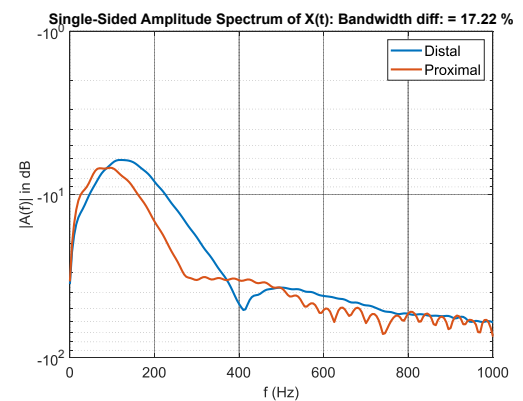


Figure B6-9: Nerve disease based on TD.

References

- [Bo00] J. Bork, H. Hahlbohm, R. Klein, The 8-layered magnetically shielded room of the PTB: Design and construction. (2001).
- [Bu04] M. Burghoff et al., Discrimination of multiple sources using a SQUID vector magnetometer. *Neurol Clin Neurophysiol* 2004, 67 (2004).
- [Bu99] R. M. Buschbacher, Mixed nerve conduction studies of the median and ulnar nerves. *Am J Phys Med Rehabil* 78, S69-74 (1999).
- [Cl06] J. Clarke, A. I. Braginski, Eds., *Applications of SQUIDS and SQUID systems*, (WILEY-VCH, Weinheim, 2006).
- [Ki91] J. Kimura, R. Kaji, Comment from the editorial office. 14, 867-868 (1991).
- [Ma04] B. M. Mackert, Magnetoneurography: Theory and Application to peripheral Nerve Disorders. *Clinical neurophysiology: official journal of the International Federation of Clinical Neurophysiology* 115, 2667-2676 (2004).
- [Re93] M. Reincke, Magnetomyography with the SQUID. *Biomedizinische Technik* 38, 276-281 (1993).
- [Sc01] W. Schulte-Mattler, T. Muller, D. Georgiadis, M. E. Kornhuber, S. Zierz, Length dependence of variables associated with temporal dispersion in human motor nerves. *Muscle & Nerve* 24, 527-533 (2001).
- [Sc06] W. Schulte-Mattler, in *Handbook of Clinical Neurophysiology*, J. Kimura, Ed. (Elsevier, 2006), vol. 7, pp. 405-419.
- [Sc99] W. Schulte-Mattler, M. Jakob, S. Zierz, Assessment of temporal dispersion in motor nerves with normal conduction velocity. *Clin. Neurophysiol.* 110, 740-747 (1999).
- [St06] K. Sternickel, A. I. Braginski, Biomagnetism using SQUIDS: status and perspectives. *Superconductor Science and Technology* 19, S160-S171 (2006).
- [Tr89] L. Trahms, S. N. Ern , Z. Trontelj, G. Curio, P. Aust, Biomagnetic functional localization of a peripheral nerve in man. *Biophysical Journal* 55, 1145-1153 (1989).

3.2.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [B6-1] F. Weitkamp, Kartierung von Nervopathologien mittels Mehrkanalelektroneurographie, Dissertation, Christian-Albrechts-Universit t zu Kiel (CAU) (2019).
- [B6-2] E. Elzenheimer, H. Laufs, T. Sander-Th mmes, G. Schmidt, Magnetoneurography of an Electrically Stimulated Arm Nerve, *Joint Journal of the German Society for Biomedical Engineering in VDE and the Austrian and Swiss Societies for Biomedical Engineering and the German Society of Biomaterials*. vol. 4, pp. 363 (2018).
- [B6-3] E. Elzenheimer, H. Laufs, W. Schulte-Mattler, G. Schmidt, Signal Modelling and Simulation of Temporal Dispersion and Conduction Block in Motor Nerves. *IEEE Transactions on Biomedical Engineering*, 1-1 (2019).

[B6-4] E. Elzenheimer, **H. Laufs**, W. Schulte-Mattler, **G. Schmidt**, Magnetic Measurement of Electrically Evoked Muscle Responses with Optically Pumped Magnetometers (OPMs), IEEE Transactions on Neural Systems and Rehabilitation Engineering, revision submitted (2019).

b) Other Publications

[B6-5] F. Weitkamp, E. Elzenheimer, W. Schulte-Mattler, **G. Schmidt**, **H. Laufs**, P15. Multimodal mapping of nerve pathology with a multichannel approach. Clin. Neurophysiol. 129, e72-e73 (2018).

3.3 Funding

Funding of this project within the Collaborative Research Centre started in 07/2016. The project focused on magnetic nerve signals will be completed by the end of the current funding period. A knowledge transfer will be requested by a separate proposal that focuses on electrical signals.

3.3.1 Project staff in the ending funding period

	Se- quen- tial no.	Name, academic degree, position	Field of re- search	Department of university or non-university institution	Commit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	Laufs, Helmut, PD, PhD, Dr. med., project co-ordinator	Neurology	UKSH neuro	4		UKSH/ Core support
	2.	Schmidt, Gerhard, Prof. Dr.-Ing., project co-ordinator	System Theory	EIE	4		Core support
Non-research staff	3.	Prehn, Kevin Lab Engineer		EIE	4		Core support
Staff funded with approved grant money							
Research staff	4.	Elzenheimer, Eric, M.Sc., Researcher	System Theory	EIE		E13	
	5.	Clinical Neurophysiologist (rotating)	Neurology	UKSH neuro		Ä1	

Job descriptions of staff (supported through existing funds):

1. PD PhD Dr. med. Helmut Laufs was responsible for the coordination and scientific management of the research project B6 in agreement with Gerhard Schmidt. He advised the scientific employees with respect to planning, execution and evaluation of the tasks, in particular in matters of actual data acquisition (placement of sensors and stimulation device, stimulation paradigm), result interpretation, ethics, patient selection and recruitment.
2. Prof. Dr.-Ing. G. Schmidt was also responsible for the coordination and scientific management of the research project B6 in agreement with Helmut Laufs. He advised the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of system design and the signal processing applications involved.
3. K. Prehn supported the research project in the areas database and IT infrastructure.

Job descriptions of staff (funded with approved grant money):

4. M.Sc. E. Elzenheimer: This person handled the scientific tasks with a focus on engineering tasks in this project.
5. Clinical Neurophysiologist (25 %): This M.D. handled the scientific tasks concerned with patient-related and medical aspects of this project. Specifically, he oversaw patient recruitment and data handling, acquired and improved skills in nerve ultrasonography together with the technician from B5, and assisted in patient identification, classification, and recruitment. He conducted the patient measurements (conventional NCS, ultrasound, ME sensor recordings).

3.1 General information about Project B7

3.1.1 Project title: 3D-Imaging of magnetically labelled cells

3.1.2 Research area(s):

406-02 Synthesis and Properties of Functional Materials, 406-05 Biomaterials

3.1.3 Project leader(s)

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Do any of the abovementioned persons hold fixed-term positions? No.

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material	no
2.	clinical trials	no
3.	experiments involving vertebrates	no
4.	experiments involving recombinant DNA	no
5.	research involving human embryonic stem cells	no
6.	research concerning the Convention on Biological Diversity	no

3.2 Summary

This project aims at investigating the potential of magnetoelectric sensors for the detection of living cells, which are tagged with magnetic micro- or nanoparticles. We are working on two methods to achieve this goal. In the first method, superparamagnetic nanoparticles are excited by a magnetic AC field and higher harmonics of the excitation frequency are generated due to their magnetic nonlinearity that can be detected by magnetoelectric sensors in resonance. Our low-cost magnetic particle mapping (MPM) technique avoids large magnetic field gradients and the resulting forces on the magnetic particles, and it does not involve high AC frequencies, which require high-power units and give rise to significant heat dissipation. In the current funding period, we have demonstrated the feasibility of this approach. In particular, it has been shown how the sharp resonance and the vector characteristics of the magnetoelectric sensors can be used to minimize effects from the excitation signal. Moreover, the reconstruction of the particle distribution has been achieved for a quasi-2D particle arrangement by solution of the forward problem, analysis of the system function, and solution of the inverse problem. The minimum detectable amount of nanoparticles is about 300 ng at a distance of 2 mm between sensor and sample. Our second method, named magnetic susceptibility particle mapping (MSPM), employs instead of AC fields a motion-modulated DC field. This field is used to magnetize magnetic particles, but also to provide a bias field for a ΔE -effect sensor, which records the resulting low frequency magnetic field. With this measurement system, the magnetic field originating from 20 μg magnetic nanoparticles can be detected at a sensor-sample distance of 8 mm.

In the second funding period, we plan to extend our investigations with MPM and MSPM to 3D measurements to further improve their sensitivities and spatial resolutions. For MPM, a strong increase in sensitivity of the setup is expected by moving from 2D to 3D measurements by measuring the second harmonic instead of the third harmonic, replacing individual sensors with sensor arrays and multichannel detection, and employing inhomogeneous and bias fields, which will also increase the spatial resolution. For MSPM, we intend to investigate several measures for increasing the signal to noise ratio such as the 3D measurements, advanced magnetic shielding as well as the use of sensors with high bias fields and sensor arrays. For the solution of the inverse problem, which is relevant for both approaches, we also plan to apply artificial intelligence concepts at a later stage. In addition, we will perform magnetorelaxometry measurements to distinguish cell-internalized magnetic particles from freely moving particles.

The abovementioned methods are applied for detecting cell distributions in various soft biomaterial scaffolds in which cell imaging is difficult to achieve by optical means. In the current funding period, we have monitored relatively simple cell distributions in biomaterial matrices. In the second funding period, dynamic investigations of magnetically labelled cells in complex 3D biomaterial scaffolds are envisaged. An important question from the biomaterials side of the project will be to investigate cell growth and migration in 3D scaffolds as a function of their mechanical properties. This will not only provide knowledge of the impact of scaffold mechanics on cells, but can, in the long run, also be relevant to organ-on-a-chip and clinical applications which we plan to explore in the third funding period.

3.3 Project progress to date

3.3.1 Report and current state of research

The subject of this project is mapping magnetically labeled cell distributions in three-dimensional biomaterial scaffolds by means of resonant magnetoelectric (ME) and ΔE -effect sensors [Na08, Ja13, Go11, B7-8, B7-10] which have been investigated throughout the CRC 1261 and particularly in **A3** and **A4** of the current funding period. The techniques have been developed within the CRC and are called magnetic particle mapping (MPM) [B7-1] and magnetic susceptibility particle mapping (MSPM).

As discussed in detail in our initial application, three-dimensional biomaterial scaffolds are very promising materials for tissue engineering. In such scaffolds, cells are grown with the aim of conditioning cells or generating implantable tissue-replacement materials [Ma15]. It is not self-evident that cells grow in biomaterial scaffolds, as their migration and growth can be impaired by pores that are too small, a lack of nutrients (e.g. due to too little porosity), the specific chemistry of a scaffold, or its mechanical properties [Gr02]. To employ a scaffold for biomedical purposes, it is essential to ensure cell growth in the entire scaffold or at least in designated areas. It is still a challenging and time-consuming procedure to investigate cell growth in the often non-transparent scaffold materials, as conventional methods like optical microscopy and scanning electron microscopy (SEM) that allow cell detection in 3D volumes require a destructive sample preparation [la19], making many replications necessary in scaffolds that are often not 100 % identical. Furthermore, destructive methods make the further use of cell-loaded scaffolds, e.g. as implants, impossible. To test cell growth in scaffolds that are typically several cm in size, it is initially sufficient to detect about 1000 cells with a spatial resolution of about 1 mm. As there is still research necessary both in biomaterials science (for generating novel scaffolds for cell growth and conditioning) and on the systems side (for non-destructively investigating cells in such scaffolds by MPM or MSPM), both aspects are addressed in this project. The experiments on cells in scaffolds also serve as a quality check for the magnetic detection systems. In the following, we describe our results achieved during the first funding period both in pushing the detection of magnetic particles in cells and the investigation of cells in biomaterial scaffolds forward.

a) Magnetic particle mapping (MPM)

Magnetic nanoparticles have been studied extensively for biomedical applications [Th12]. In particular, they have been investigated for *in vivo* diagnostics and cell imaging. A well-established technique is magnetic resonance imaging (MRI), which is very expensive and requires strong magnetic fields. Furthermore, there has been much interest in so-called magnetic particle imaging (MPI) [Gl05]. In this technique, the nanoparticles are accumulated in the biological object to be imaged and are magnetized in an AC magnetic excitation field. The resulting signals from the magnetic nanoparticles are detected and the three-dimensional distribution of the nanoparticles is reconstructed by solving an inverse problem. The central idea of MPI is to take advantage of the nonlinear nature of the nanoparticle magnetization curve, which produces higher harmonics of the excitation field frequency. These higher harmonics are used to discriminate the weak signals of the magnetic nanoparticles from the strong excitation field. Several variants of MPI have been reported [We08][Sa09][We18]. Generally, they employ large DC gradient fields to produce a field-free point or line.

The AC excitation fields ranging from several tens to hundreds of kHz needed to generate sufficient signal in the pick-up coils require huge power supplies, and the heat dissipation is a real challenge. Moreover, the large DC gradient fields give rise to significant forces on the nanoparticles.

In the present project, we follow a different concept (*Figure B7-1A*), using our novel magnetic nanoparticle mapping technique (MPM) which requires neither particularly high AC frequencies nor strong magnetic field gradients. As in MPI, we use higher harmonics of the signal generated by the nanoparticles for detection; currently, the third harmonic is used because it gives the largest nanoparticle signal in the spectrum. For the discriminating between the strong excitation signal and the weak signal of the magnetic nanoparticles, we use the very sharp resonance of the magnetoelectric (ME) sensors developed within the CRC and adjust the third harmonic to the resonance frequency, which is about 7.5 kHz. Furthermore, we use the strong vector characteristics of the ME sensor for additional discrimination, particularly with respect to the in-plane and out-of-plane directions. In *Figure B7-1 B*, a light microscopy image and reconstructed MPM data of magnetically labelled cells (approximately 800,000 cells in a matrigel scaffold) are shown. Hence, cell distributions can indeed be mapped and reconstructed with very close resemblance to the real distribution. In general, we are currently able to detect a minimum amount of 300 ng of magnetic nanoparticles.

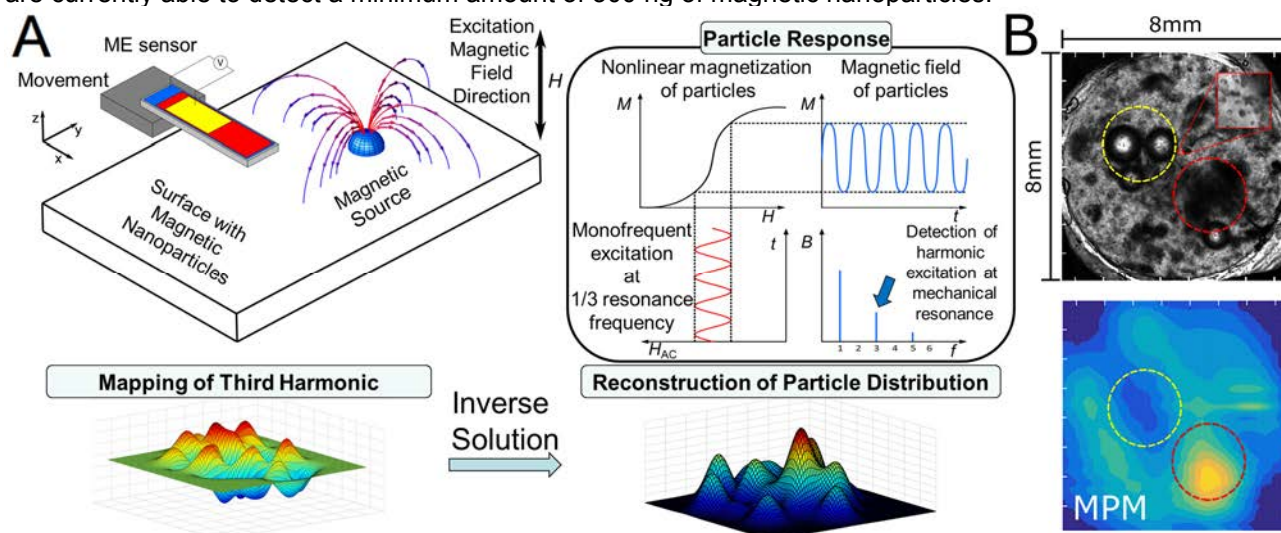


Figure B7-1 (A) Schematic of the working principle of MPM. The sample is moved with respect to the sensor's position. The 2D sample contains the magnetic nanoparticles that are magnetized by the externally applied monofrequent magnetic AC field with an amplitude of about $10 \text{ mT}/\mu_0$. The nonlinear response of the nanoparticles is detected by measuring the third harmonic excitation of the magnetic field of the nanoparticles. This magnetic field is mapped in space and can be used to reconstruct the particle distribution by solving the inverse problem. For this, a forward model was developed that considers the sensor's properties and sample geometry [B7-1] (B) 800.000 cells labelled for 24 h with magnetic nanoparticles (fluidMAG-CT, $\varnothing 100 \text{ nm}$, Chemicell, Berlin) embedded in matrigel (Matrigel Matrix Phenol Red Free 10 ml, Corning) imaged with light microscopy (top) and MPM (bottom) (from [B7-1]). The yellow dashed circle in the images shows a region where air bubbles are present, which is a region of low cell concentration. Here, the region in the MPM image shows low amplitude. The red dashed circle shows a region of high cell density, as is indicated from the dark region in the light microscopy image and the high amplitude in the MPM image.

b) System modelling and spatial reconstruction

The inverse problem has been fully described for the MPM system and can be solved for arbitrary geometries and sizes of the solution vector subjected to a nonnegativity constraint, which is necessary because negative particle concentrations do not exist. The imaging system can be described as a spatially shifted invariant linear system, i.e. the imaging system has an impulse response and the forward problem can be described as a convolution of the particle distribution. Initial computations of the inverse solution were done in cooperation with **B3**. In collaboration with the group of Prof. Hansen (DTU, Denmark), an iterative description for the computation of the inverse solution has been implemented. In this regard, a research stay of the PhD student Ron-Marco Friedrich at DTU was very helpful. The strategy allows for the investigation of useful system geometries for better reconstruction of the particle distribution, and an approach for a future 3D setup has been designed.

c) Characterization of magnetic nanoparticles

To investigate magnetic nanoparticle samples for their suitability as imaging agents in MPM, magnetic particle spectroscopy (MPS) can be used as it directly provides the harmonic spectrum for a given excitation

frequency and AC field amplitude [Bi09]. We have applied AC susceptibility (ACS) up to 1 MHz, multivariate MPS (varying the excitation field amplitude and frequency, as well as the magnitude of a superimposed DC field) and static magnetization measurements for the comprehensive characterization of representative magnetic nanoparticle samples. Particle behavior depends on many properties, such as viscosity, magnetic anisotropy, particle shape, magnetic core size, hydrodynamic size, temperature, magnetic field strengths, and frequency [Lu17]. The particles we use in this project are fluidMAG (Chemicell, Berlin). These particles were characterized with respect to their dynamic responses in cooperation with Prof. Meinhard Schilling and Prof. Frank Ludwig from TU Braunschweig using MPS and ACS. *Figure B7-2* shows the effective magnetic moment of the magnetic nanoparticles at 2.5 kHz for different excitation amplitudes. The increase in effective magnetic moment is due to the larger magnetic field amplitudes that allow for the emerging larger nonlinear response.

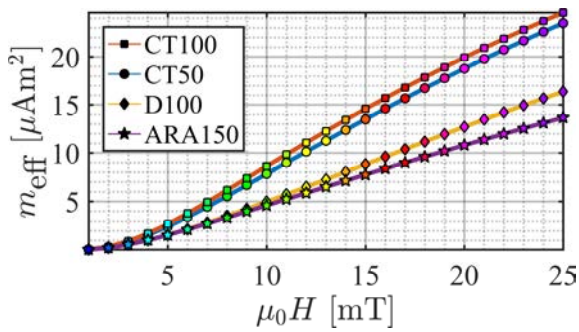


Figure B7-2 Effective magnetic moment m_{eff} of the third harmonic excitation of four types of magnetic nanoparticles (names in the legend, number indicates particle size in nm) from fluidMAG Chemicell (150 μl of 25mg/ml concentration) as a function of excitation amplitude at 2.5 kHz. Larger values are favorable, such that CT100 is used for most MPM and MSPM measurements. The data were obtained in cooperation with Prof. Meinhard Schilling and Prof. Frank Ludwig via magnetic particle spectrometry. At even higher magnetic field amplitudes, the effective magnetic moment will saturate.

d) Magnetic susceptibility particle mapping (MSPM)

In addition to MPM, we have established a completely different method that does not require a high-frequency magnetic field and only uses a DC field which is modulated by the signal from a sample moving over the sensor at a frequency in the Hz range. The signal is recorded with a ΔE -effect sensor developed in **A4**. Permanent magnets are used to magnetize the particles and at the same time provide the bias field necessary for shifting the operating point of the ΔE -effect sensor to its most sensitive region. The sensor is operated in its second bending mode at a frequency of 45 888 Hz. In this mode the bandwidth of the sensor is around 40 Hz. This setup (*Figure B7-3*) can directly measure the fields generated by the magnetized particles which are moved periodically over the sensor. This is a clear advantage compared to MPI and MPM, where the excitation field needs to be separated from the field generated by the particles [Gl05], and a significant part of the particle signal is lost by filtering. As MSPM does not require any filtering and directly measures the field originating from the particles, the method should achieve a high sensitivity, although ΔE -effect sensors have a higher LOD than resonant ME sensors.

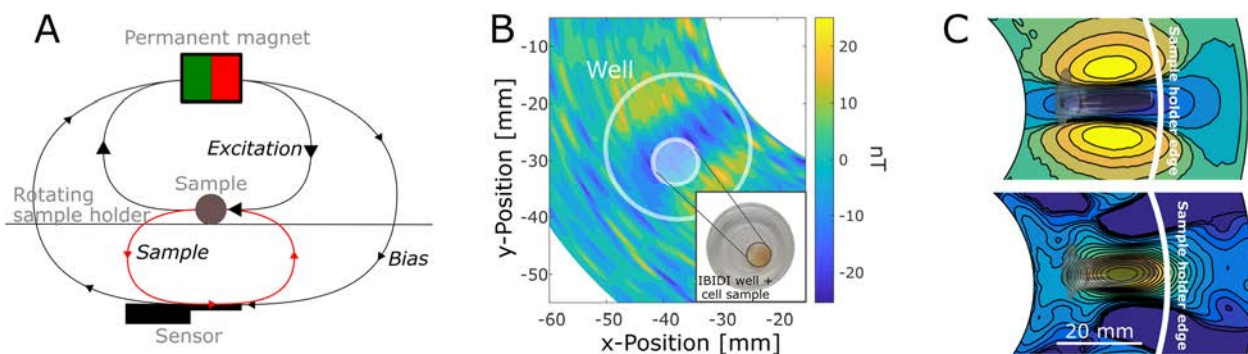


Figure B7-3 (A) Sketch of the working principle of the magnetic susceptibility particle mapping (MSPM) setup. Bias and excitation fields for the ΔE -effect sensor and the magnetic particles, respectively, are generated at the same time by a permanent magnet which is located approximately 21 mm above the sensor in a field of 1.7 mT. The sensor position is fixed in the field of the permanent magnet, and the direction of the magnetic field of the magnet is parallel to the long axis of the cantilever. Moving a sample on a rotating disc between the permanent magnet and the sensor aligns the magnetic moments of the particles, thus resulting in a motion-modulated magnetic field. (B) Measured field of a cell sample at a distance of 8 mm above the sensor. The sample consists of $\sim 1.4 \times 10^6$ cells labelled with magnetic nanoparticles (fluidMAG-CT, $\varnothing$ 100 nm, Chemicell, Berlin) and embedded in a gelatin/alginate matrix. Sample time at each radial position was 8 s. (C) Top: Field distribution measured with MSPM of a cylindrical sample containing 5 mg of nanoparticles

(same as above) diluted in 200 μL of water. Bottom: Reconstruction of the particle distribution from the measured field. A clear accumulation of particles is observable at the position of the sample. In both cases, an image of the sample (tube) is graphically overlaid. The white line shows the edge of the sample holder disc.

The working principle of MSPM is depicted in *Figure B7-3*. In the current setup, the sample (located on a disc) is rotated at 2.5 Hz through the gap between the permanent magnet and the sensor which measures the field generated by the magnetic nanoparticles. For a 2D measurement of the field distribution, the sensor is moved radially. At the moment, the minimum detectable iron content is 20 μg , and the spatial resolution is around 5 mm at a sample-to-sensor distance of 8 mm. Depending on sample size and the acquisition time, the full sample area is scanned within several minutes in the present setup.

e) Magnetorelaxometry measurements

Magnetorelaxometry allows for gathering information about the size of magnetic particles, their aggregation state, and their coupling to the environment [Wi12]. It makes use of the magnetization properties of superparamagnetic particles, where an ensemble of particles only shows a magnetic field when it is inside a magnetic field. After switching off this external field, the magnetization vanishes over time due to thermodynamic relaxation effects (Néel relaxation, Brownian relaxation). The time constant of relaxation changes when particles are internalized by cells [Ca18]. For magnetic cell detection it would be extremely helpful to be able to distinguish between freely moving particles and particles internalized by cells, as only the latter are of interest. We have developed a magnetorelaxometry apparatus using a self-biased ΔE -effect sensor in a setup similar to that for MSPM. Preliminary experiments demonstrate that the magnetic relaxation behavior of the particles depends on their environment (*Figure B7-4*).

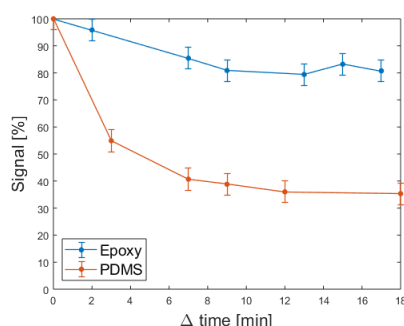


Figure B7-4 Signals detected from iron nanoparticles (diameter 50-100 nm) embedded in a stiff epoxy resin (double bubble, Henkel) and in a soft uncured silicone (Sylgard 184 (Polydimethylsiloxane, PDMS), Dow Corning). The signal measured from particles in a low viscosity environment (uncured PDMS) decays faster than that from bound particles in an epoxy resin.

f) Biomaterial scaffolds for tissue engineering

Systems for non-destructively detecting living cells in biomaterial scaffolds are crucial in many applications, including bone and soft tissue engineering. Therefore, we have also been pursuing research on porous biomaterials. To generate unique and specifically structured fibrous scaffolds, we have employed aerographite as well as some of its spin-offs (collaboration with **A2**). This strategy has allowed us to extend our studies to other carbon-based materials, including carbon-nanotube-tube networks (CNTT) and graphene-coated aerographite [B7-2]. The structure of the materials resembles that of collagen and can be adapted and chosen according to the requirements of the application. All materials generated are biocompatible and allow for cell growth (*Figure B7-5*). To make the materials bioactive, we have investigated procedures to integrate bioactive nanoparticles, such as hydroxyapatite nanoparticles and bioactive glass [B7-9, B7-3]. On such materials we could even demonstrate that pre-osteoblast cells grow and show osteogenic behavior, demonstrating the feasibility of our scaffolds for bone tissue engineering. We have furthermore extended our portfolio of scaffold materials by carrying out research on the inverse materials of the abovementioned fibrous materials, i.e. on microchannel-containing materials. [B7-4, B7-P1].

To understand whether magnetic particles influence cell dynamics, we have carried out systematic studies of cell migration in relation to intracellular motion both with and without intracellular artificial particles. As a first step, we established methods to track cells and intracellular particles and found highly exciting properties from single particle trajectories [B7-5] and from statistical analysis [B7-6]. We also observed that phagocytosed particles influence cell motion in structured extracellular environments [B7-7]. Hence, the size of magnetic particles chosen for our experiments on live cells needs to be adapted to the pore size of the scaffold to make sure that the magnetic particles are not influencing the cell experiment by reducing cell migration. We are therefore here working with nanoparticles instead of microparticles.

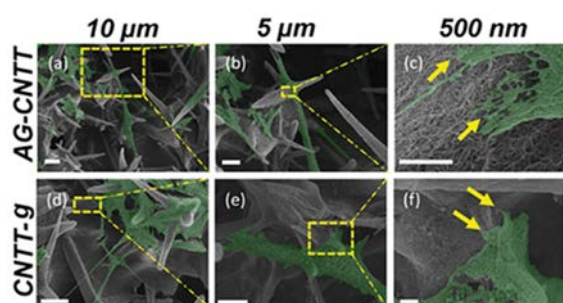


Figure B7- 5 SEM images of REF52wt cells after 7 days of culturing on (a–c) an aerographite-CNT composite and on (d–f) carbon-supported carbon-nanotube networks (CNTT). Left: medium-sized overview images illustrating the growth of cells between the fibers in different directions and planes; middle: zoomed-in images showing well-stretched cells along the fibers and their elongation; and right: close-up images on the adhesion sites, proving the presence of strong contacts between the materials and the cell membrane (yellow arrows) [from B7-2].

References

- [Bi09] S. Biederer, T. Knopp, T. F. Sattel, K. Lüdtke-Buzug, B. Gleich, J. Weizenecker, J. Borgert, T. M. Buzug, Magnetization response spectroscopy of superparamagnetic nanoparticles for magnetic particle imaging. *Journal of Physics D: Applied Physics* **42**, 205007 (2009).
- [Ca18] D. Cabrera, A. Coene, J. Leliaert, E. J. Artés-Ibáñez, L. Dupré, N. D. Telling, F. J. Teran, Dynamical Magnetic Response of Iron Oxide Nanoparticles Inside Live Cells. *ACS Nano* **12**, 2741-2752 (2018).
- [Gl05] B. Gleich, J. Weizenecker, Tomographic imaging using the nonlinear response of magnetic particles. *Nature* **435**, 1214-1217 (2005).
- [Go11] B. Gojdka, R. Jahns, K. Meurisch, H. Greve, R. Adelung, E. Quandt, R. Knöchel, F. Faupel, Fully integrable magnetic field sensor based on delta-E effect *Appl. Phys. Lett.* **99** (2011)
- [Gr02] L. G. Griffith, G. Naughton, Tissue Engineering--Current Challenges and Expanding Opportunities. *Science* **295**, 1009-1014 (2002).
- [Ia19] D. Iandolo, F. A. Pennacchio, V. Mollo, D. Rossi, D. Dannhauser, B. Cui, R. M. Owens, F. Santoro, Electron Microscopy for 3D Scaffolds--Cell Biointerface Characterization. *Advanced Biosystems* **3**, 1800103 (2019).
- [Ja13] R. Jahns, A. Piorra, E. Lage, C. Kirchhof, D. Meyners, J. L. Gugat, M. Krantz, M. Gerken, R. Knöchel, E. Quandt, Giant Magnetoelectric Effect in Thin-Film Composites. *Journal of the American Ceramic Society* **96**, 1673-1681 (2013).
- [Ja15] K. A. Jansen, D. M. Donato, H. E. Balcioglu, T. Schmidt, E. H. J. Danen, G. H. Koenderink, A guide to mechanobiology: Where biology and physics meet. *Biochimica et Biophysica Acta (BBA) - Molecular Cell Research* **1853**, 3043-3052 (2015).
- [Li14] M. Liebl, U. Steinhoff, F. Wiekhorst, J. Hauelsen, L. Trahms, Quantitative imaging of magnetic nanoparticles by magnetorelaxometry with multiple excitation coils *Phys. Med. Biol.* **59** 6607–20 (2014).
- [Li96] Y. Li, D. Oldenburg., 3D inversion of magnetic data *Geophysics* **61** 394–408 (1996)
- [Lu13] Luo, K. Mohan, P. A. Iglesias, D. N. Robinson, Molecular mechanisms of cellular mechanosensing. *Nature Materials* **12**, 1064 (2013).
- [Lu17] F. Ludwig, C. Balceris, C. Jonasson, C. Johansson, Analysis of AC Susceptibility Spectra for the Characterization of Magnetic Nanoparticles. *IEEE Transactions on Magnetics* **53**, 0-3 (2017).
- [Ma15] V. Marx, Organs from the lab. *Nature* **522**, 373 (2015).
- [Na08] C.-W. Nan, M. I. Bichurin, S. Dong, D. Viehland, G. Srinivasan, Multiferroic magnetoelectric composites: Historical perspective, status, and future directions. *Journal of Applied Physics* **103**, 031101 (2008).
- [Po16] W.C. Poller, N. Löwa, F. Wiekhorst, M. Taupitz, S. Wagner, K. Möller, G. Baumann, V. Stangl, L. Trahms, A. Ludwig, Magnetic particle spectroscopy reveals dynamic changes in the magnetic behavior of very small superparamagnetic iron oxide nanoparticles during cellular uptake and enables determination of cell-labeling efficacy *J. Biomed. Nanotechnol.* **12** 337–46 (2016)
- [Ra15] J. Rahmer, A. Halkola, B. Gleich, I. Schmale, J. Borgert, First experimental evidence of the feasibility of multi-color magnetic particle imaging *Phys. Med. Biol.* **60** 1775–91 (2015)
- [Sa09] T. F. Sattel, T. Knopp, S. Biederer, B. Gleich, J. Weizenecker, J. Borgert, T. M. Buzug, Single-sided device for magnetic particle imaging. *Journal of Physics D: Applied Physics* **42**, 022001 (2008).
- [Se18] M. Sekino, A. Kuwahata, T. Ookubo, M. Shiozawa, K. Ohashi, M. Kaneko, I. Saito, Y. Inoue, H. Ohsaki, H. Takei, M. Kusakabe, Handheld magnetic probe with permanent magnet and Hall sensor for identifying sentinel lymph nodes in breast cancer patients. *Scientific Reports* **8**, 1195 (2018).
- [Ta15] S. Tanaka, H. Murata, T. Oishi, Y. Hatsukade, Y. Zhang, H. Horng, S. Liao, H. Yang, Imaging of Magnetic Nanoparticles Using a Second Harmonic of Magnetization With DC Bias Field. *IEEE Transactions on Magnetics* **51**, 1-4 (2015).
- [Th12] N.T.K. Thanh, Magnetic Nanoparticles From Fabrication to Clinical Applications *CRC Press* **54** 243–276 (2012)

- [We08] J. Weizenecker, B. Gleich, J. Borgert, Magnetic particle imaging using a field free line. *Journal of Physics D: Applied Physics* **41**, 105009 (2008).
- [We18] M. Weber, J. Beuke, A. von Gladiss, K. Gräfe, P. Vogel, V.C. Behr, T.M. Buzug, Novel Field Geometry Using Two Halbach Cylinders for FFL-MPI *Int. J. Magn. Part. Imaging* **4** (2018).
- [Wi12] F. Wiekhorst, U. Steinhoff, D. Eberbeck, L. Trahms, Magnetorelaxometry Assisting Biomedical Applications of Magnetic Nanoparticles. *Pharmaceutical Research* **29**, 1189-1202 (2012).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [B7-1] R.-M. Friedrich, S. Zabel, A. Galka, N. Lukat, J.-M. Wagner, C. Kirchhof, E. Quandt, J. McCord, C. Selhuber-Unkel, M. Siniatchkin, F. Faupel, Magnetic particle mapping using magnetoelectric sensors as an imaging modality. *Scientific Reports* **9**, 2086 (2019).
- [B7-2] M. Taale, F. Schütt, T. Carey, J. Marx, Y. K. Mishra, N. Stock, B. Fiedler, F. Torrisi, R. Adelung, C. Selhuber-Unkel, Biomimetic Carbon Fiber Systems Engineering: A Modular Design Strategy To Generate Biofunctional Composites from Graphene and Carbon Nanofibers. *ACS Applied Materials & Interfaces* **11**, 5325-5335 (2019).
- [B7-3] M. Taale, D. Krüger, E. Ossei-Wusu, F. Schütt, M. A. U. Rehman, Y. K. Mishra, J. Marx, N. Stock, B. Fiedler, A. R. Boccaccini, R. Willumeit-Römer, R. Adelung, C. Selhuber-Unkel, Systematically Designed Periodic Electrophoretic Deposition for Decorating 3D Carbon-Based Scaffolds with Bioactive Nanoparticles. *ACS Biomaterials Science & Engineering*, **5**, 4393-4404 (2019).
- [B7-4] S. B. Gutekunst, K. Siemsen, S. Huth, A. Möhring, B. Hesseler, M. Timmermann, I. Paulowicz, Y. K. Mishra, L. Siebert, R. Adelung, C. Selhuber-Unkel, 3D Hydrogels Containing Interconnected Microchannels of Subcellular Size for Capturing Human Pathogenic *Acanthamoeba Castellanii*. *ACS Biomaterials Science & Engineering* **5**, 1784-1792 (2019).
- [B7-5] D. Krapf, N. Lukat, E. Marinari, R. Metzler, G. Oshanin, C. Selhuber-Unkel, A. Squarcini, L. Stadler, M. Weiss, X. Xu, Spectral Content of a Single Non-Brownian Trajectory. *Physical Review X* **9**, 011019 (2019).
- [B7-6] S. Thapa, N. Lukat, C. Selhuber-Unkel, A. G. Cherstvy, R. Metzler, Transient superdiffusion of poly-disperse vacuoles in highly motile amoeboid cells. *The Journal of Chemical Physics* **150**, 144901 (2019).
- [B7-7] M. Timmermann, N. Lukat, L. P. Schneider, C. W. Shields IV, G. P. López, C. Selhuber-Unkel: Migration of microparticle-containing amoebae through constricted environments. *ACS Biomaterials Science & Engineering* (2019), DOI: 10.1021/acsbiomaterials.9b00496.
- [B7-8] B. Spetzler, C. Kirchhof, J. Reermann, P. Durdaut, M. Höft, G. Schmidt, E. Quandt, F. Faupel, Influence of the quality factor on the signal to noise ratio of magnetoelectric sensors based on the delta-E effect. *Applied Physics Letters* **114**, 183504 (2019).
- [B7-9] M. Taale, F. Schütt, K. Zheng, Y. K. Mishra, A. R. Boccaccini, R. Adelung, C. Selhuber-Unkel, Bioactive Carbon-Based Hybrid 3D Scaffolds for Osteoblast Growth. *ACS Applied Materials & Interfaces* **10**, 43874-43886 (2018).
- [B7-10] S. Zabel, J. Reermann, S. Fichtner, C. Kirchhof, E. Quandt, B. Wagner, G. Schmidt, F. Faupel, Multimode delta-E effect magnetic field sensors with adapted electrodes. *Applied Physics Letters* **108**, 222401 (2016).

b) Patents

- [B7-P1] Gutekunst, S.; Hölken, I.; Adelung, R.; Selhuber-Unkel, C.: (2016) Microporous hydrogels, Europäisches Patentamt, EP3291971.

3.4 Project plan

Objectives

The goal of the present project is to investigate magnetoelectric sensors, developed in the CRC 1261, for the detection of living cells which are tagged with magnetic micro- or nanoparticles. We will pursue three methods developed in the current funding period: magnetic particle mapping (MPM), magnetic susceptibility particle mapping (MSPM), and magnetorelaxometry. In MPM, similar to conventional magnetic particle imaging (MPI), magnetic marker particles, consisting of superparamagnetic nanoparticles in a biocompatible polymer encapsulation, are stimulated by a magnetic AC field. Higher harmonics of the stimulation frequency are generated which can be detected by magnetoelectric sensors in resonance. The very effective suppression of the excitation frequency is achieved by the sharp resonance and the strong vector characteristics of the dedicated magnetoelectric thin film sensors. Our newly developed magnetic particle mapping technique does

not use pick-up coils and, hence, does not require high AC fields generated by high-power units, nor does it resort to large magnetic field gradients. Thus, the method has great potential for the realization of a compact, very cost-effective apparatus that avoids forces on the magnetic particles and eliminates the heat dissipation problem present in other methods. This holds even more for MSPM, where only a weak DC field is needed to simultaneously bias the sensor to its operating point and align the magnetic nanoparticles. The DC field is motion-modulated and the resulting low-frequency AC field is detected by a sensor based on the ΔE effect. In magnetorelaxometry, the magnetic moments of the nanoparticles are aligned in a DC field and the decay of the net magnetic moment of the sample is measured. It not only provides information on size and aggregation of the magnetic particles but also on their environment and will be used in particular to discriminate between particles inside and outside cells.

After having demonstrated the feasibility of our three methods for the detection of magnetic nanoparticles, we now plan to increase the sensitivity and spatial resolution and aim for 3D imaging. Depending on the specific method, approaches to address this goal include the extension from 2D to 3D measurements, use of multichannel and array techniques, employment of inhomogeneous fields for alignment of the magnetic nanoparticles, advanced shielding measures, resonant detection of the 2nd instead of the 3rd harmonic (MPI, WP1), and use of sensors with a higher bias field (MSPM). The objective for MSPM (WP2) is to increase the current sensitivity of the method by a factor of 100 such that about one thousand magnetically labelled cells are detectable in 200 mm³. We expect that a detailed simulation of the full measurement system will be able to predict the influence of each contributing parameter, which we will verify in experiments. Moreover, in WP6 we will investigate enhanced solutions of the inverse problem including nonlinear problems and, at a later stage, artificial neural networks. In addition, we expect significant progress by advanced characterization of the magnetic nanoparticles (WP4) in order to use the best markers for the specific measuring techniques. In magnetorelaxometry (WP3), we aim to build a setup that is able to distinguish between the signal originating from freely moving and from cell-internalized particles. We expect that the relaxation signal will enable us to distinguish between intracellular and extracellular particles.

The different techniques will be applied for detecting cell distributions in various soft biomaterial scaffolds. Our objective is to first generate fibrous and porous scaffold materials with distinct structural and mechanical properties (WP7), such as aero-polymers and 3D-printed hydrogels. As both scaffold mechanics and structure have a strong impact on cells, we here hypothesize that there is an optimum for both parameters. We further aim (WP8) to identify if our magnetic particle detection methods hold their promises in experiments on living cells and if they are suitable for replacing conventional destructive methods for detecting cells in biomaterial scaffolds. Our aim is to carry out dynamic investigations of magnetically labelled cells with a temporal resolution of a few minutes and a spatial resolution in the mm range. We expect that certain conventional methods can be replaced.

Proposed research methods and work plan

The technical, chemical and biological methods proposed to reach the abovementioned objectives are described in detail in the work plan, which also addresses envisioned challenges and mentions the major co-operation partners. In addition, it contains a timeline that includes prospects for the 3rd funding period.

Table B7-1: Work schedule

	2020		2021				2022				2023				2024	
	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2
WP1 3D-MPM:																
Setup build and measurement																
DC Bias /2 nd Harmonic																
Inhomogeneous fields																
Sensor Arrays																
WP2 MSPM:																
Shielding																
Sensor unit modifications																
WP3 Magnetorelaxometry																
WP4 Magnetic particle markers																
WP5 Excitation Electronics																
WP6 Modelling, inverse problems																
WP7 Scaffolds with tailored structure, mechanics																
Cell investigation																

WP8 Magnetic cell imaging: in 3D scaffolds																			
dynamic measurements																			
relaxometry measurements																			

Doctoral researcher 1 (Faupel)

Doctoral researcher 2 (Selhuber-Unkel)

WP1 3D-MPM Setup

WP1 deals with modifying the existing MPM setup towards 3D imaging. Here, we will implement more measures to enhance the imaging system:

1. Alteration of sample geometry to a cylindrical sample for improving spatial sensitivity,
2. inhomogeneous magnetic fields for selective excitation,
3. usage of the second harmonic excitation for larger signals, and
4. larger magnetic fields using high power coils for larger nonlinear responses of MNP.

To evolve the existing MPM setup to be able to measure 3D samples effectively, we intend to alter the sample geometry such that deeper lying magnetic nanoparticles can contribute more to the measurable signal. This geometry is in the form of a rotating cylinder (see *Figure B7- 6*). For the currently available quasi-2D detection system, 3D imaging cannot be done efficiently because the signal from deep sources is very weak. Furthermore, the signals originating from several particles can cancel each other out because of the particular projection of the magnetic nanoparticles that is measured. Choosing a 3D cylindrical geometry for the sample allows for the measurement of a specific projection of the magnetic field of the magnetic nanoparticles from which deeper sources can contribute more to the measurement signal. Furthermore, it is not possible for the particle signals to cancel each other by measuring this projection as shown in *Figure B7- 6*. Furthermore, the solution of the inverse problem does not reflect the real distribution of magnetic particles because a surface bias of the reconstructed distribution exists, i.e. the reconstructed particle distribution is closer to the surface than in reality [Li96]. To accommodate for this surface bias, cylindrical geometry allows for a better reconstruction in 3D while also allowing for a larger measurable magnetic field from the MNP because of the larger spatial sensitivities.

In addition, incorporation of inhomogeneous fields can lead to a vast enhancement of the proper reconstruction of the particle distribution because the magnetic sources are selectively excited [Li14]. Based on these considerations, a setup will be investigated for the evaluation of such an imaging system. An example is shown in *Figure B7- 6*. Here, the bias coils will be used to introduce a magnetic offset field that shifts the operating point on the magnetization curve of the particles to the region where the second harmonic dominates and thus allows for the alteration of the magnetic particle spectra. In this way, instead of the third harmonic excitation, the second harmonic excitation can be measured, which has a larger amplitude and should therefore lead to a higher sensitivity of the imaging system. The relative factor in amplitude between the third and second harmonics is at least 1.5 [Ta15], though this depends on the amplitude of the excitation field and is larger for smaller excitation amplitudes. Investigation of magnetic particle spectra while applying a magnetic bias field will be done for optimal bias choice and will be part of WP4. Furthermore, the excitation coils can be used either in series or selectively, and thereby enabling homogeneous or inhomogeneous magnetic fields.

The excitation field amplitude for the setup as shown in *Figure B7- 6* is only about 2 mT with the current electronics because of the unavailability of a cooling system. An excitation field amplitude of 25 mT would increase the sensitivity of the imaging system more than an order of magnitude (because the effective magnetic moment increases strongly, c.f. *Figure B7- 62*) and lead to a strongly increased sensitivity of the imaging system. Using the data from *Figure B7- 62* for the particles CT100, we can estimate the magnetic field at a distance of 5 mm for an excitation field of 2 mT per μg particles to have a maximum value of 58 pT/ μg , whereas for 25 mT excitation it is 4300 pT/ μg . This is an increase by a factor of 74. It is thus essential to increase the excitation amplitude for the 3D imaging system. For such a system to operate at larger excitation amplitudes, the electronics must be chosen appropriately, as outlined in WP5.

Such a strong increase in the excitation amplitude will also give rise to a modulation of the bias field of the magnetoelectric sensor that could drive the sensor away from its operating point. If this should turn out to affect the solution of the inverse problem, nonlinear approaches will be addressed in WP6. In case of severe nonlinearities, we plan to use artificial neural networks already in the second funding period because they are not affected by nonlinearities.

The 3D setup design that has been theoretically investigated (see 1.3.1 b)) is based on an altered sample geometry involving a rotating cylinder. This geometry allows a useful magnetic field projection to be measured, because spatial sensitivities (i.e. the coefficients of the system matrix, which is the field B that a particular position in space generates at the sensor position per mass of particle content) are overall larger and reach deeper than in the already existing 2D setup. This imaging approach with the rotating cylinder for 3D imaging will also be applied to the MSPM measurements.

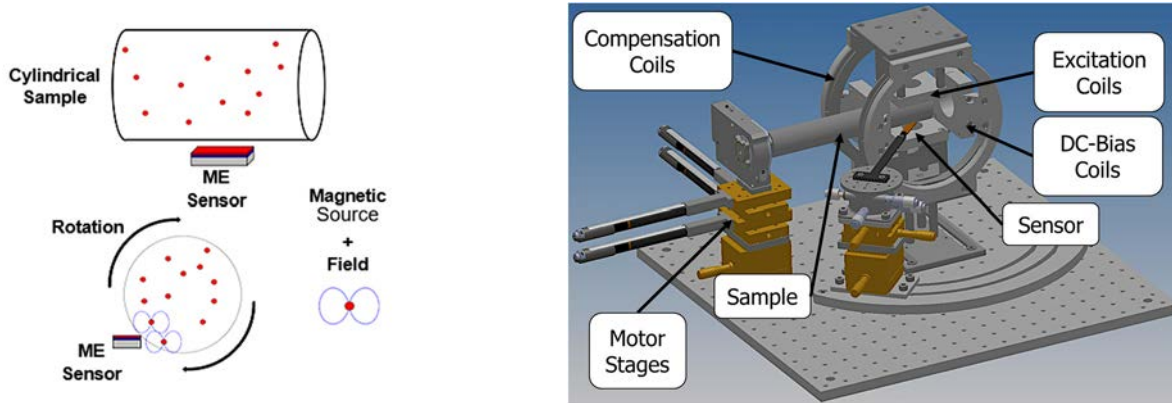


Figure B7- 6 Schematic Principle of the sample geometry for 3D measurements (left) and possible setup for the 3D measurements (right). The dipole field of the particles is indicated. The sensor configuration is only possible due to the change in the sample geometry. Deeper lying sources contribute to the measurement signal more strongly with this configuration. In addition, all particles in the sample contribute additively to the signal, unlike a planar sample geometry where signals can cancel each other out. This imaging approach will also be used in WP2 for MSPM. DC bias coils will be used to shift the operating point of the magnetic nanoparticles into a region of strong nonlinearity such that a larger signal can be measured.

Another important aspect is the implementation of sensor arrays for faster measurements or higher sensitivity in the MPM system. Multichannel detection with sensors mounted at different positions will also enhance spatial resolution. At the moment, measuring a grid of 50 x 50 measurements takes about 2 hours, but faster motors will also enable a shorter measurement time. Sensor arrays and multichannel detection (collaboration with **A4**, **B1**, **B2**, and **Z1**) will reduce the measurement time more than one order of magnitude.

WP2 Magnetic susceptibility particle imaging (MSPM)

As shown in 1.3.1, our MSPM setup shows great potential for detecting small magnetic particle concentrations. We will carry out a detailed simulation of the full measurement system to predict the influence of each parameter that influences sensitivity and spatial resolution of the setup. The simulation will be verified by experiments. Currently, the limit of detection is not given by the sensor noise but by a magnetic background signal. Reducing this background signal can be achieved by electric and magnetic shielding. We will also work on three strategies to further decrease the LOD of MSPM by modifying the sensor unit itself. These strategies include (1) the usage of a stronger permanent magnet and arrangements of multiple magnets for the excitation, (2) a specific adaptation of the sensor for the MSPM method (with **A4**), and (3) the use of sensor arrays and multichannel detection in cooperation with **A4**, **B1**, **B2**, and **Z2**. In detail, this means:

- (1) Permanent magnets for excitation: The choice for the ideal excitation is closely linked to the sample size and the minimum particle concentration that should be detected. On the one hand, an enhanced magnetic field in the sample region will generate a larger particle signal from the sample and result in a larger magnetic field at the sensor. On the other hand, the gradient of the magnetic field is also crucial as it defines the distance from the magnet with a suitable bias field for the sensor. Therefore, a single magnet or an arrangement of magnets with a high gradient down to the position where the required bias field should be located will be employed. With this, the magnetization of the sample will be increased and result in a stronger signal at the sensor. Alternatively, we will modify the magnetic field distribution by an arrangement of a permanent magnet and soft magnetic materials.
- (2) Sensor adaptation: We will use a sensor with a working point at a larger bias field, as it can be located closer to the magnet and thus to the sample, which is between sensor and magnet (with **A4**). We also plan to explore the use of surface acoustic wave (SAW) sensors from **A9**. Like ΔE -effect sensors, they are based on the ΔE -effect and are suitable for the detection of low-frequency magnetic fields.
- (3) Sensor arrays and multichannel detection with sensors at different positions: These will be used for collecting more spatial information in less time. The sensor arrays will be integrated into the setup in collaboration with **A4** and **B1**.

We expect a further significant increase in sensitivity of the setup by reducing the distance between the sample and the sensor by modifying the setup such that the sample is no longer located between magnet and sensor. Instead, the sensor and the excitation permanent magnet will be located on one and the same side of the sample (single-sided detection). This should be possible, as the particles in the sample are mainly magnetized by the field component that is perpendicular to the sensor plane. Due to the magnetic shape anisotropy of the sensor, its sensitivity is not affected by this component. The challenge here is to generate an excitation field where the perpendicular component for particle magnetization is large and where the parallel component is in the range of the bias field that is required by the sensor. Single-sided setups with good sensitivities would be very beneficial, as they would enable imaging on surfaces of larger volumes. This is highly relevant in the clinical context, e.g. in sentinel lymph node detection [Se18].

In total, we increase the current sensitivity of the method from 20 μg (measured in water in a volume of 200 μl ; projected area of 50 mm^2) by a factor of 100. This would correspond to a few thousand magnetically labelled cells in the same volume [Po16]. We expect an increase in sensitivity due to the usage of specifically designed fields from permanent magnets by a factor of two, due to a reduction of sensor-sample distance by a factor of 10, and due to electrical shielding by a factor of 5. A reduction of the sensor-sample distance will also decrease the current spatial resolution from the range of several mm to the sub-mm regime.

So far, MSPM has only been used for 2D imaging. To achieve 3D imaging, we plan to combine our MSPM with the 3D-MPM setup described in WP1 (Figure B7-8), where a cylindrical sample is measured to enhance the spatial resolution in 3D. Data analysis will involve complex aspects of the inverse problem and will be performed in WP6.

WP3 Magnetorelaxometry

In WP3, we plan to build a setup similar to the MSPM setup (Figure B7-3) that is able to distinguish between the signal originating from freely moving particles and cell-internalized particles. The difference between this setup and MSPM is that the point of the highest excitation field in the sample layer is not located perpendicular above the sensor but is shifted to the opposite point of the disc (Figure B7-7). Depending on the relaxation time and the distance between excitation magnet and the sensor, a magnetic signal will be measured. Particles with a longer relaxation time (e.g. particles in cells) will contribute stronger to this signal, while the contribution from particles with short relaxation times (i.e. freely moving particles) will be small. We expect that a detailed magnetorelaxometry study will, in the end, allow for choosing a particle size and type such that only cell-internalized particles contribute to the measured signal because the magnetization of the freely moving particles will have already decayed at the sensor position. For choosing the right particle system, WP3 will strongly benefit from the results of WP4 on magnetorelaxometry. So far, our setup has only been used for measuring the drastically different relaxation times of particles in epoxy resin and uncured silicone (Figure B7-7). Crucial setup parameters are the rotation speed of the sample, the spatial gradient of the exci-

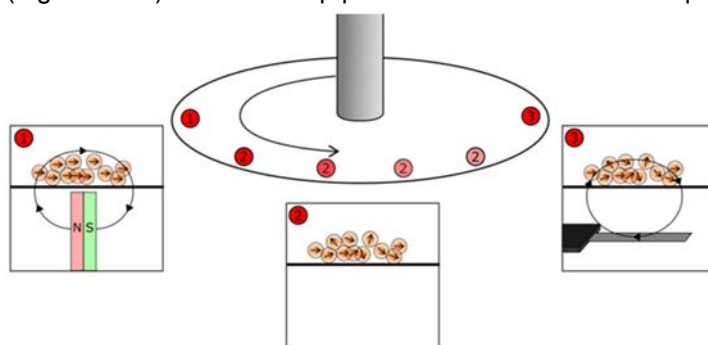


Figure B7- 7 Working principle of the relaxometry setup. The rotating sample is magnetized at one location and the magnetic field of the sample is measured at another position. After having left the field of the permanent magnet, the magnetization of the magnetic labels decays due to relaxation processes. The relaxation time is a function of the mechanical coupling of the particle to its environment.

tation magnet in the direction of sample movement, and the time that the particles stay in the excitation field. For this setup, we also plan to use ΔE -effect sensors. If the distance between the region of particle magnetization and sensor is too large to provide the bias-field for the ΔE -effect sensors, self-biased ΔE -effect sensors or electrically modulated ME sensors (A7) will be employed.

WP4 Magnetic particle markers

WP4 deals with the behavior of magnetic nanoparticles (MNP) internalized by cells and the proper choice of MNP for the cell experiments. MPM measurements will be done on magnetically labeled cells and their magnetic response will be analyzed. First steps to sensitivity measurements with reference samples in aqueous media have already been performed, as shown in Figure B7- 8, where point-shaped samples were measured at a sample-sensor distance of 2 mm and an excitation amplitude of 9 mT. The minimum detectable result was 300 ng of particles. Different particles and particle environments will give different sensitivities and these will be investigated, thereby enabling the figure of merit for the choice of MNP for cell measurements.

Complementary to that, a cooperation with Prof. Meinhard Schilling and Prof. Frank Ludwig (TU Braunschweig) will allow us to perform *in situ* magnetic particle spectroscopy (MPS) measurements on living cells. Thus, the change in the particle dynamics can be tracked and a more complete picture of particle incorporation into cells can be established. Furthermore, second harmonic generation in presence of a magnetic DC bias will be investigated for improved sensitivity.

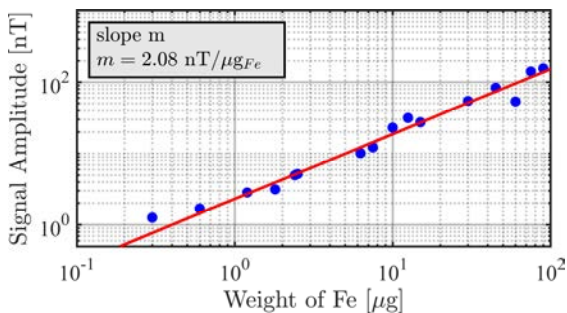


Figure B7- 8 Linear response of measured magnetic field for different amount of MNP. The sensitivity gives a measure of the particles' (CT100, Chemicell fluidMAG) usefulness for MPM. The particles were excited at about 2.5 kHz with an amplitude of 9 mT at a distance of 2 mm. The inset shows the parameters of the linear fit. The slope is the sensitivity of the setup with the aforementioned characteristics.

WP5 Excitation electronics

In this work package we plan to improve the electronics of the magnetic excitation system. Linearity of the excitation signal and stable amplitudes are a must for the MPM setup. Therefore, filter stages need to be developed that can attenuate the amplifiers' nonlinearities. These filter stages will be developed together with the group of Prof. Buzug (Institute of Medical Engineering, University of Lübeck), who is an expert on magnetic particle imaging systems and their corresponding electronics.

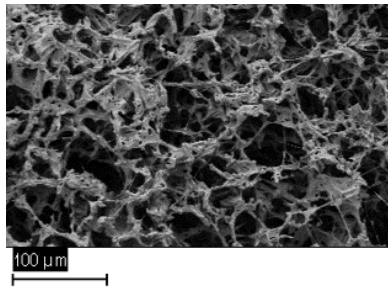


Figure B7- 9 Aero-polymer made of PDMS.

Larger field amplitudes will lead to a larger nonlinear response of the magnetic nanoparticles, thereby increasing the sensitivity of the imaging system. For the 3D setup as outlined in WP1, we expect to improve the sensitivity by more than one order of magnitude. To drive the excitation coils with greater power, we need to cool the coils because the input power will be several hundred watts. Therefore, an enhanced setup will be developed that will be able to sustain continuous operation of a high-power input.

Also, the filter stages need to be able to withstand large currents running without nonlinearities. In addition, a shielding chamber for the setup will be built to reduce external effects on the measurements.

WP6 Modelling and inverse problems

WP6 deals with improving the solution of the inverse problem. For this, a detailed model of the imaging system is needed. At the moment, all MPM and MSPM data can be analyzed via a multitude of algorithms and constraints. Even the size of the data is not an issue because the algorithms used are iterative, as are the computations of the forward problem. For the second funding period, the following points have to be addressed with regards to the inverse problem:

1. The influence of inhomogeneous fields,
2. the behavior of the MNP for different AC-excitation amplitudes in inhomogeneous fields,
3. incorporation of phase relations of the particles to investigate the binding state of MNP,
4. additional factors for the influence of the sensor geometry on the system function, and
5. inclusion of several magnetic field projections for a combined inversion of the data.

At the moment, only homogeneous fields are used. To gain more robustness in 3D, inhomogeneous fields can be used to excite areas with MNP more selectively. The measured data will be used appropriately because the system function changes. This needs to be modelled accordingly by modification of the system matrix. Because the MNP response depends on the strength of the applied magnetic field, this MNP behavior has to be included in the system function as well if inhomogeneous magnetic fields are used. For this, the MNP need to be characterized and their behavior will be encoded in the coefficients of the system function.

In this context, the phases of the measured data also depend on the binding state of the particles, such that, similar to MPI, "colored MPM" will be investigated [Ra15]. Here, one separates different particle behaviors from each other, to make a map of local binding states of the MNP. For this situation, also the forward model will be adapted to deal with the inverse problem in this regard.

Another factor that needs to be included is the influence of the sensor geometry on the system function. Here, the sensor averages the inhomogeneous magnetic fields of the MNP. Therefore, the sensor can be

described as a spatial filter, and because the sensor itself is magnetic, this spatial filter may be nonlinear with respect to the field averaging such that neural networks could be used to express this nonlinearity. Other artificial intelligence approaches can also be used on top of the already existing description of the imaging system because nonlinearities can be expressed this way.

Lastly, in WP1 and WP2, arrays of ME sensors and multichannel detection will be used for the MPM and MSPM system. For this, different projections of the magnetic field will be measured and used for the reconstruction of the MNP distribution which needs to be implemented in the system model.

WP7 Scaffolds with tailored mechanical and structural properties for tissue engineering

An important application field for the magnetic particle mapping methods is the monitoring of cells growing in porous biomaterials. In the first funding period, we have mainly investigated rather stiff scaffolds with Young's moduli up to several 10 MPa [B7-2]. An important question in biomaterials science is, however, the influence of material mechanics on cells ("mechanosensing") in three-dimensional environments [Ja15, Lu13]. Here, we aim to study the role of soft 3D polymer scaffolds. We will focus on two types of porous scaffolds: fibrous "Aero-polymers" and porous 3D-printed hydrogels. Aero-polymers are the non-conductive polymer counterparts of the fibrous carbon-based scaffolds investigated during the first funding period. They are investigated and fabricated in collaboration with **A2**. Due to their fibrous nature, they can mimic the structure of collagen (Figure B7- 9). The mechanical properties of the aero-polymers will be changed by using different cross-linker concentrations during the polymerization of the polymer (e.g. Sylgard 184 PDMS) so that biologically relevant Young's moduli between ≈ 1 kPa and 100 kPa are reached. In addition, we will also vary the porosity and fiber properties and will make the scaffolds structurally, mechanically, and chemically inhomogeneous, e.g. by photopolymerization and locally adding biofunctionalization agents. This should mimic inhomogeneous conditions in the body and allow for exploring aspects that are necessary for future organ-on-a-chip investigations. In addition to fibrous scaffolds, we will 3D print well-defined structures of hydrogel scaffolds (e.g. GelMA) with different mechanical properties using a 3D hydrogel printer (CellInk). In this way, we will generate well-defined pores and also co-print the cells directly into the scaffolds. The 3D printed scaffolds will be particularly able to serve as samples for exploring the limits of our cell detection methods (MPM, MSPM, and magnetorelaxometry).

All scaffolds will be sterilized prior to cell seeding. To test the cellular response (including cell growth, migration, mechanotransduction) on cell lines well-established in the group (e.g. REF52wt), it will here be characterized by standard methods (light microscopy, SEM). *In situ* information on cell growth and migration will be collected with 3D-MPM and MSPM in WP8.

WP8 Magnetic cell imaging

Here, the main questions to answer with both MPM and MSPM are: i) Do the cells grow homogeneously in 3D scaffolds? ii) How fast do cells migrate into the scaffolds? (iii) How long are cells detectable with our set-ups and at which spatial and temporal resolution? (iv) Which method is most suitable for which problem?

Prior to cell experiments we will magnetically label the cells with magnetic nanoparticles and either seed them onto the scaffolds or print them into the scaffolds (WP7). In the ideal case, a cell can take up 100 pg of magnetic material [Po16]. We will start off by investigating cells in small sample volumes (several mm³) that contain well-defined, simple structures for cell growth. We will then extend their complexity and size step-by-step. This will involve more complex 3D-printed structures and aero-polymers, both with volumes up to the cm³ regime and internal structures in the micro- to millimeter size. Presumably, no larger samples than those in the lower cm³ range can be imaged, as the magnetic field originating from the magnetic particles decreases significantly with distance. We will carry out a systematic investigation of spatial and temporal resolution with our setups. We hypothesize that there is a difference in the suitability of each of the methods for specific research questions and scaffold types. For example, we expect that MPM is more suitable for imaging large volumes, whereas MSPM should be able to achieve a higher temporal resolution due to the shorter measurement time. However, the setup-induced limits in temporal or spatial resolution are certainly overlaid by biological processes. For example, cells distribute their magnetic load over their daughter cells in cell division and they might also be influenced by longer measurements that involve tiny field gradients. These aspects will also be investigated.

In addition, we will also carry out magnetorelaxometry experiments (see WP3). These experiments are important because they could ensure that only the signal of cell-internalized magnetic particles is detected. We expect that most particles will be bound to cells if cells are co-printed into the scaffolds with the 3D printer. However, if magnetic particles are added while the cells are already present in the scaffolds, we expect to find some freely moving particles or particles stuck to the scaffolds. We will therefore determine the best method to pre-load cells with magnetic particles.

Future Prospects

The methods investigated in this project have great potential for the realization of compact systems for detecting magnetically labelled cells that avoid large forces on the magnetic particles and eliminate the heat dissipation problem present in other methods. Clinical applications could benefit greatly from such cost-efficient, precise, and handy systems, for example in tumor margin detection. Therefore, the long-term aim for the third funding period will be the development of compact systems for applications in life science. To reach this goal, we will address particularly challenging problems, such as dynamic measurements at high temporal and spatial resolution in clinical applications. We also plan to use artificial intelligence approaches for a fast and precise solution of the inverse problems involved. We are also considering applying for a transfer project in the third funding period.

3.5 Role within the Collaborative Research Centre

B7 takes ME sensors towards bioengineering applications. As the project is based on the expertise of a number of other projects (e.g. on sensor design, fabrication, simulation), there are many connections to and interactions with other projects. In detail, collaborations with the following projects are planned:

- A2:** Aero-polymer networks.
- A4:** ΔE -effect sensors for MSPM and magnetorelaxometry experiments.
- A7:** Electrically modulated ME sensors for magnetorelaxometry experiments.
- A8:** Simulations of small resonant sensors and their response to small magnetic dipole fields.
- A9:** SAW sensors for MSPM and magnetorelaxometry experiments.
- B1:** Front-end development for sensor arrays and multichannel systems.
- B2:** Multichannel system signal processing
- Z1:** Resonant sensors for 3D-MPM.
- Z2:** Non-magnetic motor concepts, sensor characterization and multichannel systems for arrangements of multiple sensors.

B7 contributes to the focus groups “Concepts based on ΔE effect”, “Biomedical applications” and “Modelling”.

3.6 Differentiation from other funded projects

C. Selhuber-Unkel and her group are currently supported by several third-party funded projects that are listed in the general part of this proposal. All these projects are clearly different from the project proposed here.

F. Faupel and his group are currently supported by the DFG through various projects listed in the general part of the CRC1261 proposal. None of the projects are related to magnetoelectric materials and sensors, except for the projects within the CRC1261.

3.7 Project funding

3.7.1 Previous funding

Funding of this project within the Collaborative Research Centre started in 07/2016.

3.7.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral Re-researcher, 100 %	2	68.40	2	136.80	2	136.80	2	136.80	2	68.0
Total		68.40		136.80		136.80		136.80		68.40
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables	20.00		20.00		16.00		16.00		8.00	
Total	20.00		20.00		16.00		16.00		8.00	
Instrumentation	Sum		Sum		Sum		Sum		Sum	

Instrumentation up to k€ 50	0	0	0	0	0
Total	0	0	0	0	0
Grand total	86.30	152.60	148.60	148.60	74.30

(All figures in k€)

3.7.3 Requested funding for staff for the new funding period

	Se- quen- tial no.	Name, academic degree, position	Field of research	Department of university	Project com- mitment (h/week)	Catego- ry	Funding source
Existing staff							
Research staff	1.	Faupel, Franz, Prof. Dr. rer. nat., Professor	Functional materials	IMS	4		Core support
	2.	Selhuber-Unkel, Christine, Prof. Dr. rer. nat., Professor	Biomateri- als	IMS	4		Core support
Non-research staff	3.	Lieb, Manuela, Dipl.-Ing. Techni- cian		IMS	4		Core support
	4.	Rehders, Stefan, Dipl.-Ing. (FH), Lab Engineer		IMS	4		Core support
	5.	Sommer, Peter, Dipl.-Inf. IT Technician		IMS	2		Core support
Requested staff							
Research staff	6.	N.N., doctoral researcher	Composite Materials	IMS		E13	
	7.	N.N., doctoral researcher	Biomateri- als	IMS		E13	

Job description of staff (supported through available funds):

1. Prof. Dr. rer. nat. Franz Faupel will be responsible for the coordination and the scientific management of that part of **B7** which deals with magnetic particle mapping, the characterization of the magnetic particle markers, and the sensor electronics. He will represent together with Prof. Selhuber-Unkel the project within the CRC and externally. He advises the scientific staff participating in the project and in planning and executing the tasks within the project (mainly WP1, WP4, WP5, WP6, and WP8).
2. Prof. Dr. rer. nat. Christine Selhuber-Unkel will be responsible for the coordination and the scientific management of that part of **B7** which deals with the fabrication, chemical modification and biological application of biomaterial scaffolds as well as with the magnetic detection of cells in the scaffolds. She will represent together with Prof. Faupel the project within the CRC and externally. She will advise the scientific staff participating in the project and in planning and executing the tasks within the project (mainly WP2, WP3, WP7, and WP8).
3. Dipl.-Ing. Manuela Lieb will support the doctoral researcher in the Selhuber-Unkel group in all issues regarding cell culture, chemicals, and lab maintenance.
4. Dipl.-Ing. (FH) Stefan Rehders will help with the design and construction of the MPM scanner.
5. Dipl.-Inf. Peter Sommer will give IT support by computer configurations.

Job description of staff (requested):

6. In the first year Ron-Marco Friedrich and later N.N. will work on WP1, WP4, WP5, WP6, and WP 8 as indicated in the work plan on the development of the MPM technique, including the characterization of the magnetic particles and their suitability for MPM, improving the electronics, enhancements for the solution of the inverse problems, and measurements on real 3D cell scaffolds labelled with magnetic particles.
7. N.N. will be responsible for research on MSPM, magnetorelaxometry, biomaterial scaffolds and cell detection in the scaffolds. The doctoral researcher will work on WP2, WP3, WP7, and WP8.

3.7.4 Requested funding for direct costs for the new funding period

(All figures in k€)	2020/2	2021	2022	2023	2024/1
IMS: existing funds from core support	2.50	5.00	5.00	5.00	2.50
Sum of existing funds	2.50	5.00	5.00	5.00	2.50
Sum of requested funds	20.00	20.00	16.00	16.00	8.00

Equipment up to k€ 10, software, consumables for financial year 2020/2

Non FDA approved biocompatible magnetic particles (e.g. from Chemicell)	k€	1.00
Biolab consumables (e.g. cell lines, cell medium, buffers, cell culture dishes)	k€	3.50
Polymers for aero-polymer fabrication (e.g. silicones)	k€	2.00
Proteins and peptides for scaffold coating (e.g. collagen, fibronectin, RGD)	k€	2.00
Hydrogels for scaffold fabrication (e.g. inks for 3D printer, proteins)	k€	5.00
Cleanroom costs (photolithography for simple structure scaffolds)	k€	2.00
AFM cantilevers for measuring the mechanical properties of the scaffolds	k€	2.00
Mechanical and electrical parts for 3D-MPM setup (e.g. power supply, capacitors, coils)	k€	2.50

Equipment up to k€ 10, software, consumables for financial year 2021

FDA approved magnetic particles (e.g. Resovist, Gadolinium)	k€	2.00
Biolab consumables (e.g. cell lines, cell medium, buffers, cell culture dishes)	k€	3.00
Polymers for aero-polymer fabrication (e.g. silicones)	k€	2.00
Proteins and peptides for scaffold coating (e.g. collagen, fibronectin, RGD)	k€	2.00
Hydrogels for scaffold fabrication (e.g. inks for 3D printer, proteins)	k€	5.00
Cleanroom costs (photolithography for simple structure scaffolds)	k€	2.00
AFM cantilevers for measuring the mechanical properties of the scaffolds	k€	2.00
Materials for electrical and magnetic shielding (e.g. Mu-metal, Cu plates, special cables)	k€	2.00

Equipment up to k€ 10, software, consumables for financial year 2022

FDA approved magnetic particles (e.g. Resovist, Gadolinium)	k€	2.00
Biolab consumables (cell medium, buffers, cell culture dishes)	k€	2.50
Consumables for the biological characterization of the scaffolds (dyes, antibodies, PCR kits)	k€	3.00
Polymers for aero-polymer fabrication (e.g. silicones)	k€	1.00
Proteins and peptides for scaffold coating (e.g. collagen, fibronectin, RGD)	k€	2.00
Hydrogels for scaffold fabrication (e.g. inks for 3D printer, proteins)	k€	1.00
Cleanroom costs (photolithography for simple structured scaffolds)	k€	2.00
AFM cantilevers for measuring the mechanical properties of the scaffolds	k€	0.50
Mechanical and electrical parts for magnetorelaxometry setup (stepper motors, bearings, controller board, DC motors, aluminum profiles, power supply, coils)	k€	2.00

Equipment up to k€ 10, software, consumables for financial year 2023

FDA approved magnetic particles (e.g. Resovist, Gadolinium)	k€	2.00
Biolab consumables (cell medium, buffers, cell culture dishes, dyes)	k€	3.00
Consumables for the biological characterization of the scaffolds (dyes, antibodies, PCR kits)	k€	4.00
Polymers for aero-polymer fabrication (e.g. silicones)	k€	2.00
Peptides for scaffold coating (e.g. RGDs with different linker lengths)	k€	1.00
Hydrogels for scaffold fabrication (e.g. inks for 3D printer, proteins)	k€	2.00
AFM cantilevers for measuring the mechanical properties of the scaffolds	k€	0.50
Chemicals for scaffold fabrication and coating (chemicals, inks for 3D printer, proteins)	k€	1.50

Equipment up to k€ 10, software, consumables for financial year 2024/1

Various types of magnetic particles (e.g. from Chemicell, Resovist, Gadolinium)	k€	1.00
Biolab consumables (cell medium, buffers, cell culture dishes, dyes, antibodies)	k€	2.00
Consumables for the biological characterization of the scaffolds (dyes, antibodies, PCR Kits)	k€	3.00
Polymers for aero-polymer fabrication (e.g. silicones)	k€	1.00
Peptides for scaffold coating (e.g. RGDs with different linker lengths)	k€	1.00

3.1 General information about Project B9(N)

3.1.1 Project title: Magnetoelectric Sensors for Movement Detection and Analysis

3.1.2 Research areas:

206-08 Clinical Neurosciences I - Neurology, Neurosurgery, Neuroradiology,
408-02 Communications, High-Frequency and Network Technology, Theoretical Electrical Engineering

3.1.3 Project leaders

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09.09.1971, Austrian

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Do any of the above mentioned persons hold fixed-term positions? No

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	yes
	A copy of the required approval of the responsible ethics committee is included with the proposal.	yes
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

Neurological diseases associated with pathological movements (NDPMs) such as Parkinson's disease, stroke, and multiple sclerosis affect millions of people worldwide. The evaluation of these diseases is typically performed by medical professionals in a clinic or doctor's practice using qualitative or, at best, semi-quantitative approaches.

Two quantitative movement assessment techniques have already found their way into clinical research and, at least with pilot systems, into clinical management: complex stationary lab assessments and inertial measurement units (IMUs). Complex stationary lab assessments are extremely accurate and allow detailed, time-synchronized, comprehensive analyses of movement patterns. Disadvantages are high cost and relatively inflexible and time-consuming assessments. In contrast, IMUs, most often based on acceleration assessment with accelerometry and angular measurement with gyroscopes, have the advantage of flexible application. Disadvantages are data synchronization difficulties and time-related signal drift. Moreover, these techniques do not provide a comprehensive picture of body movements, neither in a global coordinate system nor in relation to a specific part of the body, e.g. the lower back.

We propose here an entirely novel movement detection strategy based on magnetoelectric (ME) sensors (combined with IMUs) that has the potential to combine almost all advantages of the movement detection techniques currently in use (e.g. flexible use, relatively cheap, unobtrusive, exact, and objective), while overcoming most of the respective disadvantages (e.g. not bound to a specific environment). This system will

substantially add to our general understanding of physiological and pathological human movement under supervised and unsupervised conditions. It will eventually add to the quality of treatment evaluation of NDPMs (significant reduction of drift, improved localization performance).

3.3 Research rationale

3.3.1 Current state of research and preliminary work

1.3.1.1 Neurological diseases associated with pathological movements (NDPMs)

Neurological diseases associated with pathological movements (NDPMs) are clinical syndromes resulting from deficits of the central and peripheral nervous systems. Examples are Parkinson's disease (PD), stroke, and multiple sclerosis (MS). Pathological movements can include hyperkinetic (excess of movements; e.g. chorea, myoclonus, tremor, akathisia, and dyskinesia) and hypokinetic elements (reduction of velocity and extent, and rarity of movements; e.g. bradykinesia and hypokinesia). The prevalence of NDPMs in women and men aged 50-89 years in the general population is 28%, sharply increasing with age [We05], and close to 100% in NDPMs.

1.3.1.2 Quantitative assessment of neurological disorders

To quantitatively collect, analyse, and deliver complementary movement data to the clinical information, a large number of quantitative movement assessment tools have been developed in the last two decades to allow accurate and objective assessment of movement patterns in NDPMs [B9-1, B9-2, Au15, Ci16]. Measures obtained from quantitative movement assessment tools can (i) support supervised assessment in the clinic and laboratory, where outcome measures mainly reflect **functional capacity** ("How well can you perform?"), and (ii) can easily be used under unsupervised conditions in ecologically natural environments where the outcome measures reflect mainly **functional activity** ("How do you usually perform?"). Based on very recent literature, functional capacity and functional activity movement data provide – at least partly – complementary information [B9-1, Lu16, Hi19].

Functional capacity assessment for movement is mainly performed with stationary equipment such as multi-camera systems, instrumented walkways, and treadmills. Disadvantages of this stationary equipment are relatively high costs and time-consuming assessments, as well as data capture issues (e.g. data loss due to occluded markers and limited overall space volume to assess). Moreover, the systems are bound to explicit locations and often have specific requirements for the space where they operate.

Accelerometers and gyroscopes (i.e. inertial measurement units, IMUs) are currently the most regularly used mobile health technologies [B9-2, B9-3]. Accelerometers measure linear acceleration; gyroscopes measure angular velocity. These different types of sensors are often combined within one device and are relatively low-cost, lightweight, and easy-to-use instruments. A vastly and dynamically increasing number of studies indicate the usefulness of such devices for the assessment of functional activity aspects in the home environment of healthy people and patients with NDPMs [B9-1, B9-2, El17, Sh14].

1.3.1.3 Motivation for magnetoelectric (ME) sensor-based movement analysis studies

The accelerometers and gyroscopes currently used still have some disadvantages, such as an offset error, i.e. an intrinsic signal drift that has to be addressed with complex digital signal post-processing approaches. This proves to be problematic when, e.g., raw acceleration signals are integrated to velocity (1st integral) and even more to position (2nd integral) [Ri16]. Moreover, communication between the sensors depends on complicated techniques and a 100% synchronization status is difficult [Ol10]. Eventually, this technique has clear limitations concerning the provision of local and global individual movement patterns, i.e., they cannot provide information about the relative movement of one part of the body (e.g. the feet) in relation to another part (e.g. the lower back [Br19]). Therefore, it makes sense to explore alternative options for measuring movements in patients with NDPMs.

Due to specific characteristics, ME sensor-based movement detection systems have the potential to complement the currently used ambulatory movement detection techniques. Compared to stationary movement detection systems, ME sensor-based movement detection systems can be non-stationary and, therefore, not be limited to specific laboratories and environments. This reduces data capturing issues and can improve system usability. Compared to the IMUs, ME-based systems can produce 100% synchronized data and no drift occurs that compromises data quality. Signal-to-noise ratio of the ME sensors is high because they measure an individual and specific high-frequency magnetic field sent from the respective coils. Due to the cantilever structure, the ME sensors proposed for the current project are resonant at distinct frequencies. For example, a 3mm-by-1mm sensor has its second resonance at approximately 50 kHz (for a thickness of about 25 μm). This high frequency leads to extreme robustness with respect to disturbing magnetic fields, such as the earth's magnetic field as well as acoustic distortions. Further advantages are the small size of the ME sensors (Fig. B9-3), a



cost-effective micro-electro-mechanical systems (MEMS) fabrication production and low operating costs.

Figure B9-1: A piece of clothing (here presented as a jacket on the left) will be equipped with electric coils (green buttons) located at positions of the body relevant for movement detection (forearms, upper arms, shoulders, upper and lower back, thighs, lower legs; see also work package 1 and 2). These coils (the "transmitter") will send individual magnetic signals (e.g. separable in time and/or frequency, or code-based separation) to ME sensors (the "receivers") which will be positioned at the trunk and operate in resonance. A hardware box for sensor readout and excitation of coils and ME sensors will be positioned at the lower back. On the right, a first prototype of such a jacket with two coils and two ME sensors is shown. In addition, inertial measurement units (IMUs) and reflecting units for a multi-camera system for gold standard assessment will be added.

It is thus proposed to develop garment equipped with ME and IMU sensors (Fig. 9-1). The idea is to design within this CRC phase (2020 – 2024) a mobile movement detection system consisting of multiple ME and IMU sensors embedded into garments (i.e., a jacket and trousers). This system will then be investigated with regard to clinical feasibility, acceptability, and usefulness in cohorts of older adults and NDPM patients. Moreover, it will be validated against data obtained from a validated, state-of-the-art synchronized multi-camera system in a motion lab, which is the current gold standard in human movement research. Tab. B9-1 summarizes the pros and cons of current ambulatory systems (IMU- and magnetometer-based) as well as systems based on ME sensors.

Table B9-1: Advantages and disadvantages of IMUs, magnetometers, and ME sensors.

	Accelerometers/Gyroscopes	Magnetometers	ME Sensors
Advantages	Already established for movement measurements	Allow for solving horizontal plane non-uniqueness	Very robust and sensitive at resonance frequency (e.g. at around 7 or 50 kHz)
Disadvantages	- Offset error - Synchronization difficult	Often disturbed by DC magnetic fields	- Not established yet - Requires energy for coils

Research on magnetoelectric sensors

Within the CRCs 855 (2010 – 2014) and 1261 (2016 – 2020) several types of ME sensors were and are investigated and great progress has been achieved in recent years in terms of sensitivity and limit of detection (LOD) improvement. The most relevant sensor principles for this research project are cantilever-based sensor structures with magnetostrictive and piezoelectric layers. An ME sensor as shown in Fig. B9-2A and B is already available [Za15] and will be considered for the proposed project. It is based on a polysilicon cantilever, where the top is coated with piezoelectric material (AlN) and the bottom with magnetostrictive material (FeCoSiB). This electromechanical resonator is utilized as a magnetic field sensor because it uses the mechanical coupling between magnetostrictive material and a piezoelectric material in a resonant structure. A change in the external magnetic field strength causes a strain in the magnetostrictive component which is then mechanically transferred to the piezoelectric component. Hereby, the resulting electrical signal from the piezoelectric material is proportional to the primary magnetic field change. The existing first resonance frequency (see Fig. B9-2C) of an ME sensor (typically in the range of 800 Hz to 8 kHz) can be adjusted by the thickness and dimension of the substrate. The small dimensions of an ME sensor, including the clamping printed circuit board (PCB, Fig. B9-2B), is especially advantageous for this project because it can be included in a very small housing and reach a sensitivity that is sufficient for the proposed project (Fig. B9-4).

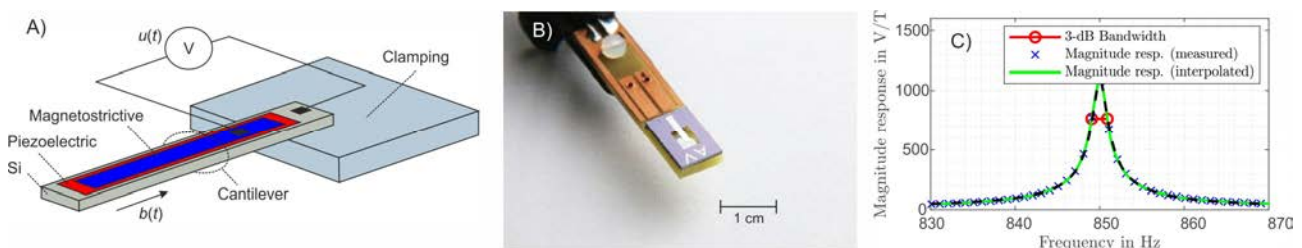


Figure B9-2: A) Typical layout of a magnetoelectric (ME) sensor. B) ME sensor as currently used in the CRC 1261. C) Resonance curve of a typical ME sensor (width: 2.2 mm, length: 25.2 mm).

In contrast to competing sensor principles that are suitable for magnetic signal amplitudes in the pT range such as SQUIDS [Kö16] or optically pumped magnetometers [Bo17], ME sensors can operate both at room temperature (i.e. without cooling) and in “normal”, unshielded environments. Currently, the ME sensor principle achieves LODs in the low pT/Hz^{1/2}-range at low frequencies (e.g. 30 pT/Hz^{1/2} at 10 Hz, see A7), but at several resonance frequencies (the “modes” of the cantilever), sensitivities are higher. LODs of about 1 pT/Hz^{1/2} and below were recently measured [Rö15, Ya16]. However, these resonances appear at approximately 7 kHz for the first mode and approximately 50 kHz for the second mode (note that such values can vary, depending on, e.g., the cantilevers’ geometry and thickness). These resonances are too high for most medical applications but are actually an advantage for movement analysis as shown below.

ME sensor positioned on jackets and trousers will not only measure the signal of interest but will create disturbances (artefacts) during movements due to acceleration of the cantilever. However, this will not lead to saturation effects due to their large dynamical range. Furthermore, such disturbances are usually low-frequency-dominated (below 100 Hz). In addition, ME sensors can detect acoustic signals, which must be considered a further disturbance for the actual setting and system proposed here. Acoustic signals typically occur within the range of 10 Hz to 20 kHz. If we use a signal transmission frequency in the range of the second mode (e.g. about 50 kHz), acoustic signals will only marginally influence the transmission from the coils (the “transmitters”) to the receiving ME sensors.

Preliminary work within the field and in own lab

We are not aware of any study that reports about movement detection using the proposed approach. In our own pilot experiments, movement data have been successfully recorded by use of ME sensors and coils mounted on a jacket. A change of the magnetic field was achieved by moving a coil (green buttons in Fig. B9-1, Fig. B9-3) that was mounted on the jacket depicted on the right of Fig. B9-1 and worn by a person while walking.



Figure B9-3: Electric coil designed as a small button, which can be easily sewn to garment.

The coil generated a sine signal at a frequency of approximately 800 Hz (Fig. B9-4), which is the resonance frequency of an ME sensor with

a size of 3 mm by 20 mm (first mode). Since this experiment was performed with only one coil, no signature signal was applied here. The magnetic field created was several orders of magnitude higher than a “biological” human signal. In more detail, a coil was worn at the wrist, and we applied a sinusoidal current of about 10 mA (RMS) and a constant frequency of 775 Hz (Fig. B9-4), which leads to an amplitude at the sensor of about 500 pT. The magnetic signals could be easily recorded with a sensor located at the trunk (red squares in Fig. B9-1). We thus conclude that the current above is sufficient to generate a recognizable magnetic field in a normal unshielded environment, without being saturated by disturbing magnetic fields such as the earth’s magnetic field or fields created by power supplies or loudspeakers.

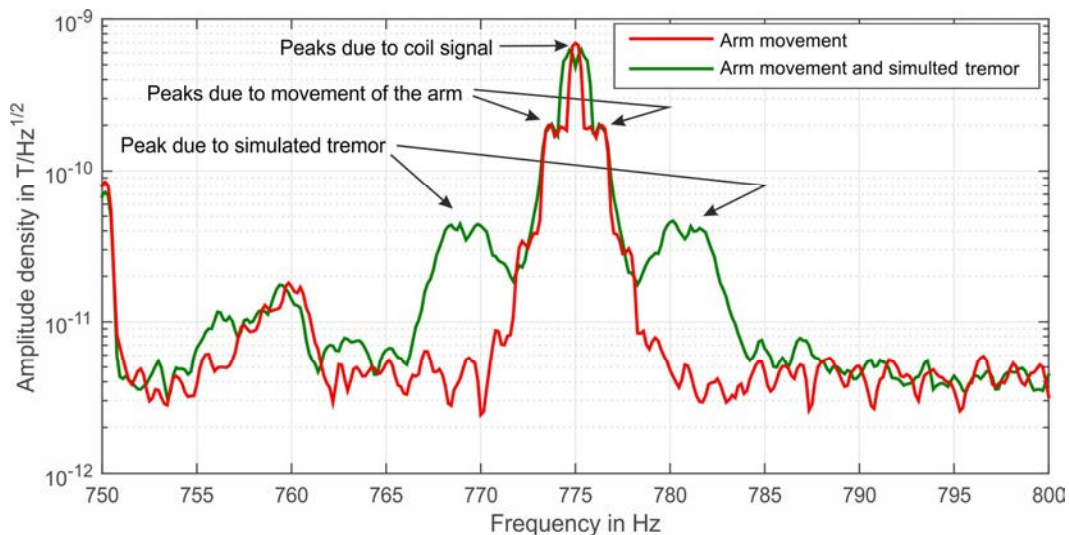


Figure B9-4: Power spectral densities of physiological movement (arm swing with approximately 1 Hz frequency) without imitating tremor by shaking of hands and forearms (red line) and with this “pathological” movement performed with approximately 7 Hz frequency (green line). Both arm swing and shaking the hands plus forearms are visible as distinct amplitude modulations (“deviations”) from the mean frequency of the coil (775 Hz) in the upper and lower direction.

References

- [Au15] K. Austen, What could derail the wearables revolution? *Nat. News* 525 **22**, (2015)
- [Be18] F. P. Bernhard, J. Sartor, K. Bettecken, M. A. Hobert, C. Arnold, Y. G. Weber, S. Poli, N. G. Margraf, C. Schlenstedt, C. Hansen, W. Maetzler, Wearables for gait and balance assessment in the neurological ward - study design and first results of a prospective cross-sectional feasibility study with 384 inpatients. *BMC Neurol.* **18**(1):114, (2018).
- [Bo17] E. Boto, S. S. Meyer, V. Shah, O. Alem, S. Knappe, P. Kruger, T. M. Fromhold, M. Lim, P. M. Glover, P. G. Morris, R. Bowtell, G. R. Barnes, M. J. Brookes, A new generation of magnetoencephalography: Room temperature measurements using optically-pumped magnetometers. *Neuroimage* **149**, 404–414 (2017).
- [Br19] S. M. Brice, E. J. Phillips, E. L. Millett, A. Hunter, B. Pilippa, Comparing inertial measurement units and marker-based biomechanical models during dynamic rotation of the torso. *European Journal of Sport Science*, 1-9 (2019).
- [Ci16] A. Cifu, V. Prasad, Wearables, Smartphones and Novel Anticoagulants: We Will Treat More Atrial Fibrillation, but Will Patients Be Better Off? *J. Gen. Intern. Med.* **31**, 1367–1368 (2016).
- [CI16] T. W. Cleworth, M. G. Carpenter, Postural threat influences conscious perception of postural sway. *Neurosci. Lett.* **620**, 127–131 (2016).
- [De03] F. Debaere, N. Wenderoth, S. Snaert, P. Van Hecke, S. P. Swinnen, Internal vs external generation of movements: differential neural pathways involved in bimanual coordination performed in the presence or absence of augmented visual feedback. *Neuroimage* **19**, 764–76 (2003).
- [El17] M. El-Gohary, D. Peterson, G. Gera, F. B. Horak, J. M. Huisinga, Validity of the Instrumented Push and Release Test to Quantify Postural Responses in Persons With Multiple Sclerosis. *Arch. Phys. Med. Rehabil.* **98**, 1325–1331 (2017).
- [Fi16] M. Filippi, M. A. Rocca, O. Ciccarelli, N. De Stefano, N. Evangelou, L. Kappos, A. Rovira, J. Sastre-Garriga, M. Tintorè, J. L. Frederiksen, C. Gasperini, J. Palace, D. S. Reich, B. Banwell, X. Montalban, F. Barkhof, MRI criteria for the diagnosis of multiple sclerosis: MAGNIMS consensus guidelines. *Lancet Neurol.* **15**, 292-303 (2016).

- [Go08] C. G. Goetz, B. C. Tilley, S. R. Shaftman, G. T. Stebbins, S. Fahn, P. Martinez-Martin, W. Poewe, C. Sampaio, M. B. Stern, R. Dodel, B. Dubois, R. Holloway, J. Jankovic, J. Kulisevsky, A. E. Lang, A. Lees, S. Leurgans, P. A. LeWitt, D. Nyenhuis, C. W. Olanow, O. Rascol, A. Schrag, J. A. Teresi, J. J. van Hilten, N. LaPelle, Movement Disorder Society-sponsored revision of the Unified Parkinson's Disease Rating Scale (MDS-UPDRS): scale presentation and clinimetric testing results. *Mov Disord* **23**, 2129–2170 (2008).
- [Hi10] I. Hillel, E. Gazit, A. Nieuwboer, L. Avanzino, L. Rochester, A. Cereatti, U. D. Croce, M. O. Rikkert, B. R. Bloem, E. Pelosin, S. Del Din, P. Ginis, N. Giladi, A. Mirelman, J. M. Hausdorff, Is every-day walking in older adults more analogous to dual-task walking or to usual walking? Elucidating the gaps between gait performance in the lab and during 24/7 monitoring. *Eur Rev Aging Phys Act.* **16:6**, eCollection (2019).
- [Kö16] R. Körber, J.-H. Storm, H. Seton, J. P. Mäkelä, R. Paetau, L. Parkkonen, C. Pfeiffer, B. Riaz, J. F. Schneiderman, H. Dong, S. Hwang, L. You, B. Inglis, J. Clarke, M. A. Espy, R. J. Ilmoniemi, P. E. Magnelind, A. N. Matlashov, J. O. Nieminen, P. L. Volegov, K. C. J. Zevenhoven, N. Höfner, M. Burghoff, K. Enpuku, S. Y. Yang, J.-J. Chieh, J. Knuutila, P. Laine, J. Nenonen, SQUIDs in biomagnetism: a roadmap towards improved healthcare. *Supercond. Sci. Technol.* **29**, 113001 (2016).
- [Lu83] J. F. Kurtzke, Rating neurologic impairment in multiple sclerosis: an expanded disability status scale (EDSS). *Neurology* **33**, 1444–52 (1983).
- [Me02] B. C. Meyer, T. M. Hemmen, C. M.; Jackson, P. D. Lyden, Modified National Institutes of Health Stroke Scale for Use in Stroke Clinical Trials. *Stroke* **33**, (2002).
- [Ni17] A. Nieuwenhuys, R. R. Oudejans, Anxiety and performance: perceptual-motor behavior in high-pressure contexts. *Curr. Opin. Psychol.* (2017).
- [Ol10] E. Olson, A passive solution to the sensor synchronization problem. *IEEE/RSJ International Conference on Intelligent Robots and Systems*, 11689706 (2010).
- [Po17] W. Poewe, K. Seppi, C. M. Tanner, G. M. Halliday, P. Brundin, J. Volkmann, A.-E. Schrag, A. E. Lang, Parkinson disease. *Nat. Rev. Dis. Prim.* **3**, 17013 (2017).
- [Po15] R. B. Postuma, D. Berg, M. Stern, W. Poewe, C. W. Olanow, W. Oertel, J. Obeso, K. Marek, I. Litvan, A. E. Lang, G. Halliday, C. G. Goetz, T. Gasser, B. Dubois, P. Chan, B. R. Bloem, C. H. Adler, G. Deuschl, MDS clinical diagnostic criteria for Parkinson's disease. *Mov. Disord.* **30**, 1591–1601 (2015).
- [Ri16] L. Ricci, F. Taffoni, D. Formica, On the Orientation Error of IMU: Investigating Static and Dynamic Accuracy Targeting Human Motion. *PLoS ONE* **11(9)**, e0161940 (2016).
- [Rö15] V. Röbisch, E. Yarar, N. O. Urs, I. Teliban, R. Knöchel, J. McCord, E. Quandt, D. Meyners, Exchange biased magnetoelectric composites for magnetic field sensor application by frequency conversion. *J. Appl. Phys.* **117**, 17B513 (2015).
- [Sh14] P. B. Shull, W. Jirattigalachote, M. A. Hunt, M. R. Cutkosky, S. L. Delp, Quantified self and human movement: A review on the clinical impact of wearable sensing and feedback for gait analysis and intervention. *Gait Posture* **40**, 11–19 (2014).
- [Sh10] L. M. Shulman, A. L. Gruber-Baldini, K. E. Anderson, P. S. Fishman, S. G. Reich, W. J. Weiner, The clinically important difference on the unified Parkinson's disease rating scale. *Arch. Neurol.* **67**, 64–70 (2010).
- [Lu15] R. C. van Lummel, S. Walgaard, M. Pijnappels, P. J. M. Elders, J. Garcia-Aymerich, J. H. van Dieën, P. J. Beek, Physical Performance and Physical Activity in Older Adults: Associated but Separate Domains of Physical Function in Old Age. *PLoS One* **10**, e0144048 (2015).
- [We05] G. K. Wenning, S. Kiechl, K. Seppi, J. Müller, B. Högl, M. Saletu, G. Rungger, A. Gasperi, J. Willeit, W. Poewe, Prevalence of movement disorders in men and women aged 50–89 years (Bruneck Study cohort): a population-based study. *Lancet Neurol.* **4**, 815–820 (2005).
- [Wu11] T. Wu, L. Wang, M. Hallett, Y. Chen, K. Li, P. Chan, Effective connectivity of brain networks during self-initiated movement in Parkinson's disease. *Neuroimage* **55**, 204–215 (2011).
- [Ya16] E. Yarar, S. Salzer, V. Hrkac, A. Piorra, M. Höft, R. Knöchel, L. Kienle, E. Quandt, Inverse bilayer magnetoelectric thin film sensor. *Appl. Phys. Lett.* **109**, 22901 (2016).
- [Za15] S. Zabel, C. Kirchhof, E. Yarar, D. Meyners, E. Quandt, F. Faupel, Phase modulated magnetoelectric delta-E effect sensor for sub-nano tesla magnetic fields. *Appl. Phys. Lett.* **107**, 152402 (2015).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [B9-1] E. Warmerdam, J. M. Hausdorff, A. Atrsaie, Y. Zhou, A. Mirelman, K. Aminian, A. J. Espay, C. Hansen, L. J. W. Evers, A. Keller, C. Lamothe, A. Pilotto, L. Rochester, **G. Schmidt**, B. R. Bloem, **W. Maetzler**, Long-term unsupervised mobility assessment in movement disorders. *Lancet Neurol.* In press (2019).
- [B9-2] A. J. Espay, J. M. Hausdorff, Á. Sánchez-Ferro, J. Klucken, A. Merola, P. Bonato, S. Paul, F. B. Horak, J. A. Vizcarra, T. A. Mestre, R. Reilmann, A. Nieuwboer, E. R. Dorsey, L. Rochester, B. R. Bloem, **W. Maetzler**, A roadmap for implementation of patient-centered digital outcome measures in Parkinson's disease obtained using mobile health technologies. *Mov. Disord.* **34**, 657-63 (2019).
- [B9-3] S. Del Din, M. Elshehabi, B. Galna, M. A. Hobert, E. Warmerdam, U. Suenkel, K. Brockmann, F. Metzger, C. Hansen, D. Berg, L. Rochester, **W. Maetzler**, Gait analysis with wearables predicts conversion to Parkinson disease. *Ann. Neurol.* **86**, 357-67 (2019).
- [B9-4] M. H. Pham, E. Warmerdam, M. Elshehabi, C. Schlenstedt, L.-M. Bergeest, M. Heller, L. Haertner, J. J. Ferreira, D. Berg, **G. Schmidt**, C. Hansen, **W. Maetzler**, Validation of a Lower Back "Wearable"-Based Sit-to-Stand and Stand-to-Sit Algorithm for Patients with Parkinson's Disease and Older Adults in a Home-Like Environment. *Front. Neurol.* **9**, 652 (2018).
- [B9-5] M. H. Pham, M. Elshehabi, L. Haertner, S. Din, K. Srulijes, T. Heger, M. Synofzik, M. A. Hobert, G. S. Faber, C. Hansen, D. Salkovic, J. J. Ferreira, D. Berg, A. Sanchez-Ferro, J. H. van Dieën, C. Becker, L. Rochester, **G. Schmidt**, **W. Maetzler**, Validation of a Step Detection Algorithm during Straight Walking and Turning in Patients with Parkinson's Disease and Older Adults Using an Inertial Measurement Unit at the Lower Back. *Front. Neurol.* **8**, 457 (2017).
- [B9-6] J. M. T. van Uem, K. S. Maier, S. Hucker, O. Scheck, M. A. Hobert, A. T. Santos, Ø. Fagerbakke, F. Larsen, J. J. Ferreira, **W. Maetzler**, Twelve-week sensor assessment in Parkinson's disease: Impact on quality of life. *Mov. Disord.* **31**, 1337-8 (2016).
- [B9-7] J. Reermann, **G. Schmidt**, I. Teliban, S. Salzer, M. Höft, R. Knöchel, A. Piorra, E. Quandt, Adaptive Acoustic Noise Cancellation for Magnetolectric Sensors. *IEEE Sensors Journal* **10**, 5804–5812 (2016).
- [B9-8] P. Hayes, S. Salzer, J. Reermann, E. Yarar, V. Röbisch, A. Piorra, D. Meyners, M. Höft, R. Knöchel, **G. Schmidt**, E. Quandt, Electrically Modulated Magnetolectric Sensors. *Applied Physics Letters* **108**, (2016).
- [B9-9] J. Reermann, C. Bald, S. Salzer, P. Durdaut, A. Piorra, D. Meyners, E. Quandt, M. Höft, **G. Schmidt**, Comparison of Reference Sensors for Noise Cancellation of Magnetolectric Sensors. *IEEE Sensors* (2016).
- [B9-10] J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, F. Faupel, **G. Schmidt**, Adaptive Readout Schemes for Thin-Film Magnetolectric Sensors Based on the delta-E Effect. *IEEE Sensors Journal* **16**, 4891-4900 (2016).

3.4 Project plan

Objectives

The aim of this project is to develop, test, and validate an ambulatory ME- and IMU-based movement detection and analysis system in older adults and patients with three different NDPMs. Our working hypothesis is that the ME-based sensor system – due to its capability to precisely estimate distances between coils and ME sensors - can collect complementary information compared to pure IMU-based systems, and therefore with a combined system, more detailed and accurate information can be delivered to medical professionals and patients with the eventual aim of providing more effective disease management.

The following objectives of the project are defined, which will be completed at the end of the work packages listed (WP):

- Hardware development for the ME sensors/coils movement detection system (WP 1);
- Data collection for the development and training of the movement detection algorithms by simultaneous application of the ME sensor/coil movement detection system and a high-end IMU system to older adults and patients with NDPMs (WP 2); evaluation of the performance of both systems via a multi-camera based gold-standard (WP 2);

- Development of algorithms for common, everyday human movement patterns (overall activity, walking, postural transitions, turning, and fine motor movements such as tooth brushing) using ME sensor-derived data from WP 2 (WP 3);
- Validation of the novel ME-based algorithms in cohorts of older adults and NDPM patients, including sensitivity to change (treatment response) aspects and comparison with IMU-derived data (WP 4).

Proposed research methods

Among the various types of ME sensor principles investigated within the current CRC1261, we will focus on the cantilever-based approaches that will be read out in resonance. These sensors (the “receivers”) will be combined with coils (the “transmitters”). For feasibility reasons, we will include up to but no more than 12 ME sensor/coil combinations, which is comparable to a high-end IMU system. This ME sensor system will be embedded in a garment (jacket, Figure B9-1) with up to 8 ME sensor/coil combinations and trousers with up to 4 ME sensor/coil combinations. An existing Noraxon® IMU system consisting of 16 synchronized IMU devices communicating among each other will be applied to all study participants during all assessments. Sensors in the jacket and trousers will be connected via cables or, if technically feasible, with a short-range wireless link (e.g. Bluetooth). Four different cohorts will be tested and used for validation of the algorithms derived from the above-mentioned systems: healthy older adults and patients with PD, stroke, and MS. Validation will be performed against the current gold standard in movement assessment, i.e. stationary optical multi-camera systems (Qualisys®, available in the movement analysis lab of the applicants). For cleaning of ME sensor data, statistical signal processing attempts for enhanced pre-processing (cleaning) will be applied. Afterwards, hypothesis-driven analysis methods as well as pattern recognition approaches for (i) detecting and (ii) describing defined movements will be used for the development of algorithms for the detection and description of aspects of common movements. An iterative optimization process addressing, e.g. data interference, and multichannel and power consumption issues, will be applied. Analysis of IMU-derived data will be done in parallel with already available and validated algorithms [e.g. B9-3, B9-6, B9-5]. The individual WPs are described in the following. Fig. B9-5 shows an overview of the ME-based movement recording equipment, including the planned detection and analysis approaches.

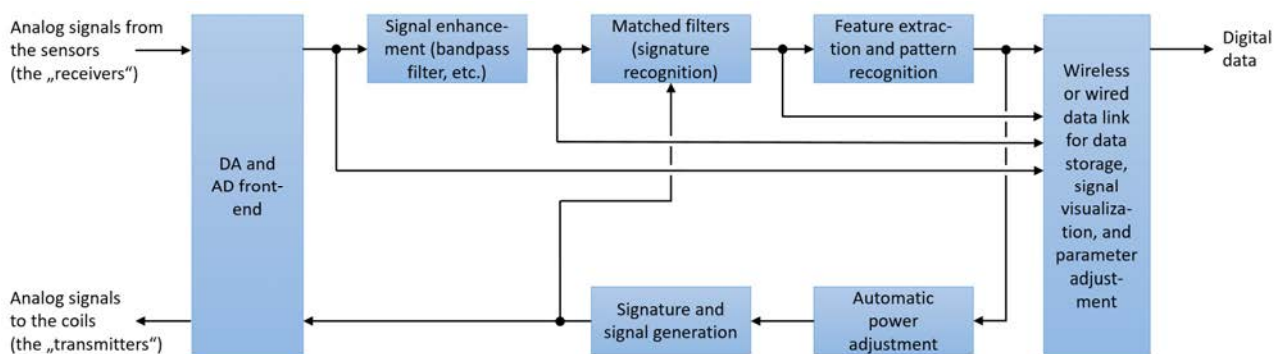


Figure B9-5: Overview of the structure and function of the proposed ME-based movement detection system, including the most relevant signal processing steps necessary for the testing and improvement of the hardware. AD: analogue-to-digital; DA: digital-to-analogue.

Work plan

In the following, the four work packages (WPs) are described in detail. All of them will be performed in close collaboration with the ME sensor systems for medical applications projects, such as **B10** and **T1**, with the signal processing projects **B1** and **B2**, and with the central projects **Z1** and **Z2** for sensor production and characterization. A time schedule for the work is provided in Tab. B9-2.

WP 1: Hardware development

WP 1A will cover the hardware development of the ME sensor-based movement detection system. The system will consist of up to 12 ME sensors (“receivers”) and 12 coils (“transmitters”, Fig. B9-2) that will be connected by small cables and will be excited by one or two central boxes positioned at the lower back (jacket and trousers). This approach will also allow the collection, synchronization, and pre-processing of all ME sensors. Each coil will be fed with a sinusoidal current at a frequency near the resonance frequency of the sensor (e.g.

7 kHz for the first mode or about 50 kHz for the second mode). Consequently, each coil will generate a small magnetic flux of about 1 nT peak amplitude at the sensor at greatest distance. Such amplitudes are far below the European rules for the exposure of electromagnetic fields (1999/519/EC). Note that the signal processing in terms of matched filters will allow obtaining reliable signals even below 0 dB signal-to-noise ratio. Movements of the coils relative to the ME sensors will induce a change of this magnetic flux that can be measured (for details see next paragraphs). Low-power processing hardware with advanced digital signal processing can be used afterwards to estimate relevant movement parameters.

Table B9-2: Work schedule

No	Work package	2020		2021				2022				2023	
		III	IV	I	II	III	IV	I	II	III	IV	I	II
WP 1	Hardware development												
	A: System development												
	B: System optimization												
WP 2	Data collection for algorithm development												
	Database, recruitment, and assessment												
WP 3	Algorithm development												
	A: Algorithm development / training												
	B: Graphical user interface												
WP 4	Algorithm validation												
	Recruitment and assessment												
	Analyses												

 Engineer PhD (100%)  Movement scientist (25%) and Clinician (25%)

A particular aim of this WP is to enable a *specific* detection of movement data coming from defined coils and collected with defined ME sensors. With this multichannel approach, a high spatial resolution of movements will be possible, perfectly complementing the given 100% time resolution of the data. Standard multiple access methods (e.g. frequency division multiple access (FDMA) / time division multiple access (TDMA) / code division multiple access (CDMA)) realized with so-called matched filters (optimal receivers in Gaussian noise) will be considered and compared.

The advantages of this principle are demonstrated with the simulation presented in Fig. B9-6. Two coils periodically emit a signature signal of 50 ms duration with a center frequency of 40 kHz and with a bandwidth of 600 Hz. Both signals are designed to be mutually orthogonal (CDMA principle). The distance between the first coil and the sensor are changed periodically with a frequency of 2 Hz, and, in parallel, between the second coil and the sensor with a frequency of 3 Hz. Afterwards, the sensor signal is filtered with two matched filters optimized to the respective signatures. The second and third diagram of Fig. B9-6 present the effective separation properties of this principle even at a signal-to-noise ratio of 0 dB. A further advantage of matched filters is that they help to compress all signal energy onto specific time points. This can be used to (further) improve the signal-to-noise ratio or, alternatively, to adjust the signal power provided for the transmitters (the coils).

If this new readout principle does not work adequately (e.g. due to too small frequency ranges available resulting from too high Q factors of the ME sensors), we will switch back to conventional readout schemes [B9-7, B9-8] by using, e.g., different carrier signals for the individual schemes. This might lead to decreased robustness of the signal separation and temporal compression performance. In this case, we will apply higher signal power and reduce the proposed number of sensors and coils. We are confident that even with this smaller set of transmitter-receiver pairs, clinically relevant movement detection and analysis will be possible because current literature suggests that even one body-worn sensor can provide clinically relevant information [B9-3, B9-6, B9-5].

WP 1B investigates possible cross-talk and interference between different transmitters and receivers depending on their distance or location. It is probable that a too close physical localization of two ME sensors leads to interaction effects and, consequently, to an increase in noise and artefacts. This aspect will be evaluated and controlled in detail with (i) different positions of the coils and sensors, (ii) with signal control (e.g. with automatic power adjustment of specific coils that are relevant for the actual movement) and (iii) with adaptive cancellation approaches [B9-8, B9-9, B9-10].

WP 2: Data collection for algorithm development and training

For the development of the algorithms, data will be collected from 5 healthy older adults and from patients with NDPMs (5 patients with PD, 5 with stroke, 5 with multiple sclerosis; note that larger numbers will be recruited for validation of the algorithms in WP 4). Participants will be recruited from the Department of Neurology, UKSH, Campus Kiel, and from the general population. The recruitment will be based on the review of recent medical records and on personal communications with the responsible physicians. An ethical approval for this task is already in place (D18/438). The database for collection of data and source for analyses, based on RedCap®, is finished and fulfills the current EU *General Data Protection Regulation (GDPR)*. We do not expect any issues related to recruitment and assessment: For PD, stroke and MS, the Neurology Department has per year more than 1000 patients each; the study can also be done with inpatients. Study participants will have to fulfill the following criteria:

- *all*: male or female, 40 – 85 years of age; able to: communicate well with the investigator, understand and comply with the requirements of the study, provide written informed consent to participate in the study, understand the right to withdraw their consent at any time without prejudice to future medical care, and require no walking aid;
- *PD*: Diagnosis according to [Po15], Hoehn & Yahr stage I-III (i.e. mild postural stability deficits are allowed), medication-associated fluctuations of mobility with ≥ 5 points change in the motor part of the Revised Unified PD rating scale (UPDRS, equals moderate clinically important difference [Sh10]);
- *Stroke*: Vascular event within the last 12 months or at least moderate subcortical arteriosclerotic encephalopathy based on Fazekas Scale, confirmed by imaging (cerebral computer tomography or magnetic resonance imaging), associated with clinically visible handicap and spasticity of at least one leg;
- *Multiple Sclerosis*: Diagnosis according to [Fi16]. Expanded Disability Status Scale (EDSS) 3.5 to 5.5 (walking affected but still able to walk without aid);
- *Healthy older adults*: exclusion of acute and chronic diseases that interfere with everyday mobility.

Participants will be equipped with the following three systems in parallel, which makes assessment in a research mobility laboratory necessary (available at UKSH, Campus Kiel):

- 16 reflexive markers for the assessment with the Qualisys® camera system (10-camera-system), worn on both wrists, both ankles, both dorsal feet, sternum, lower back;

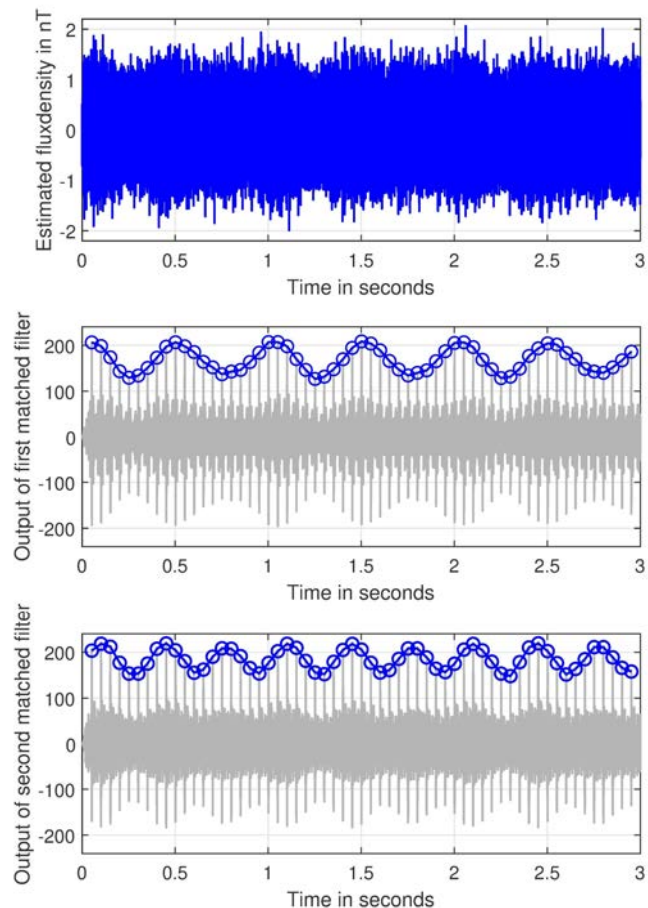


Figure B9-6: Simulation to show the benefits of the proposed readout scheme. The top diagram shows the signal received by an ME sensor being resonant at 40 kHz (third mode). This signal consists of two coil signals that were moved in distance with 2 Hz (first coil) and 3 Hz (second coil) plus measurement noise with a signal-to-noise ratio of about 0 dB. The second plot shows the same sensor signal but processed with a filter that was matched to the first signal signature. Sampling the signal at the signature rate (blue circles) leads to a very good recovery of the first sending signal. The third plot shows the same data, but now matched to the second coil signature.

- 16 conventional synchronized IMUs (Noraxon®), worn on both wrists, both ankles, both dorsal feet, sternum, lower back;
- ME-based movement detection garment (see WP 1).

The study protocol will be adapted to validation studies already performed in the frame of the EU projects SENSE-PARK (2011-2014, PI W. Maetzler [B9-4, B9-5, B9-6] and KEEP CONTROL (2017-2021, PI W. Maetzler). It will include a neurological examination (including the MDS-UPDRS part III as a measure of motor function that we have already successfully used in PD and in NDPMs in general [Be18]) and standardized and well-established tests for the assessment of functional performance and mobility. Examples are the Timed-up-and-Go test and the Short Physical Performance Battery. In addition, all participants will undergo a standardized daily activity-like assessment with procedures such as free walking, opening and closing doors, climbing stairs, transfers, brushing teeth, making coffee, drinking a cup of tea, ironing, sitting quietly, sitting and counting coins, and sleeping.

PD patients will be assessed twice to evaluate whether algorithms can detect responsiveness to treatment. They will first be assessed during their OFF phase (i.e. 12 hours after intake of the last medication) and then in medication ON phase (i.e. the situation when medication allows optimal mobility, this is normally the case 1-2 h after medication intake).

The entire assessment will be videotaped to allow an exact classification and interpretation of movements. The entire procedure will take about 2 hours (4 hours for PD patients with ON/OFF assessment). There is a small risk that the simultaneous application of all three systems may be too burdensome for some participants; in such cases, we will recruit a new participant to maintain the proposed group size.

WP 3: Algorithm development and training

WP 3A will cover the development and training of both hypothesis-driven and (semi-) unsupervised algorithms for the detection of three predefined movement patterns: (i) walking, (ii) fine motor movements such as tooth brushing, and (iii) transitions, turning, and overall daily activity with data obtained from the ME-based system as described in WP 2. We chose these movement patterns because they allow a stepwise “evolution” of algorithm development according to the complexity of the respective movements. Walking can be considered a kind of “2D” movement pattern (antero-posterior), tooth brushing as a “3D” movement pattern (including all 3 axes), and transitions, turning, and overall activity as irregular movement patterns. The algorithm development and training will consist of two parts: (i) identification of the movement pattern within a dataset consisting of a reasonable number of movement patterns performed during an everyday activity assessment (see WP 2), and (ii) the qualitative appraisal of the movement pattern (i.e. the definition of relevant parameters describing the quality / dysfunction of the movement). For the first part, specific movement features will be extracted from datasets obtained (i) from lab members wearing the system in the first development phase, and (ii) from older healthy adults and NDPM patients. The feature extraction will be performed in close collaboration between engineers, algorithm developers, movement scientists, and clinicians to ensure that the most feasible and useful features will serve as references and that a highly accurate movement classification can be achieved.

For the hypothesis-driven algorithm development, signal pattern evaluation methods already established in our lab [B9-3, B9-5, B9-6] will be applied. For the automatized classification process, Gaussian mixture models (GMMs) for approximating the multi-variate probability density functions of the individual features and/or neural networks combined with Hidden Markov Models (HMMs) to model the temporal behaviour and the transition probabilities of the individual actions will be used. During this phase, further adaptation of the signal control programming (automatic power adjustment, see WP 1) and possibly the hardware itself will be necessary, e.g. to increase signal-to-noise ratio. This adjustment does not put the project at relevant risk as we have experience with 2 ME sensor/coils pairs and have seen that useful data is extractable with excellent signal-to-noise ratio; however, it may be possible that the analysis of *all* 12 ME sensor/coil pairs may not be possible due to the above-mentioned reasons.

The second part of the algorithm development and training will be devoted to the qualitative evaluation of respective movements (e.g. determination of step frequency and variability) with comparison of the ME-sensor-derived algorithms against clinical scales and the optical camera system (see WP 2). The same process will then be performed with data obtained from the IMU system (Fig B9-7). Of note, we have already excluded an interaction effect between the IMU and the ME hardware (own unpublished results), i.e. these systems can be worn simultaneously by the same participant without interference effects.

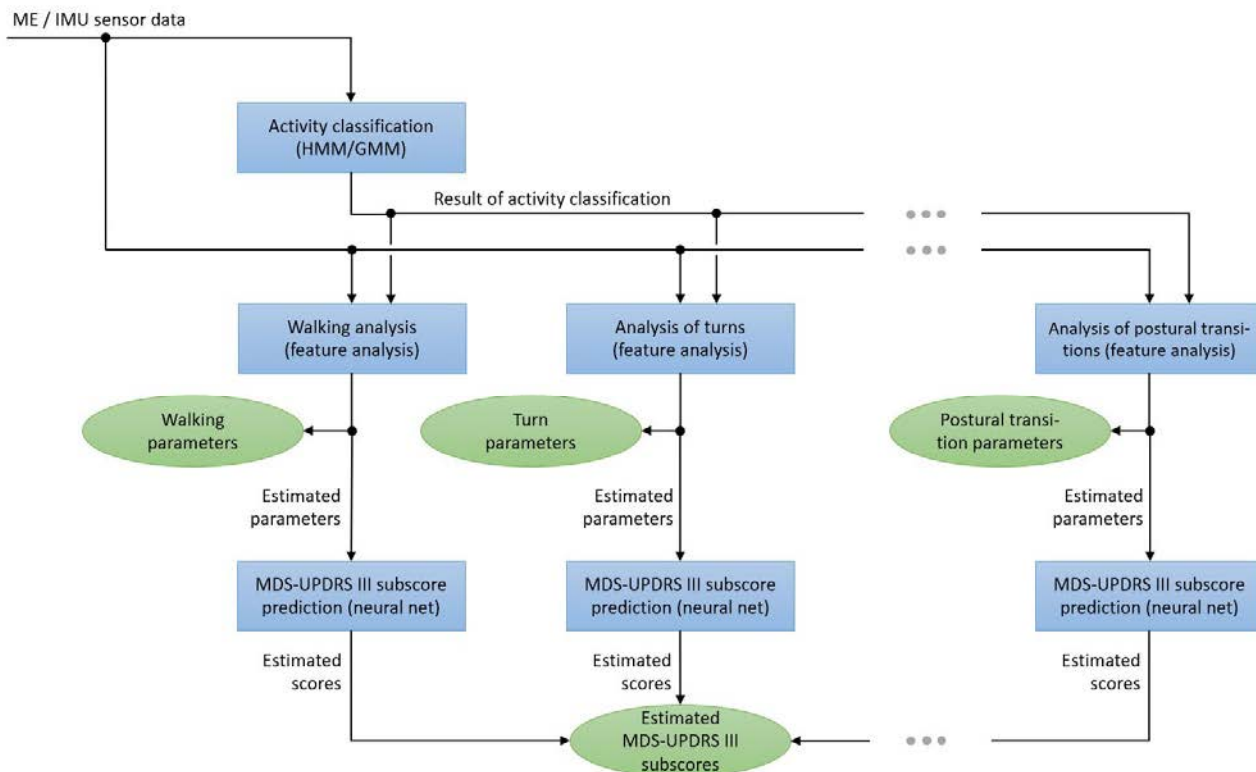


Figure B9-7: Work package 3: Proposed scheme for movement classification, based here on feature extraction and pattern recognition. The lower part of the figure presents the overall analysis plan of the extracted data (compare Fig. B9-5). GMM: Gaussian mixture model; HMM: Hidden-Markov model; MDS-UPDRS: Movement disorder society-revised version of the Unified Parkinson's disease Rating Scale.

WP 3B will cover the development of a real-time analysis approach. For this purpose, a graphical user interface (GUI) will be designed and implemented. Such a GUI will provide effective and comprehensive patterns in real time and facilitate the pattern classification. The aim is to present the acquired data in time-, frequency-, modulation-, and correlation-based graphs. The modulation-based approach has particularly high potential to present the complex data obtained from the freely moving magnetic fields of the coils during human movement in an understandable way.

We expect the new feature extraction methods, such as correlation- and modulation-based approaches (part of WP 3B), to outperform conventional methods (such as the short-term power of individual frequency ranges), especially if combined with deep learning methods (part of WP 3A) that can also be used partly without labelling the data (semi-supervised learning methods). However, if this new approach does not show the expected results, we will return to conventional movement analysis methods that are performed in the state-space domain using, e.g., Kalman filters with parameters optimized for dedicated movement patterns.

The eventual aim of WP 3 is the provision to WP 4 of algorithms for the detection and qualitative evaluation of walking, tooth brushing, turning, transitions, and overall activity based on data extracted from ME sensors/coils. WP 3 will also analyse IMU-derived data associated with ME-derived data, using already established algorithms [e.g. B9-3, B9-5, B9-6].

WP 4: Algorithm validation

WP 4A: For validation purposes, we will recruit 15 participants each from the above-mentioned four cohorts. We will apply the same inclusion and exclusion criteria to the study participants and assess them with the same movement detection systems as described in WP 2. An ethical approval for this task is already in place (D18/438). The database for collection of data and source for analyses, based on RedCap®, is also available and fulfills the actual EU *General Data Protection Regulation (GDPR)*. As soon as the cohorts are assessed and data are available for analyses, we will perform the following validation steps.

The ME sensor system, including the newly developed algorithms, will be considered valid with regard to detection / qualitative evaluation of a certain movement when the following requirements are fulfilled:

- **Detection** of specific mobility periods (e.g. detection of walking / transitions / turning / tooth brushing episodes; further episodes can be added during the project if applicable): sensitivity and specificity of ME-derived algorithms compared to optical camera system >0.8 ;
- **Correlation** of specific mobility parameters (e.g. stride time, stride length, gait variability, turning extent, mean and maximum turning velocity, repetitive movement during tooth brushing) compared to optical camera system: $r>0.7$;
- **Responsiveness to treatment**: Correct classification of ON / OFF phases of $\geq 12/15$ PD patients using the above-mentioned mobility parameters; differences of certain movement parameters >20 ;
- **Differential diagnosis**: Correct classification of cohorts using the above-mentioned mobility parameters (e.g. with cluster or discriminant and area under the receiver operating characteristic curve analyses), AUC >0.8 .

The same approach will then be applied to IMU-derived data analysed with the already available algorithms. Values will be compared with those derived from ME-sensors / algorithms, to compare accuracies of the respective systems and to detect and evaluate normal and everyday movement patterns. Special emphasis will be put on the evaluation of how technical assets and limitations of the respective systems influence validation outcomes (e.g. ME-sensor/coil system: + high resolution of movements relative to a certain point of the body, lack of drift; - uncertainty due to distance and orientation; IMUs system: + better absolute orientation, independent evaluation of one IMU possible; - data drift over time, no/low relative localisation resolution).

Prospects

We expect that the project will allow developing and validating a device for the detection and analysis of movements in humans with far-reaching consequences for movement detection and classification in general. After data collection and the generation and implementation of the first ME-based movement detection algorithms in healthy individuals and patients with NDPMs (PD, stroke, MS), which is the aim of the first phase of the proposed project, the second phase will be dedicated to the validation of these algorithms in these cohorts. The study protocol also allows the evaluation of the efficiency of the system with regard to responsivity to treatment, as PD patients will be evaluated under optimal treatment and lack thereof. The project, if successful, will open entirely novel avenues for accurate assessment of patients with movement disorders in the clinic / practice environment *and* the home environment where clinicians do not normally have access to any objective data. Further development into practical use of an ME-system, beyond the project proposed here, needs answers to the following questions:

- How can the system be evaluated and validated in real-life environments?
- Can the system provide real time feedback, e.g., for patients during specific training sessions through, e.g., a moving skeleton on a screen?
- Do ME sensors have useful potential in detecting muscle activity ("magnetomyography") and can this feed into clinical relevant assessment strategies?
- May permanent magnets (including specific coding; advantage would be no/very low energy consumption) instead of electricity-consuming coils may also be usable transmitters?
- What is the minimal / optimal number of ME / IMU sensors for specific and valid assessment of movement / movement deficits in the above cohorts?

We anticipate these as relevant questions for a potential third phase of the CRC. The eventual aim will be to develop a device for the individualized diagnosis and management of NDPMs and, potentially, also other age-related conditions associated with impaired movement based on quantitative clinical and home-acquired data. We will decide during the upcoming CRC phase whether the project should continue as a pure research or rather as a transfer project.

3.5 Role within the Collaborative Research Centre

Close cooperation is planned with the following partners:

Z1	This project is closely interlinked with the ME-sensor projects, especially those that operate in resonance. Such sensors are mainly produced in Z1 .
B1, Z2	B9 will benefit from B1 and Z2 adapting system frontends and small sensor arrays to the requirements of B9 . In turn, we will communicate test results back to B1/Z2 to facilitate the development of suitable measurement systems after transfer of mature sub-systems to Z2 .
B2, B10	The project will use the same real-time framework as projects B2 and B10 . Thus, all extensions made in either one of the projects will benefit the other and immediately speed up development.
B10, T1	All study participant management and data acquisition procedures will be shared with project B10 and T1 .
T1	T1 and B9 will recruit PD patients jointly and evaluate at least 2 patients together.

B9 participates in the focus group “Biomedical Applications”.

3.6 Differentiation from other funded projects of the project leader(s)

Walter Maetzler holds research grants from the European Union (Horizon 2020 Marie Skłodowska-Curie grant No 721577, ITN towards age-related gait and balance deficits; Horizon 2020 FAIR-PARK II, grant No 633190, NCT02655315, towards evaluation of an iron chelator in PD; Horizon 2020 IMI project Mobilise-D, grant No 820820 for the development of a Real World Walking algorithm derived from a lower back IMU, and Horizon 2020 IMI project IDEA-FAST (negotiation phase) for the evaluation of mobile health technologies for the detection of non-motor features of neurodegenerative and rheumatoid diseases), from BMBF (grant No 031L0188A, GUIDE-IBD, towards IMU-based assessment of inflammatory bowel disease in real life) and from Lundbeck (progression markers of PD). These projects include cross-sectional evaluation of healthy older adults as well as patients with PD IMUs. None of these funded projects use ME sensors for movement detection.

3.7 Project funding

3.7.1 Previous funding

This project is currently not funded and no funding proposal has been submitted to other funding bodies.

3.7.2 Requested funding

Funding for	2020 (2 nd half)		2021		2022		2023		2024 (1 st half)	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral candidate, 100%	1	34.2	1	68.4	1	68.4	1	68.4	1	34.2
Postdoc, 25%	1	8.9	1	17.8	1	17.8	1	17.8	1	8.9
Medical research associate, 25%	1	12.0	1	23.9	1	23.9	1	23.9	1	12.0
Total		55.1		110.1		110.1		110.1		55.1
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment (up to 10,000 Euro), software and consumables	8.0		10.0		9.0		9.0		4.0	
Total	8.0		10.0		9.0		9.0		4.0	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
None	0.0		0.0		0.0		0.0		0.0	
Total	0.0		0.0		0.0		0.0		0.0	
Grand total	63.1		120.1		119.1		119.1		59.1	

(All figures in k€)

3.7.3 Requested funding for staff

	Se- quen- tial no.	Name, academic degree, position	Field of research	Department of university or non-university institution	Project commit- ment in hours per week	Category	Funding source
Existing staff							
Research staff	1.	Maetzler, Walter, Prof. Dr. med., Pro- ject coordinator	Neurology	CAU / UKSH neuro	4		Core sup- port
	2.	Schmidt, Gerhard, Prof. Dr.-Ing.	System Theory	EIE	4		Core sup- port
	3.	Berg, Daniela, Prof. Dr. med.	Neurology	CAU / UKSH neuro	1		Core sup- port
	4.	Schlenstedt Chris- tian., Dr. rer. nat.	Neurology	CAU / UKSH neuro	4		Core sup- port
Non-re- search staff	5.	Kevin Prehn		EIE	3		Hardware core sup- port
Requested staff							
Research staff	6.	N.N., Doctoral Re- searcher	Neurology	EIE / UKSH neuro		Doctoral candidate	
	7.	Clint Hansen, Dr., Movement scientist	Neurology	CAU / UKSH neuro		Postdoc	
	8	Markus Hobert, Medical research assistant	Neurology	CAU / UKSH neuro		Medical re- search as- sociate	

Job descriptions of staff for the proposed funding period (supported through existing funds):

1. Prof. Dr. med. Walter Maetzler will be responsible for the coordination and scientific management of the research project B9. He will advise the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of actual data acquisition (placement of sensors in the ME device, typical characteristics of movements of interest as observed in healthy individuals and patients with NDPMs, support with design of hypothesis-driven algorithms), interpretation of results, ethics, study participant selection and recruitment as well as clinical evaluation. The state-of-the-art movement lab of the Neurology Department of the UKSH, Campus Kiel will be available for the assessment of the cohorts described in the proposal.
2. Prof. Dr.-Ing. Gerhard Schmidt will be responsible for the coordination and scientific management of the research project B9 in agreement with Walter Maetzler. He advises the scientific employee with respect to planning, execution, and evaluation of the tasks, in particular in matters of digital system design, pattern recognition approaches and involved signal processing applications. Moreover, the real-time framework available at the chair can be used for the project.
3. Prof. Dr. med. Daniela Berg will contribute to the feature extraction process and to the recruitment of participants for the prospective study.
4. Dr. phil. Christian Schlenstedt will provide support for the prospective validation study by introducing and maintaining the Neurology motion lab and will support respective data analysis.
5. Kevin Prehn will give support for development of the hardware and for programming the described classification algorithms.

Job descriptions of staff for the proposed funding period (requested funds):

6. N.N. (E13, engineer, 100%): This person will mainly handle the engineering and algorithm development tasks in this project as described in the work packages. This person will be jointly supervised by W. Maetzler und G. Schmidt and will have working places both at the Neurology Department and the Faculty of Engineering.
7. Dr. Clint Hansen (E13/6, 25%) is a movement scientist with a strong background in clinical evaluation of physiological and pathological movement patterns in young and old adults as well as in algorithm development. He will handle the scientific tasks concerned with movement pattern-related aspects of this project. Specifically, he will contribute 1) to the hardware development by adding practical information and input from a movement scientist's point of view (WP 1), 2) algorithm development for the ME-based data by providing movement science and clinically relevant information for the hypothesis-driven algorithms and for the feature extraction task (WP 2), and 3) validation process by supporting writing of the ethical proposal, recruitment, and investigation of study participants and data analysis.
8. Markus Hobert (TVÄ1/2, 25%) works currently as a resident at the Neurology Department, UKSH Campus Kiel and has extensive experience with the design and execution of movement-associated studies in healthy older adults and patients with NDPMs. He will primarily be responsible for the clinical input during the development of the ME-based movement detection system, for bringing in clinical aspects of movement analysis (WP 2), and for the recruitment and clinical investigation of the study participants as described in WP 3.

3.7.4 Requested funding of direct costs

	2020/2	2021	2022	2023	2024/1
Existing funds	1.5	3.0	3.0	3.0	1.5
Sum of requested funds	8.0	10.0	9.0	9.0	4.0

(All figures in k€)

Available funds will be used for the acquisition of (i) garments and associated material (textile, button tapes, subtasks for the adaptation of the clothing), (ii) the portable hardware for sensor readout and excitation, (iii) the small mechanical parts, electrical circuits, cables, shielding and damping material, (iv) the clinical database, and (v) material for / execution of the prospective studies. The remaining funds will be used for the manufacturing of mechanical components required for the ME-based movement detection system and for publication costs. In total this will require about 40 000 Euros (12 000 Euros paid by the university).

Equipment up to k€ 10, software, consumables for 2020 (2 quarters)

Portable readout hardware, electronic consumables, small appliances, and support materials	k€	4.0
Clothing, including adaptation and subtasks	k€	2.0
Installation and maintenance of the clinical database	k€	2.0

Equipment up to k€ 10, software, consumables for 2021

Electronic consumables, small appliances, and support materials	k€	6.5
Consumables for the setup of the prospective clinical study	k€	3.5

Equipment up to k€ 10, software, consumables for 2022

Electronic consumables, small appliances, and support materials	k€	4.0
Consumables for the prospective clinical study	k€	5.0

Equipment up to k€ 10, software, consumables for 2023

Electronic consumables, small appliances, and support materials	k€	4.5
Consumables for the prospective clinical study	k€	4.5

Equipment up to k€ 10, software, consumables for 2024 (2 quarters)

Electronic consumables, small appliances, and support materials, publication costs	k€	4.0

3.7.5 Requested funding for instrumentation

none

3.1 General information about Project B10(N)

3.1.1 Project title: Magnetolectric Sensors for Localization of Cardiac Arrhythmias

3.1.2 Research area(s):

407-06 Ingenieurwissenschaften: Systemtechnik: Biomedizinische Systemtechnik,
205-12 Lebenswissenschaften: Medizin: Kardiologie, Angiologie

3.1.3 Project leader(s)

Frey, Norbert, Prof. Dr. med.
15.10.1966

Schmidt, Gerhard, Prof. Dr.-Ing.
23.11.1971

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Do any of the above mentioned persons hold fixed-term positions? no

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	yes
	a copy of the required approval of the responsible ethics committee is included with the proposal.	No, application is in progress
2.	clinical trials.	yes
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

Current standard electrocardiography is a useful and easily applicable method that has been in clinical use for more than hundred years. However, it is hampered by low spatial resolution. Thus, precise electro-anatomical mapping of arrhythmias still has to be conducted by invasive catheterization. The main long-term objective of this project is to answer the question whether invasive mapping of arrhythmic substrates (current standard) can be replaced by a non-invasive alternative, namely analyses using signals obtained from ME sensors combined with electric measurements.

We will thus investigate if a multi-channel combined ECG/MCG (electrocardiogram/magnetocardiogram) approach allows for reliable non-invasive localization of the origin of cardiac arrhythmias. This is becoming even more important, as recently stereotactic body radiation therapy was successfully applied for ablation of ventricular tachycardia, promising a completely non-invasive way to cure arrhythmias in the future.

To perform the required measurements with a multitude of magnetic (both ME sensors originating from this CRC [B10-3, B10-6] and already established systems) as well as electric sensors, individual real-time signal-to-noise ratio estimations of all involved sensors will be investigated that permit optimal sensor placement, sensor signal combination, and parameter extraction. An appropriate automatic signal quality analysis should guarantee a minimum recording time for patients. To answer these research questions, forward modelling and

a solution of the inverse problem is necessary. Here the results of the former CRC project **B3** will be used and further extended. To evaluate the accuracy and clinical utility of this approach, we plan to compare it with results from electrophysiological studies (current standard) in 3 different groups of patients: (1) premature ventricular contractions, (2) idiopathic ventricular tachycardia, (3) ischemic ventricular tachycardia. For each patient, magnetic resonance imaging (MRI) and computed tomography (CT) for anatomy and electric and magnetic measurements will be performed.

3.3 Research rationale

3.3.1 Current state of research and preliminary work

3.3.1.1 Electrophysiological studies and ablation therapy

Cardiac arrhythmias ultimately originate from altered membrane potentials and electrically unstable individual cardiomyocytes leading to irregular activation of surrounding cells [B10-4]. On the organ level, precise diagnostics to localize the origin of cardiac arrhythmias usually depend on invasive procedures such as electrophysiological studies (EPS). In these procedures, special catheters capable of sensing cardiac action and stimulating the myocardium are introduced into the cavity of the right or left atrium or ventricle under fluoroscopy. While the risk of these diagnostic procedures is low, it still is not negligible (1-2% of relevant complications such as pericardial effusion or vascular complications [Hu15]) and it would thus be a great advancement for affected patients to potentially replace invasive procedures with non-invasive alternatives. For the curative ablation of cardiac arrhythmias, again specific catheters are needed to apply high energy on myocardial cells causing cardiac lesions that subsequently cannot transmit the cardiac action potential anymore. One frequent application for this approach is ventricular tachycardia, a potentially life-threatening arrhythmia that is more frequent in patients with structural heart disease, e.g. ischemic, hypertrophic, or dilated cardiomyopathy. First line therapy in these patients is treatment with an implantable cardioverter defibrillator and medical antiarrhythmic therapy. For patients that are affected by frequent ventricular tachycardias and that are hemodynamically unstable during arrhythmia, radiofrequency ablation of the arrhythmic substrate is the treatment of choice. Evolving strategies of intracardiac mapping, including 3D-electroanatomical mapping of intracardiac voltage and impedance, have made this method very accurate and have influenced mechanistic approaches to the development of arrhythmias. While this therapy is relatively safe and can be done with only small amounts of radiation-time due to electromagnetic imaging, a venous and sometimes even arterial access usually via a femoral approach is still necessary. Furthermore, there is a relevant amount of ventricular arrhythmia originating from epicardial foci that are difficult to reach with a subendocardial approach. In 2017, several papers have been published describing non-invasive ablation of ventricular arrhythmia by application of stereotactic body radiation therapy (SBRT) [Cu17, Ro19]. However, for precise targeting of this therapy, non-invasive mapping of the arrhythmia is crucial. Recent studies apply complex algorithms using electrocardiographic mapping during the running ventricular tachycardia or even combining invasive mapping with non-invasive ablation. For maximum benefit concerning risk and effort, it is necessary to ultimately develop a method that allows precise non-invasive mapping with non-invasive ablation. It will be necessary to assess these new methods in probands and patients in comparison to standard techniques, which requires experience in the successful conduction of clinical trials and registries [B10-4, B10-9, B10-10].

3.3.1.2 Forward and inverse modelling

For localization of the myocardial target area that should get ablated, knowledge about the current density during specific moments in the excitation cycle is of great importance. To estimate the (time-variant) current density distribution within the heart in a non-invasive manner, dual-sensing approaches are utilized:

- As a first step, 3D-image-based approaches such as magnetic resonance imaging (MRI) or computed tomography (CT) are used for estimating the distribution of the magnetic and electric properties of the heart (the geometry) as well as the surrounding parts of the human body. This step is necessary to obtain reliable forward solutions.
- As a second step, analyses with high temporal resolution such as electro- and magnetocardiography (ECG and MCG) are utilized to obtain supporting points of the time-varying electric and magnetic fields at the surface (electric) or in the vicinity of the human body (magnetic). This step is necessary to obtain measurements that can be utilized (together with the forward solutions) to compute inverse solutions, which lead finally to the current density distribution.

Using both analyses, ECG/MCG on the one hand and CT/MRI on the other, means that one measurement approach with good spatial and one with good time resolution are combined, which allows overcoming the drawbacks of each individual attempt. This leads to very promising analysis methods.

In detail, the results of the 3D image-based methods are converted to either surface or volumetric meshes leading to surface areas or volumes of (nearly) equal electric (susceptibility) and magnetic properties (permeability). While surface meshes are used for so-called *boundary element* approaches (BEM, the letter M abbreviates “methods”), volumetric grid meshes are used for *finite-element* approaches (FEM). Of course, also mixed approaches are used.

Since the involved electromagnetic sources are active mainly in the very low frequency range (0 to 100 Hz), the quasi-static approximation of the Maxwell equations (i.e. Biot-Savart for the magnetic part and Poisson's equation for the electric part) can be used to numerically compute the solution of the forward problem to obtain the so-called *Leadfield matrix* $\underline{L}$. Such a matrix is used for a linear mapping approach

$$\underline{y}(n) = \underline{L} \underline{i}(n),$$

that maps a so-called current *super vector*

$$\underline{i}(n) = [\underline{i}^T(0, n), \underline{i}^T(1, n), \dots, \underline{i}^T(N_i - 1, n)]^T,$$

that contains current subvectors (one vector for each voxel containing the x, y, and z component of the, e.g., center current)

$$\underline{i}(k, n) = [i_x(k, n), i_y(k, n), i_z(k, n)]^T$$

to a data vector containing all measured magnetic and electric signals

$$\underline{y}(n) = [v_0(n), v_1(n), \dots, v_{N_v-1}(n), b_0(n), b_1(n), \dots, b_{N_b-1}(n)]^T.$$

The quantities N_i , N_v , and N_b indicate the number of current dipoles (one for each voxel), the number of measured voltages, and the number of measured magnetic flux density components, respectively. This linear model is used within several inverse solutions that utilize the measured data to obtain the current super vector (the current density) either at specific time points or as complete signal sequences. Methods such as minimum norm solutions, LORETA (low-resolution [brain] electromagnetic tomography¹), several types of beamformer approaches (MVDR, LCMV, etc.²), state-space-based approaches (based on Kalman filtering approaches) as well as several others can be used to estimate the vector containing the current dipoles $\underline{i}(n)$. Due to the limited size of such a proposal, we will not go into the details of the individual methods. A good overview can be found in [Oo12].

In most approaches, the estimation is based on the minimization of different vector norms of the vector containing the differences between the measured signals and the signals obtained by the forward solution if the current vectors under test are inserted. In addition, several constraints are added to the cost function, e.g. the norm of the current vector or modified versions that should lead, e.g., to spatially smooth solutions.

In recent years, very good progress has been made for solving such problems. Hardware improvement in computer technology now allows for very powerful solutions. In addition, improvements in robustness and computational efficiency of the numerical solvers showed very promising results. The main applications of such inverse solutions are for neurological applications. However, also cardiological approaches have been investigated [Oo14].

Even if very powerful software packages are freely available for research purposes, it is still very demanding to combine all steps necessary for converting the individual data formats, applying forward modelling approaches, and obtaining the inverse solutions.

Within the current period of the collaborative research center, one CRC project (**B3**) has focused on inverse problems [Ha17a, Ha17b, Ha18, Ha19, Me19]. The project mainly focused on state-space approaches combined with different numerical approaches for obtaining the required parameter matrices. The main idea of the

¹ Even if LORETA is originally made for neurological inverse problems, it can also be used for cardiological applications.

² MVDR abbreviates minimum-variance-distortionless-response, LCMV stands for linear-constraint-minimum-variance.

state-space approach is to add statistical a-priori knowledge about the current signals involved – both in terms of temporal as well as spatial knowledge. In particular, this means that the current vector is modelled as a, e.g., first-order auto-regressive process:

$$\underline{i}(n) = \underline{A}\underline{i}(n-1) + \underline{d}_i(n).$$

The term $\underline{d}_i(n)$ can be interpreted in state-space notation as the system noise. Also, the forward solution, required to compute the Leadfield matrix, is modelled in a statistical manner. Thus, measurement noise $\underline{d}_y(n)$ is added when modelling the measured signals:

$$\underline{y}(n) = \underline{L}\underline{i}(n) + \underline{d}_y(n).$$

Besides the linear approach, also non-linear extensions as well as higher-order approaches were investigated. The state-space approach allows one to use Kalman-based schemes to reduce the measurement noise on the one hand and obtain the inverse solution (the estimated state vector) in a recursive and optimal manner (in the mean-squared sense) on the other hand [Ga04]. Even if non-linear Kalman filters (unscented or extended versions) are used, the computational load of this part of the solution is rather low. Besides the estimation of the state vector $\underline{i}(n)$, the (numerically) much more complex problem is the estimation of the system matrix $\underline{A}$. Here, a variety of solutions were investigated, starting from simplex algorithms via EM approaches³ and ending at BFGS-based⁴ solvers [Bo06]. According to the findings in **B3**, a combination of simplex and BFGS approaches, applied in an iterated manner, led to a good compromise between speed and accuracy.

In order to keep the computational complexity at a moderate level, the sparseness of the system matrix $\underline{A}$ could be exploited. One can assume that only neighboring voxels have significant influence on the currents of a (center) voxel, which leads to a matrix where only the area around the main diagonal is filled with non-zero values. Instead of computing a very large equation system, a large number of small equation systems has to be solved instead, which reduces the computational load to a great extent. The same can be argued for the system noise covariance matrix.

With this approach, however, two optimizations, a Kalman filter for estimating the current density vector and a nonlinear optimization for obtaining the system matrices, have to be computed in a nested manner, which leads to an optimization loop as depicted in Fig. B10-1.

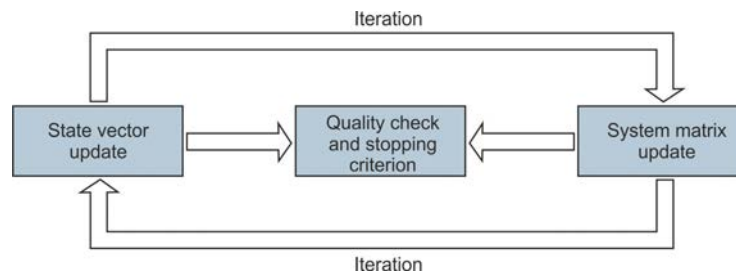


Fig. B10-1: Optimization loop performed during the computation of the inverse solutions. A Kalman filter and a solver for non-linear optimization problems (e.g. BFGS) are computed in an alternating manner. A stability and quality check (e.g. based on the Akaike information criterion) is computed after each loop cycle.

It is no trivial task to know how good the current estimation is. Besides checking the global cost function, statistical measures such as the Akaike information criterion were also evaluated. Within the project B3, the state-space framework that was already established for brain source localization was investigated for its performance for cardiological applications. Even if a lot of improvements are possible, it turned out that it performed at least in the same performance class as competitive approaches such as LORETA. In Fig. B10-2 the results of a cardiological source localization with simulated signals are shown (results in terms of precision of localization on the right, as well as the process flow on the left). Especially in good signal-to-noise (SNR) conditions as they appear in medical practice, the state-space approach performs better or at least as good as LORETA [Ha18]. This motivates that this approach should be further investigated within this funding period.

³ EM stands for “expectation maximization”.

⁴ BFGS abbreviates the last names of the inventors of the algorithm: Charles George Broyden, Roger Fletcher, Donald Goldfarb, David F. Shanno.

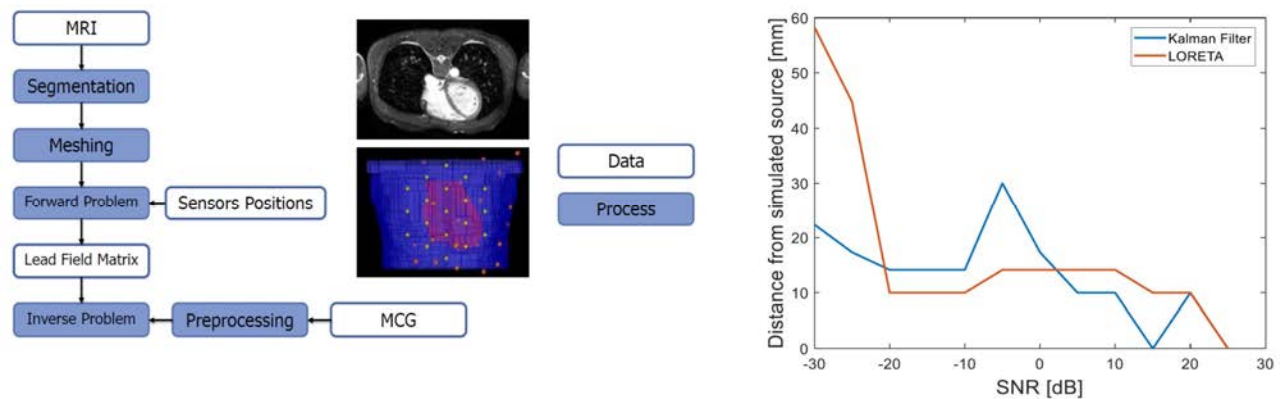


Fig. B10-2: Process flow of the Kalman-based inverse MRI/MCG approach for source localization (inverse solution) [Ha18]. Simulated data was used, allowing for precise knowledge of the positions of the sources to be localized. Even if the results were not as good as for the neurological approaches, a comparison with LORETA shows very promising results, especially in realistic SNR conditions (10 to 20 dB).

3.3.1.3 State of research for magnetic measurements for cardiologic applications

Even if the CRC has no direct cardiologic project (except the project of inverse modelling), the magnetically shielded chamber at the Faculty of Engineering was prepared for cardiologic measurements (see Fig. B10-3). This includes, first of all, the set-up of a low-channel ECG system that can be connected to the real-time system established within **B2**. This system allows using all of the ME sensor types (magnetically-modulated, electrically modulated, ΔE -based, surface-acoustic wave based) in parallel to the ECG system. Since the ME sensor systems of the CRC are not yet able to directly measure the magnetic signals of a human heart without averaging, the ECG channels can be used to determine, e.g., the R peaks and use them as temporal supporting points for averaging.

This averaging process was used for measuring the R peak using the CRC sensors in 2017 [B10-2]. Besides the CRC-based sensors, several other types of sensors were connected to the real-time system [B10-1]. While fluxgate- and magneto-impedance-based (MI) sensors still need temporal averaging, optically pumped magnetometers (OPMs) were able to measure the signal of a human heart even at a few centimetres distance in sufficient quality. Such sensors (OPMs) will be used as reference sensors in this project. The drawback of OPMs is, however, that they get saturated as soon as the magnetic flux exceeds amplitudes of more than about 50 nT. As a result, they can be used only in magnetically extremely well shielded environments - operation in standard patient rooms is not possible. There exist also OPMs that can work in non-shielded environments. However, these types of OPMs are only as sensitive as fluxgates or MI sensors, where the above-mentioned averaging process is necessary.

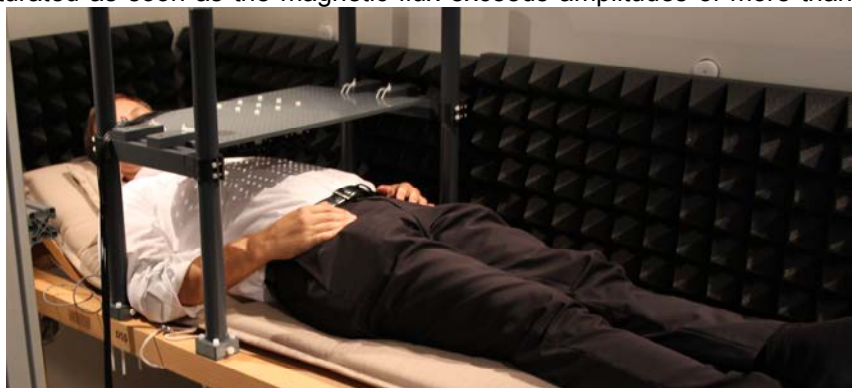


Fig. B10-3: Patient bed within the magnetically shielded chamber at the Faculty of Engineering at Kiel University. The metal-free patient bed allows parallel electric and magnetic measurements.

To prove the functionality of the real-time system, a basic R-peak detection was implemented and the resulting detection results were used for a heart-rate variability (HRV) analysis (see Fig. B10-4). These preliminary results in terms of preparation of a cardiologic measurement system within **B2** [B10-7, B10-8] and investigations of inverse solutions in **B3**, together with the recent progress in terms of ME sensor performance, made us confident in proposing this new project, which is described in the following.

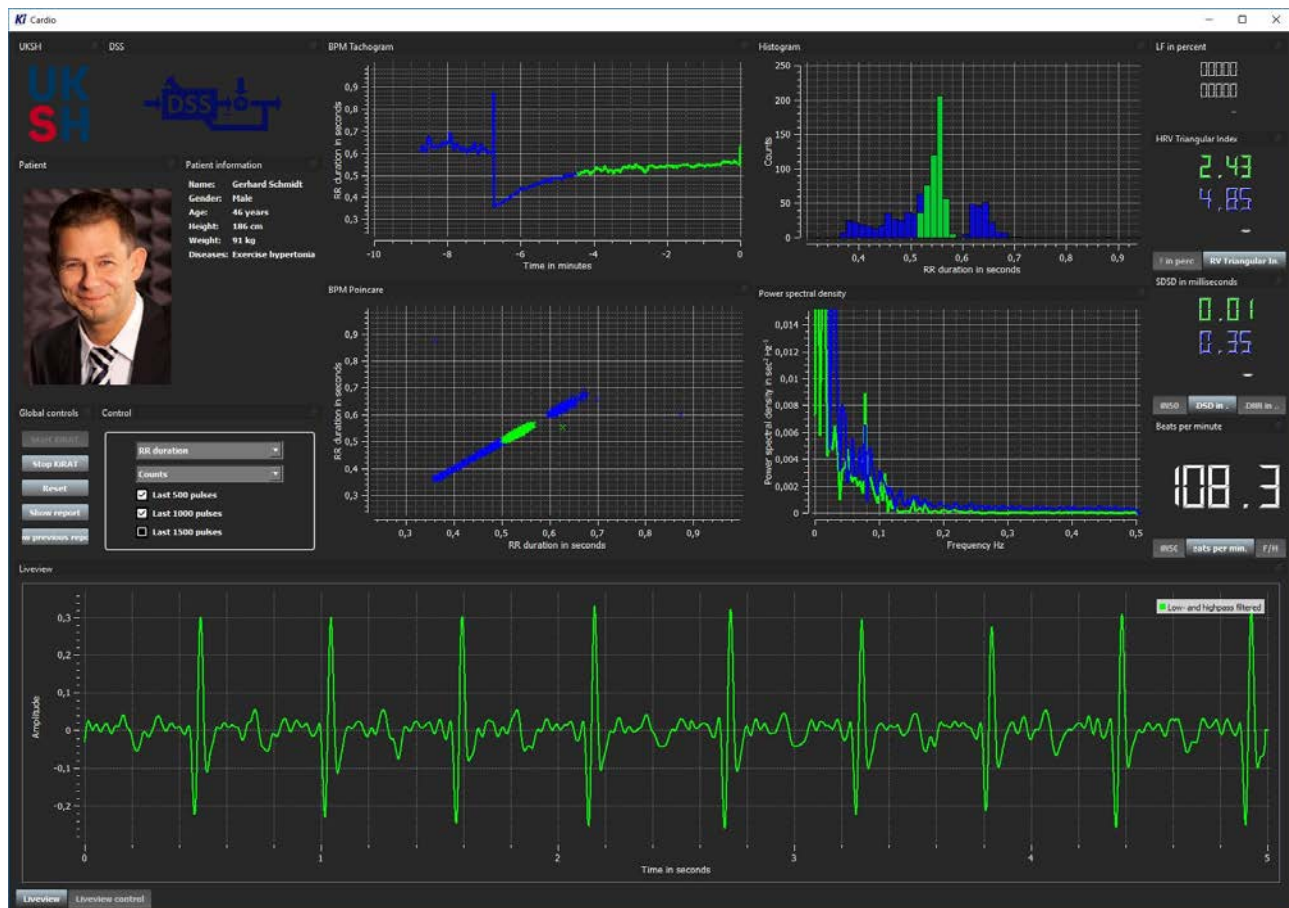


Fig. B10-4: Graphical user interface, implemented in the existing real-time framework. Similar user interfaces should be established for the MCG/ECG patient bed.

References

- [Ak71] H. Akaike, "Information Theory and an Extension of the Maximum Likelihood Principle" in *2nd International Symposium on Information Theory*, B. N. Petrov, F. Csáki, Eds., (Tsahkadsor, Armenia, USSR, 1971), pp. 267–281.
- [Bo06] J. F. Bonnans, J. C. Gilbert, C. Lemaréchal, C. A. Sagastizábal, Ed. *Newtonian Methods - Numerical Optimization: Theoretical and Practical Aspects*, (Springer, Berlin, ed. 2, 2006), pp. 51–66.
- [Cu17] P. S. Cuculich, M. R. Schill, R. Kashani, S. Mutic, A. Lang, D. Cooper, M. Faddis, M. Gleva, A. Noheria, T. W. Smith, D. Hallahan, Y. Rudy, C. G. Robinson, Noninvasive Cardiac Radiation for Ablation of Ventricular Tachycardia. *N Engl J Med* **377**, 2325-2336 (2017).
- [Ga04] A. Galka, O. Yamashita, T. Ozaki, R. Biscay, P. Valdés-Sosa, A Solution to the Dynamical Inverse Problem of EEG Generation Using Spatiotemporal Kalman Filtering. *NeuroImage* **23/2**, 435 – 453 (2004).
- [Ha18] N. Habboush, L. Hamid, M. Siniatchkin, U. Stephani, A. Galka, Pipeline for Forward Modeling and Source Imaging of Magnetocardiographic Recordings via Spatiotemporal Kalman Filtering. *Proc. EMBC*, 199-202 (2018).
- [Ha19] L. Hamid, M/EEG Source Imaging Via the Spatiotemporal Kalman Filter and Its Applications in Epileptology, disseration, *Shaker* (2019).
- [Ha17a] L. Hamid, A. A. Farawn, I. Merlet, N. Japaridze, U. Heute, U. Stephani, A. Galka, F. M. Wendling, M. Siniatchkin, Spatial Projection as a Preprocessing Step for EEG Source Reconstruction using Spatiotemporal Kalman Filtering. *39th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC), IEEE Engineering in Medicine and Biology Society*, (2017).
- [Ha17b] L. Hamid, A. A. Farawn, I. Merlet, N. Japaridze, U. Heute, U. Stephani, A. Galka, F. M. Wendling, M. Siniatchkin, Source Reconstruction via the Spatiotemporal Kalman Filter and LORETA from EEG Time Series with 32 or Fewer Electrodes. *39th International Engineering in Medicine and Biology Conference (EMBC), IEEE Engineering in Medicine and Biology Society*, (2017).
- [Hu15] S. K. Hussain, M. M. Eddy, L. Moorman, R. Malhotra, A. E. Darby, K. Bilchick, P. Mason, M. J. Mangrum, J. P. Dimarco, J. D. Ferguson, Major complications and mortality within 30 days of an

- electrophysiological procedure at an academic medical center: implications for developing national standards. *J. Cardiovasc Electrophysiol.* **26**(5), 527-531 (2015).
- [Me19] P. Mégevand, L. Hamid, M. Dümpelmann, M. Heers, New Horizons in Clinical Electric Source Imaging. *Epileptol.* **32**, 187, (2019).
- [Oe12] A. van Ooesterrom, The Inverse Problem of Bioelectricity: An Evaluation. *Med. Bio. Eng. Comput.* **50**, 891-902 (2012).
- [Oe14] A. van Ooesterrom, A Comparison of Electrocardiographic Imaging Based on Two Source Types. *EUROSPACE* **16**, iv120-iv128 (2014).
- [Ro19] C. G. Robinson, P. P. Samson, K. M. S. Moore, G. D. Hugo, N. Knutson, S. Mutic, S. M. Goddu, A. Lang, D. H. Cooper, M. Faddis, A. Noheria, T. W. Smith, P. K. Woodard, R. J. Gropler, D. E. Hallahan, Y. Rudy, P. S. Cuculich, Phase I/II Trial of Electrophysiology-Guided Noninvasive Cardiac Radioablation for Ventricular Tachycardia. *Circulation* **2019** **139**, 313-321 (2019).

3.3.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [B10-1] J. Reermann, E. Elzenheimer, **G. Schmidt**, Real-time Biomagnetic Signal Processing for Uncooled Magnetometers in Cardiology. *IEEE Sensors Journal* **15**, 4237-4249 (2019).
- [B10-2] J. Reermann, P. Durdaut, S. Salzer, T. Demming, A. Piorra, E. Quandt, **N. Frey**, M. Höft, **G. Schmidt**, Evaluation of Magnetolectric Sensor Systems for Cardiological Applications. *Measurement (Elsevier)*, 230-238 (2018).
- [B10-3] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, J. McCord, D. Meyners, E. Quandt, **G. Schmidt**, M. Höft, Improved Magnetic Frequency Conversion Approach for Magnetolectric Sensors. *IEEE Sensors Letters* **1**, 1-4 (2017).
- [B10-4] **N. Frey**, R. P. Steeds, A. Serra, E. Schulz, S. Baldus, M. Lutz, C. Pohlmann, J. Kurucova, P. Bramlage, D. Messika-Zeitoun, Quality of care assessment and improvement in aortic stenosis - rationale and design of a multicentre registry (IMPULSE). *BMC Cardiovasc Disord.* **5**;17(1):5, 1-7 (2017).
- [B10-5] J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, F. Faupel, **G. Schmidt**, Adaptive Readout Schemes for Thin-Film Magnetolectric Sensors Based on the ΔE Effect. *IEEE Sensors Journal* **16**, 4891-4900 (2016).
- [B10-6] S. Zabel, J. Reermann, S. Fichtner, C. Kirchhof, E. Quandt, B. Wagner, **G. Schmidt**, F. Faupel, Multimode Delta-E Effect Magnetic Field Sensors with Adapted Electrodes. *Applied Physics Letter* **108** (2016).
- [B10-7] J. Reermann, C. Bald, S. Salzer, P. Durdaut, A. Piorra, D. Meyners, E. Quandt, M. Höft, **G. Schmidt**, Comparison of Reference Sensors for Noise Cancellation of Magnetolectric Sensors. *IEEE Sensors* **2016**, 1-3 (2016).
- [B10-8] J. Reermann, **G. Schmidt**, I. Teliban, S. Salzer, M. Höft, R. Knöchel, A. Piorra, E. Quandt, Adaptive Acoustic Noise Cancellation for Magnetolectric Sensors. *IEEE Sensors Journal* **15**, 5804-5812 (2016).
- [B10-9] **N. Frey**, A. Linke, T. Süselbeck, J. Müller-Ehmsen, P. Vermeersch, D. Schoors, M. Rosenberg, F. Bea, S. Tuvia, J. Leor, Intracoronary delivery of injectable bioabsorbable scaffold (IK-5001) to treat left ventricular remodeling after ST-elevation myocardial infarction: a first-in-man study. *Circ. Cardiovasc. Interv.* **7**, 806-812 (2014).
- [B10-10] H. Bonnemeier, T. Demming, B. Weidtmann, J. Ortak, C. Burgdorf, M. Reppel, W. Mäuser, M. Rosenberg, **N. Frey**, Differential heart rate dynamics in transient left ventricular apical and midventricular ballooning. *2010 Heart Rhythm* **12**, 1825-32 (2010).

3.4 Project plan

Objectives

Our project plan, described in the following, is based on three working hypotheses:

- We assume that a combination of ECG and MCG will allow for better localization of arrhythmias compared to electric-only or magnetic-only approaches.
- We assume that in the near future non-invasive cardiological treatment such as cardiac irradiation for ablation of arrhythmias will be of increasing significance.

- To perform the diagnostic and therapy entirely non-invasively, precise non-invasive mapping methods of cardiac arrhythmias, e.g. by means of magnetic measurements, need to be explored.

Under the assumptions described above, we propose to improve the quality, precision, and robustness of non-invasive mapping schemes by means of extending current solutions by robust, non-cooled, and unshielded magnetic measurements as well as appropriate forward solutions and inverse models.

Research methods

For realization of the above-mentioned research objective, we will investigate in this CRC project if precise detection and localization of malfunctioning tissue regions of patients with ventricular tachycardia (VT) can be performed completely non-invasively with the ME sensors of this CRC. The main objective of this project is to investigate if a combination of structural image methods (CT and MRI) combined with spatially high-resolution MCG and ECG sensor systems can replace the invasive localization procedure and outperform ECG-only approaches, which are the current standard of care. Besides these global research questions, quantitative results on the precision of this new scheme will also be obtained. This is possible, since we are able to measure patients with ventricular tachycardia and other arrhythmias prior to the conventional invasive electro-anatomical mapping using MRI/CT, as well as ECG and MCG. After obtaining the results of our non-invasive approach, they will be compared to the results of the conventional method (gold-standard, i.e. invasive electro-anatomical mapping).

Work plan

The project is organized into four work packages that will be explained in detail in the following. Table B8-1 shows an overview of the involved researchers as well as the temporal planning of the work packages.

Table B8-1: Work schedule

No	Work package	2020		2021				2022				2023				2024	
		III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP 1 (Real-time MCG/ECG patient bed)	Engineer PhD (100%)																
	Medical doctor (50%)																
	Study nurse (25%)																
WP 2 (Data acquisition)	Engineer PhD (10%)																
	Medical doctor (50%)																
	Study nurse (25%)																
WP 3 (Forward modelling and solution of the inverse problem)	Engineer PhD (90%)																
	Medical doctor (0%)																
	Study nurse (0%)																
WP 4 (Evaluation, optimization, measurement repetition)	Engineer PhD (100%)																
	Medical doctor (50%)																
	Study nurse (25%)																

As mentioned in the previous sections, the non-invasive approach uses 3D-image-based methods as a source of information for creating surface and volumetric meshes of the magnetic and electric parameter distribution of the individual heart (and surrounding torso). In most approaches, MRI is used for that purpose, and we will also perform MRI scans of the patients that will be investigated in our project. Alternatively, high-resolution CT

will be applied, in particular in patients with contraindications for MRI (e.g. with cardiac pacemakers/defibrillators) for obtaining the tissue geometries necessary for computing the forward solution (leading to the Leadfield matrix).

For obtaining the magnetic signals (MCG), we will use a two-stage procedure:

- On one hand, we will use 32 ME sensors. Currently, ΔE -effect sensors [B10-5], electrically modulated ME sensors, as well as surface acoustic wave (SAW) sensors are close to fulfilling the quality requirements of this cardiologic application, which is a noise power spectral density of about $1 \text{ pT/Hz}^{1/2}$ within the frequency range of about 10 Hz (or less) to 40 Hz (or more). We are confident that at least one of the sensor principles will reach such requirements within this CRC funding period. The required hardware in terms of the entire sensor system consisting of low-noise amplifiers, AD converters, and pre-processing will be developed in close cooperation with **B1** (analog signal processing), **B2** (digital signal processing), and **Z2** (central project). The sensors themselves will stem from the corresponding **A** projects as well as from the central project **Z1**.
- On the other hand, we will use four optically pumped magnetometers (OPMs) that are already available in our labs. Such sensors have a sufficient noise level of about $40 \text{ fT/Hz}^{1/2}$ within the range of 5 Hz to 100 Hz. We will use them in dual-mode operation, meaning that they can measure in two orthogonal directions in parallel. Thus, we can obtain eight magnetic signals in parallel. This option allows us to start with the cardiological analysis already at the beginning of the project period. In addition, the OPM sensors can be used as references to evaluate the performance of the ME sensors.

If none of the ME sensor principles reach the required noise level, we will use temporal averaging of the ME signals and investigate if averaged signals also allow for robust solutions of the inverse problem. The required trigger for the averaging process can be performed using a single electrode placed, e.g., at the hands of the patients. This was already applied and proved to work reliably [B10-2]. Furthermore, the OPM signals can be used alone. OPMs have already proven to have a sufficiently low noise level. However, if only OPMs are used, all measurements have to be performed in magnetically shielded environments. Since a magnetically shielded chamber is available within the CRC, this does not cause severe problems from a research perspective – however, operation in shielded environments is undesirable and unpractical for clinical use, especially with instable patients.

Even if 32 sensors are used in parallel (at least for the ME sensor approach), the spatial resolution of the measurement points might not be sufficient. Thus, we will move the sensors after a sufficient recording time to obtain further signals. Time alignment (e.g. based on the QRS-peak detection or short-term cross-correlation analysis) will be used when combining all data to a full data set. This will be done for the ME sensor systems as well as for the OPMs to end up with 128 channels in total. Further details for this part of the project are described in WP 1.

In addition to the magnetic measurements, electric measurements will be performed. Currently, we have only 12-channel ECG systems. This number of channels is not sufficient for reliable localization. In order to have at least one measurement principle that is truly recorded using parallel sensors, we will use a new research ECG system with about 144 channels (see Fig. B10-5). Such a system is currently not available in our research groups, since ECG systems with such a large number of channels are not considered to be basic equipment of cardiologic and signal processing departments. Thus, we ask in this proposal for instrumentation funding. The system will be used rather often for all patient groups mentioned in this proposal.



Fig. B10-5: ECG system “g.Hlamp-RESEARCH” from g.tech with 144 electrodes [Picture source: g.tec].

The real-time system that was created during the last funding period within **B2** is in principle capable of handling this number of channels (both in terms of AD conversion hardware as well as in terms of computational complexity). However, it will be part of WP 1 to build a patient bed in our magnetically shielded chamber with all necessary signal processing capabilities.

As soon as the recording system is completed (planned one year after start of the project), MCGs and ECGs from patients will be recorded. This is done in WP 2. We plan to investigate at least $N=30$ patients with (stable) ventricular arrhythmias who suffer from frequent premature ventricular contractions (extrasystoles) ($N_{PVC}=10$)

or idiopathic ventricular tachycardia (VT) ($N_{idio}=10$). As a third group, patients with diagnosed ventricular tachycardia (ischemic cardiomyopathy) in their history will be recorded ($N_{isch}=10$). See Fig. B10-6 for typical ECG examples. Possibly, variations due to scar tissue can be seen even though a VT is not running. For all patients, three-dimensional data from thorax CT or MRI will be available. After this, we will perform multi-channel ECG recordings (144 channels) and ME/OPM sensor measurements. In the second step, invasive electroanatomic HD-mapping is performed using the RHYTHMIA-3D-Mapping-System (Boston Scientific, USA) and data will be merged with the data from the CT and/or MRI-scan. The collected data will be evaluated by a medical doctor trained in electrophysiology (EP). Of note, all invasive EP procedures are clinically indicated; the research part only involves data processing and analysis.

We plan to perform the electric and magnetic measurements in parallel. This would be the optimal data acquisition procedure. However, it might happen that the wiring and/or the power supply of the ECG system disturbs the magnetic measurements. In this case, we will perform both types of measurement sequentially and time-align the signals afterwards. Time alignment means in this case to stretch each individual beat period to a normalized fixed time (e.g. 1 s) and shift it such that, e.g., the R peak is at 0.3 s.

In parallel to WP 2, we will start with the research on efficient realization as well as on improvements of the inverse solution (WP 3). The entire processing chain explained before should be converted into the real-time framework that is created in **B2**. The conversion should be done either directly or at least as a robust interface to existing software packages. Even if comparisons with existing software packages are planned, the core of the inverse solution should be an extended version of the state-space approach that was presented before. Besides extension for improving numerical robustness and reducing computational load, algorithmic extensions are also planned. As an example, the state-space approach will be extended by investigating not only short-term correlation (as before) but also long-term correlations. This means that also the previous heart period will be used to estimate the current one:

$$\hat{i}(n) = \underline{A}_{short} \hat{i}(n-1) + \underline{A}_{long} \hat{i}(n-RR(n)) + \underline{d}_i(n).$$

$RR(n)$ describes the (time-varying) period duration of the signal, estimated, e.g., as the duration between two consecutive R peaks. Due to computational complexity, real-time operation is not possible anymore. However, the experience obtained from our real-time tool for process optimization will be used for reducing the required time to obtain the inverse solution. This includes parallel processing approaches that use either a multitude of CPU (central processing unit) cores by appropriately using threading approaches, by using GPU (graphics processing unit) approaches (having about 3000 cores per CPU), or by means of CPU clusters. Also, mixtures of the above-mentioned approaches will be investigated. However, since a further goal (WP 4) of this project

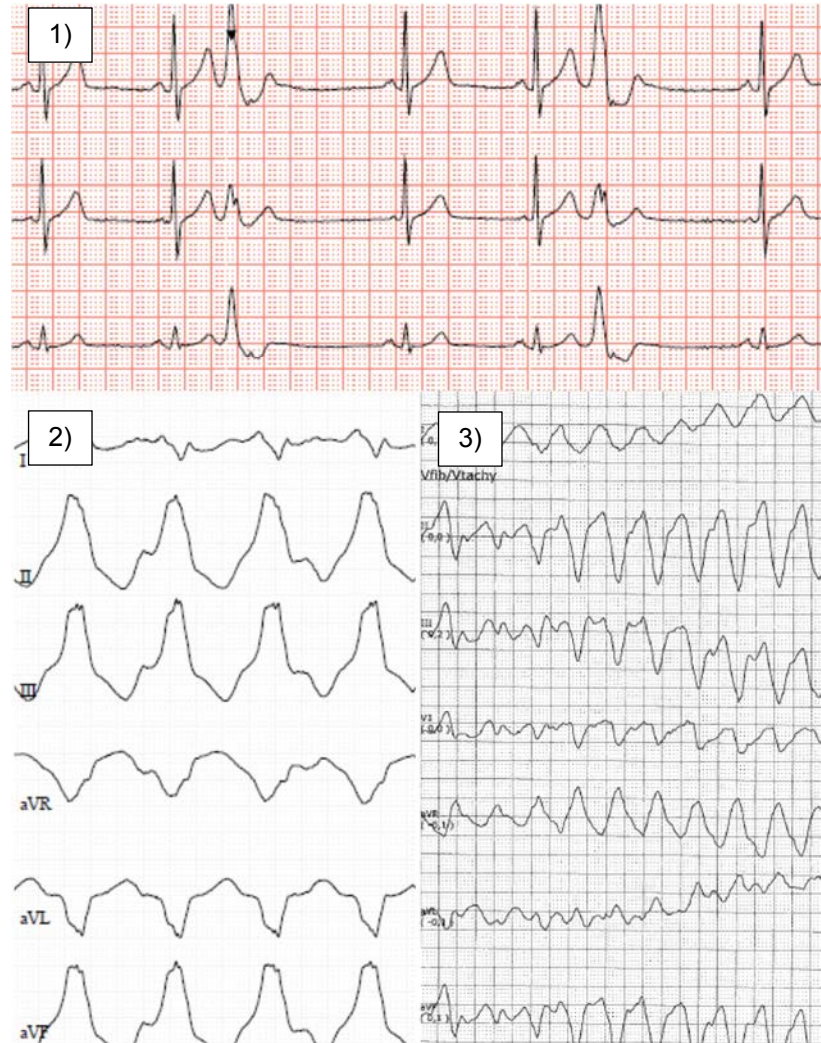


Fig. B10-6: ECG examples. 1) premature ventricular contractions (i.e. ventricular extrasystoles), heart rate: 62 bpm. 2) RVOT-ventricular tachycardia, heart rate 161 bpm; characteristics: left bundle branch block like and inferior axis. 3) Ventricular tachycardia: heart rate: 280bpm, haemodynamically instable.

is to build an open software library that can be used by many other researchers, we will focus on single PC-based solutions (with optional support of CUDA⁵ graphic cards).

This is realized in WP 3. Since this is a large amount of research, 24 months are scheduled for this project part.

It might happen that the improvement in terms of numerical efficiency will not be large enough to permit entire real-time operation, meaning that also the computation of the solution of the inverse problem will be available while performing the measurements or at least shortly after. In that case, we will make sure that at least a robust quality indication is computed in real-time. This quality indication ensures, for example, that enough sensor signals show a sufficiently high signal-to-noise ratio and that the number of artefacts is tolerable or that all measurements are artefact free. However, any improvement in numerical efficiency – even if above the “real-time threshold” – will lead to a time reduction within the treatment loop of patients.

Finally, the results of the conventional (invasive) localization should be compared with the non-invasive schemes. Besides this basic evaluation, additional approaches for improving the inverse solution should also be optimized. This includes, for example, the investigation of adaptive channel selection schemes. If, for example, only half of the electric and magnetic channels are required, the resulting reduction of computational complexity would be very large. The orthogonal information of specific signal points (electrical measurement points of equal potential [zero voltage] show often the largest amplitudes in terms of magnetic fields) can be exploited to obtain optimal sensor selections and measurement points, respectively. Furthermore, the different ME sensor principles should be compared for this cardiological application.

Finally, it is planned as part of this last work package to include the inverse solution into an open source software package, to allow scientists to use the state-space approach and compare it with their solutions. Here, interfaces to typical processing frameworks such as Matlab will be programmed. This last work package is expected to last 12 months.

WP 1 - Realization of a real-time MCG/ECG patient bed in a magnetically shielded environment

Within the first work package, a patient bed inside the magnetically shielded chamber with a combined ECG/MCG system will be built. All sensors should be connected to the existing real-time system and appropriate algorithms for SNR estimation, peak-detection, and signal quality estimation should be researched and implemented. Graphical user interfaces, as implemented for heart-rate variability analysis (see Fig. B10-4), should be established to ease the usage for the medical personnel. The basic versions described in the introduction have to be extended to handle the different types of ME sensors (before, mainly electrical signals were used – at least in terms of triggering signals for the averaging process). The averaging process will only be necessary if the limit of detection is not small enough for some sensor principles.

Each measurement will be supported by appropriate robustness and quality criteria. Examples for such criteria are background noise monitoring, artefact detection, and detection of signals that are created using coils that are integrated in the patient bed. The latter can be used to check for sensors that are not working properly. Such criteria permit minimum measurement time and assure a certain quality level of the recordings.

It is expected that the engineering researcher will work full time on the work package. He or she will be supported in the first six months by the medical doctor and the study nurse in terms of clinical relevance with respect to interface definition, patient bed design as well as cardiological signals.

Contents:

- Implementation of a 144 channel ECG system
- Implementation of an 8 channel (virtually 128) OPM-based MCG system
- Preparation of a 32 channel (virtually 128) ME sensor-based MCG system
- Time- and frequency-selective SNR estimation
- R-wave detection and time-alignment
- Investigation of quality and robustness criteria for the magnetic measurements

WP 2 - Data acquisition

⁵ CUDA stands for *compute unified device architecture* and describes a parallel computing platform and a corresponding application programming interface.

In WP 2 we plan to investigate at least 30 patients, consisting of 3 groups as mentioned above ($N=10$ each), all scheduled for ablation therapy on current guideline-directed clinical decisions:

- Patients with frequent premature ventricular contractions (PVCs) ($N_{PVC}=10$)
Patients with „idiopathic“, e.g. right ventricular outflow tract (RVOT) or other, ventricular tachycardias ($N_{idio}=10$)
- Patients with recurrent VTs and an anatomic substrate, e.g. a scar in ischemic cardiomyopathy ($N_{isch}=10$)

In all patients, we will perform both anatomic imaging (CT- or MRI-scan) as well as electrical and magnetic measurement (g.tec and ME/OPM). After this, electroanatomic HD-mapping with the RHYTHMIA-3D-Mapping-System (Boston Scientific, USA) will be performed. Besides the comparison of the different localization approaches, new insights will be used continuously for the improvement of algorithms.

The localization task for patients with PVC and idiopathic VT (e.g. RVOT-VT) can be done ‘directly’ as the extrasystoles occur frequently such that they can be recorded. VTs originating from scars do not frequently occur such that it is crucial to develop markers of arrhythmogenic scar in sine rhythm using the information about the substrate generated by 3D mapping and integrating this information with the acquired data from the ECG system and the magnetocardiographic data. Therefore, the data will be evaluated with the goal of ‘indirect’ localization by a trained electrophysiology (EP) specialist.

MRI/CT: Magnetic resonance imaging (MRI) will be used as an anatomical reference (DFG rate: € 150/hour). In patients who have an electrical device (e.g. pacemaker or defibrillator) implanted and MRI is contraindicated, computed tomography (CT) scans are necessary. With such images, size and position of different tissues can be determined.

ECG mapping (G.Hlamp-RESEARCH, g.tec): Electrical mapping using a non-invasive 144-electrode system, certified for research use, will be performed for each patient. Since the positions of the electrodes are defined in anatomical imaging (fitting to body size) the propagation map of a heart beat can be recorded for sine rhythm as well as for ventricular tachycardia/extrasystoles. This procedure can be done in the clinic as well as in the technical laboratory, ideally in parallel to MCG recordings in the shielded room. The raw data will be extracted to be used for the solution of the inverse problem.

MCG mapping (ME/OPM sensor array): Magnetic mapping using an array of 32 ME sensors in real mode (128 sensors in virtual mode) developed in the CRC will be performed at the Faculty of Engineering in the shielded room. “Real mode” means that the sensors are connected in parallel to the amplifier and analogue-to-digital converter front-end. “Virtual mode” means that several 32 channel measurements will be performed, time-aligned with appropriate temporal scaling, and combined. This latter mode requires, of course, stationarity of the signals. To start in a timely manner in case the ME sensors are not sufficient, a setup using OPMs can be realized. Since these are research setups, the medical doctor as well as the engineer will be present at all time to ensure safety.

EP study (RHYTHMIA, Boston Scientific): This is not part of this project, since only patients who are scheduled for EP study/ablation are included. The medical doctor will assist in data acquisition during the EP study such that an HD mapping of the patients’ hearts become available for the project.

This work package will mainly be done by the medical research doctor (part time, 50%) as well as by the study nurse (part time, 25%). The research engineer will help in terms of performing the ME/OPM measurements (scheduled as 10 % of his/her time).

Contents:

- Patient recordings from CT, ECG and ME/OPM sensors, invasive 3D-mapping
- Development of markers of arrhythmogenic substrate from non-invasive, non-induced studies
- Retrospective application of markers from single recordings to the full cohort

WP 3 - Forward modelling and inverse solution

This work package is core to this project. It includes the transfer and adaptation of the previous approaches from project **B3**. The forward solution workflow will be extended to support also CT (besides MRI). For the inverse solution, extended state-space approaches with non-linear parameter estimation methods will be used

as presented before. Here, the existing approaches will be modified to benefit from parallel computing hardware. Besides this approach, competing schemes such as LORETA and beamforming approaches will also be investigated. The investigated algorithms will be compared by means of convergence time as well as numerical complexity and robustness. Multi-core (CPU) approaches with GPU extensions as well as cluster-based approaches will be investigated.

The work package is mainly to be done by the engineering researcher (with medical support that is done in WP 2). Since 10 % of the research time is scheduled in WP 2, the remaining 90 % are planned for this work package.

Contents:

- Implementation of a patient-individual heart-and-torso BEM/FEM model
- Estimation of the electric and magnetic parameters from CT images
- Computing the forward solutions
- Implementation of inverse solution using state-space approaches
- Comparison of the state-space approach with existing approaches such as
 - LORETA
 - minimum-norm approaches
 - beamformer-based schemes
- Numerical optimization using parallel hardware (multi-core support and graphic card extensions)

WP 4 – Evaluation, optimization, measurement repetition

In the last work package, the localization approaches will be compared with the results of the invasive EP study. Also, setups of different numbers of sensors and sensor types (SAW, ΔE , electrically modulated, etc.) will be compared. This will lead to an answer to the original research question of whether it is possible to perform a reliable non-invasive localization of arrhythmic substrate and to what extend the CRC sensors are able to contribute to the solution. Furthermore, an open-source software package should be created that allows other researchers to use the state-space inverse solution for further research.

In order to track the results of ablation therapy in the short/medium term with regards to reoccurrence or denovo formation of arrhythmogenic substrate, the mapping procedure via the MCG (+/-ECG) approach offers a noninvasive tool that may even help in risk stratification for future ventricular tachycardia and the extraction of markers/pattern. Therefore, a follow-up measurement using the noninvasive MCG/ECG is envisioned for every patient after EP-study and ablation therapy. It is planned that the engineering researcher will work full-time on that work package, while the medical researcher and the study nurse work part-time (50 % medical doctor, 25% study nurse).

Contents:

- Comparison of the estimated source positions with the results obtained from invasive EP studies
- Investigation of a minimum / optimum set of electrical and magnetic sensors
- Open-source software publication
- Evaluation of further improvement opportunities

Prospects

We expect that the project will allow developing and validating a system for entirely non-invasive cardiological analyses and treatment for a variety of diseases in the next funding period (2024-2028). We expect that the sensor density can be increased both for electric and magnetic measurements, leading to improvements in data quality. In addition, the progress in machine learning techniques will allow for improved inverse solutions that can handle also non-linear approaches. Thus, we plan to investigate non-linearly extended analyses with a massive amount of sensor signals. Furthermore, if either adaptive shielding approaches allow for magnetically shielding only the area around the sensors (instead of the entire patient bed) or if the sensors principles that do not require shielding at all reach sufficiently low noise levels, long-term cardiological monitoring of patients without skin contact based on ME sensors is planned to be investigated. As a consequence, the system can be used without the need of magnetically shielded chambers.

3.5 Role within the Collaborative Research Centre

Close cooperation is planned with the following partners:

Z1:	This project is closely interlinked with the ME sensor projects, especially those that allow for low frequency (5 to 30 Hz) measurements.
A8:	The sensor models that are investigated in A8 , will be incorporated in the forward. A first sensor model version available in 2021 will be replaced with extended versions in 2023.
B1, Z2:	B10 will benefit from B1 adapting system front-ends and small sensor arrays to the requirements of B10 . In turn, we will communicate test results back to B1 to facilitate the development of suitable measurement systems after transfer of mature sub-systems to Z2 .
B2, B9:	The project will use the same real-time framework as B2 and B9 . Thus, all extensions made in either one of the projects will benefit the other and immediately speed up development.
B9, T1:	All study participant management and data acquisition procedures will be shared with B9 and T1 .

B10 will participate in the focus group "Biomedical Applications".

3.6 Differentiation from other funded projects of the project leader(s)

Norbert Frey holds other research grants from the DFG (e.g. FR1289/13-1) and has applied for a DFG Research Unit with a molecular cardiology focus, which is currently under review. There is no relationship to the current project proposal.

Gerhard Schmidt will guide **B2, B9** (together with W. Maetzler [Neurology Department]), and **Z2** (together with M. Höft [Faculty of Engineering]) of the CRC 1261. These projects also deal with ME sensors. However, none of these projects has direct overlap with this proposal.

3.7 Project funding

3.7.1 Previous funding

This project is currently not funded and no funding proposal has been submitted to other funding bodies.

3.7.2 Requested funding

Funding for	2020 (2 nd half)		2021		2022		2023		2024 (1 st half)	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral candidate, 100%	1	34.2	1	68.4	1	68.4	1	68.4	1	34.2
Medical doctor, 50%	1	23.9	1	47.9	1	47.9	1	47.9	1	23.9
Study nurse, 25%	1	6.4	1	12.8	1	12.8	1	12.8	1	6.4
Total		64.5		129.1		129.1		129.1		64.5
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment (up to 10,000 Euro), software and consumables	9.5		16.0		7.0		7.0		3.5	
Total	9.5		16.0		7.0		7.0		3.5	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
ECG system	62.8		0.0		0.0		0.0		0.0	
Total	62.8		0.0		0.0		0.0		0.0	
Grand total	136.8		145.5		136.5		136.5		68.0	

(All figures in k€)

3.7.3 Requested funding for staff

	Se- quen- tial no.	Name, aca- demic degree, position	Field of re- search	Department of uni- versity or non-uni- versity institution	Project commit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	Frey, Norbert, Prof. Dr. med., Project coordi- nator	Cardiology	CAU / UKSH car- dio	4		Core support
	2.	Schmidt, Gerhard, Prof. Dr.-Ing.	System Theory	EIE	4		Core support
Non-research staff	3.	Kevin Prehn		EIE	3		Hard- ware core support
Requested staff							
Research staff	4.	N.N., Doctoral Researcher	Cardiologic signal pro- cesssing	EIE / UKSH cardio		Doctoral candi- date	
	5.	N.N., Medical doctor	Cardiology	CAU / UKSH car- dio		Medical doctor	
	6.	N.N., Study Nurse	Cardiology	CAU / UKSH car- dio		Study nurse	

Job descriptions of staff for the proposed funding period (supported through existing funds):

1. Prof. Dr. med. Norbert Frey will be responsible for the coordination and scientific management of the research project. He will advise the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of conducting clinical trials.
2. Prof. Dr.-Ing. Gerhard Schmidt will be responsible for the coordination and scientific management of the research project in agreement with Norbert Frey. He advises the scientific employee with respect to planning, execution, and evaluation of the tasks, in particular in matters of digital system design, forward modelling, inverse solutions, and involved signal processing applications. Moreover, the real-time framework available at the chair can be used for the project.
3. Kevin Prehn will give support for development of the hardware and for programming of the described algorithms.

Job descriptions of staff for the proposed funding period (requested funds):

4. N.N. (E13, 100%): This person will mainly handle the engineering and algorithm development tasks in this project as described in the work packages. This person will be jointly supervised by N. Frey und G. Schmidt and will have working places both at the Cardiology Department and the Faculty of Engineering.
5. N.N. (TV-Ä1, 50%): This researcher (a medical doctor, 50%) will focus on cardiac electrophysiology. She/he will support throughout the whole research process regarding medical requirements, identify patients eligible for this pilot study, be responsible for patient information and obtaining informed consent. Finally, she/he will conduct the clinical analyses and will assist in the non-invasive measurements and invasive EP studies.
6. N.N. (E9, 25%): A part-time study nurse will assist the medical doctor in all matters of patient care and preparation for the pilot clinical trial. In particular, she/he will handle the required extensive documentation and communication with patients and legal authorities.

3.7.4 Requested funding of direct costs

	2020/2	2021	2022	2023	2024/1
Existing funds	1.5	3.0	3.0	3.0	1.5
Sum of requested funds	9.5	16.0	7.0	7.0	3.5

(All figures in k€)

Available funds will be used for the acquisition of sensor holding systems and associated material, hardware for sensor readout and excitation, small mechanical parts, electrical circuits, cables, shielding and damping material, and for the clinical setup for data acquisition and the validation study. The remaining funds will be used for the manufacture of mechanical components for the required MCG/ECG system and for publication costs. In total, this will require about 43.0 k€ (12.0 k€ paid by the University).

Equipment up to k€ 10, software, consumables for 2020 (2 quarters)

Electronic consumables, small appliances, and support materials	k€	4.0
Extension of the AD converter hardware	k€	4.5
Installation and maintenance of the clinical setup	k€	1.0

Equipment up to k€ 10, software, consumables for 2021

Electronic consumables, small appliances, and support materials	k€	5.0
Maintenance of the clinical setup	k€	2.0
CT/MRI scans (30 patients a 1 h a 150 EUR)	k€	4.5
Patient insurance (travel add-on necessary, since the magnetic measurements have to be done at the Faculty of Engineering, not at the clinic)	k€	4.5

Equipment up to k€ 10, software, consumables for 2022

Electronic consumables, small appliances, and support materials	k€	5.0
Maintenance of the clinical setup	k€	2.0

Equipment up to k€ 10, software, consumables for 2023

Electronic consumables, small appliances, and support materials	k€	5.0
Maintenance of the clinical setup	k€	2.0

Equipment up to k€ 10, software, consumables for 2024 (2 quarters)

Electronic consumables, small appliances, and support materials, publication costs	k€	2.5
Maintenance of the clinical setup	k€	1.0

3.7.5 Requested funding for instrumentation

To measure a sufficient amount of ECG channels in parallel, an ECG research system with 144 channels/sensors is required. The only one on the market fulfilling our specifications is the one from g.tec, denoted as "g.Hlamp-RESEARCH". A 144-channel ECG system is not part of the basic equipment of a cardiologic department; it will be used within the University hospital specifically for this research project. The large number of channels is required for the type of investigations and the precision of the source localization we are targeting.

Equipment > 10 k€ for 2020 (2 quarters)

144-sensor ECG system	k€	62.8

3.1 General information about transfer project T1(N)

3.1.1 Project Title: Individualized Deep Brain Stimulation

3.1.2 Research areas:

206 Neurosciences, 206-04 Systematic Neuroscience, Computational Neuroscience, Behavior, 206-08 Clinical Neurosciences I – Neurology, Neurosurgery

3.1.3 Principal investigators

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Do the above-mentioned persons hold fixed-term positions?

Prof. Dr.-Ing. M. Höft: no.

Prof. Dr. med. G. Deuschl: no; Date of retirement: 31.03.2016. He was awarded a Senior Professor position and has a contract for research with the Universitätsklinikum Schleswig-Holstein to undertake work in this project.

Dr. A.-K. Helmers: yes (commitment of extension available).

3.1.4 Application partner

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3.1.5 Legal issues

This project includes

1.	research on human subjects or human material.	yes
	A copy of the required approval of the responsible ethics committee is included with the proposal.	Submitted to ethical committee
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no

3.2 Summary

Deep brain stimulation (DBS) is a clinically effective treatment for movement disorders, including Parkinson's disease and essential tremor. The number of patients treated with DBS is rapidly increasing (> 150,000 worldwide). The knowledge of the precise position of the implanted electrode in the brain in combination with the adjustable stimulation parameters and the resulting stimulation area in the human brain are essential for the best treatment of DBS patients. The aim of this project is to detect the position of the DBS electrode in patients and additionally to determine its rotation based on the orientation marker on the electrode. This will allow for calculating the stimulated area in the brain. The magnetoelectric (ME) sensors being developed within the framework of the collaborative research center (CRC) 1261 will be used for this purpose. The position of the electrode as well as the orientation of the rotation (which is surgically uncontrollable) can be detected with this tool, thereby avoiding radiation for the patients currently exposed to MRI or CT (position) or fluoroscopy (orientation). Research in the first funding period had laid the foundations for this.

In the first work package, the (newly and continuously) developed CRC sensors will be evaluated on the basis of important characteristics of such sensors for this application. The selected sensors will then be used to perform magnetic field measurements for reconstruction of the DBS electrode that has been successfully developed for a simplified phantom in the first funding period under **B5**. This needs to be extended to the individual brain imaging (CT/MRI) of patients with implanted electrodes in the second work package of this project. The detection of the directional electrode orientation in the phantom will be an additional part of this work package. The electrophysiological localization and orientation results will then be integrated into the individual neuroimaging data (preoperative MRI and postoperative CT/MRI) in the third work package. The localization of the electrode in the brain can be performed with several software programs, e.g. by using the open-source toolbox Lead-DBS that is developed in a DFG-Emmy-Noether group (Dr. Andreas Horn, Charité Berlin) for research purposes. In the next step, also in work package two, the stimulated electrical field with respect to the anatomical structures in the brain will be calculated for the individual stimulation parameters and implemented in such a system.

We plan to develop a software package that can be wrapped into image-based software to display the magnetically measured and reconstructed electrical fields within the individual MRI of the patient. Comparing this *in silico* imaging with the best point for stimulation for specific symptoms will be a helpful tool for better programming of the DBS devices of such patients. We established a cooperation with the company Boston Scientific (producer of DBS equipment and surgical planning and programming software), which had shown interest and is ready to contribute further to this transfer project. The collaboration will ensure in this transfer project that the medical and industrial requirements are considered and that the evaluation will be performed with state-of-the-art stimulators and industrial routines. The main motivation of the company is the possibility to measure the position and rotation of the segmented electrode non-radiatively. The close collaboration will serve to design a system for the calculation of the tissue activated by deep brain stimulation and to test its accuracy in various clinical studies where the side effects and effects can be clinically measured to validate this model.

3.3 Research rationale

3.3.1 Current state of understanding and preliminary work

Deep brain stimulation (DBS) is an established therapy for movement disorders, including Parkinson's disease [De13, Li19, Sh14, T1-5], dystonia [T1-1], and tremors [Sc15, T1-6]. For 20 years increasing numbers of

patients have been treated. New indications like epilepsies and depression [Mo14] are currently being studied and may become new, established indications soon. Deep brain stimulation involves implanting electrodes into specific areas deep in the brain that are attached to an implantable pulse generator that is placed under the skin near the clavicle. If these electrodes are correctly placed, continuous stimulation with electrical impulses at 130-180 Hz may control the disease related abnormal neuronal activity in these regions. The detailed mechanisms for effects and side effects, however, are still a matter of intense research [Wi13, Sc13, T1-9, T1-10] and so far, not yet fully understood.

From a clinical point of view, the exact extent of the target area is still not precisely defined yet. The consequences may be insufficient improvement of motor symptoms and the occurrence of side effects such as muscle contractions, gait disturbances, oculomotor abnormalities as well as cognitive and emotional disturbances such as impulsivity, depression/apathy, and hypomania [Vo10]. Furthermore, higher stimulation amplitudes, which might be necessary to reach areas separate from the optimal target, might lead to higher energy consumption and, thus, shorter battery exchange cycles [T1-3]. Therefore, the detection of the stimulated region is essential. We have used a simplified phantom with the shape of a cylinder with dimensions comparable to a human head in the first funding period (see Fig. T1-1). This was done to locate the position of the electrode and to probe the stimulated area around the standard electrode. The electrode can be placed at any desired fixed position in the phantom head that is filled with saline solution, enabling measurement of the exact stereotactic position of the electrode and ensuring accuracy of this model. We used fluxgate sensors, magnetolectric (ME) sensors, and surface acoustic wave (SAW) sensors produced within the CRC for these measurements. Furthermore, we recently used SQUID sensors of a commercially available MEG device in collaboration with Prof. Schnitzler and his group, Department of Neurology, in Düsseldorf.

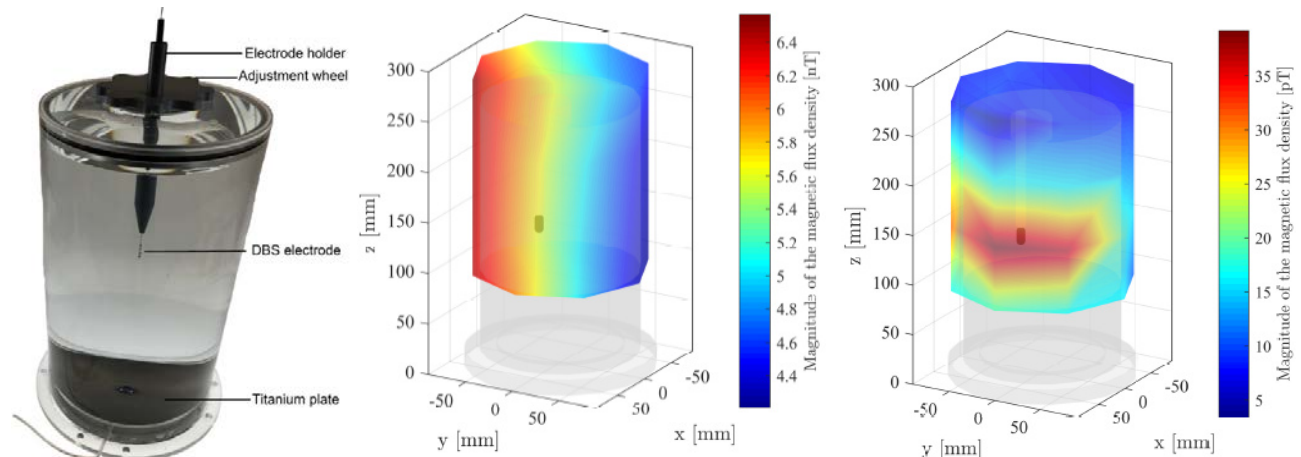


Figure T1-1: On the left side, the cylindrical phantom head filled with saline solution and with an integrated fixed deep brain stimulation electrode (at an example position) is shown. The middle and right figure show the measured magnetic field distribution for both a monopolar and bipolar electrode configuration (near-surface position). The bipolar mode generates a more focused spatial distribution that can be used for electrode localization.

Two types of DBS system were used for analysis during the first funding period. First, there is the electrode model 3387 of the company Medtronic that is voltage-controlled and powered by our electronics or the generator of the manufacturer for the tests. It has four independent circular contacts generating electrical fields around or between the desired contacts. The magnetic field which is generated in both monopolar and bipolar electrode configurations was measured with the sensor types mentioned above and the results were analyzed [T1-2]. There are differences in the magnetic properties of both configurations: The magnetic flux densities are in the pT-range in the bipolar stimulation mode and decrease quadratically with a distance of between 45 mm and 125 mm. In monopolar stimulation mode, we found the fields in the nT-range decrease linearly over the measured distances. The bipolar stimulation mode generates a more focused spatial resolution of the magnetic field around the head surface (see Fig. T1-1 on the right), which is better suited for electrode localization. The bipolar mode can subsequently be modelled as an electrical current dipole whose forward calculated fields can be fitted to the measured ones. We have shown in [T1-2] that the dipole fitting approach is able to detect the position of the electrode in the phantom head. We conclude that although the monopolar stimulation mode provides a magnetic field 100 times larger, it is less suited to be used for electrode localization due to the corresponding broad field distribution as shown in the center of Fig. T1-1. The reason is that the whole electrode with the cable serves as a dipole. There is no information about the height of the electrode (z-coordinate), which substantially limits the possibilities for localization.

Furthermore, we used the DBS system of Boston Scientific Inc. that has a current-controlled stimulator (Vercise PC) and a directional electrode (Vercise Cartesia, see Fig. T1-3). The advantage of this type of system is that the desired current amplitude is adjusted and is controlled such that the impact of differences in conductivity is minimized. The proportionality between the current and the magnetic field leads to the same magnetic field strengths in each patient with the same adjusted current. The directional lead provides multi-directional steering, and in animals the steering capabilities of the new electrode design have been demonstrated already [Ma11]. Therefore, it was essential to study the real DBS system for the magnetic characteristics. The tangential magnetic field component between 11 mm and 75 mm was measured for bipolar stimulation mode with a relatively high stimulation amplitude of 12 mA, a pulse width of 240 μ s, and a frequency of 160 Hz. The magnetic field decreases quadratically and we measured ~ 25 pT in the time domain at a distance of 40 mm. At greater distances, the resultant magnetic field of the bipolar stimulation is strongly affected by the fluxgate sensor noise, which causes fluctuation of the measurement curve in Fig. T1-2 (blue line). The quadratic decrease of the field for an amplitude of 12 mA is estimated according to the quasi-static approximation for magnetic fields with the law of Biot-Savart and can be seen in red (see Fig. T1-2). Since we measured and know the linearity of the current and the magnetic field, the estimations for 6 mA, 3 mA, and 1.5 mA were also inserted in this figure (green, pink, and black lines). Since the mean distances of the Nucleus subthalamicus (STN) to the surface of the head are approximately known (see Fig. T1-2), we expect a magnetic field of about 1 pT at a distance of 100 mm and with a stimulation amplitude of 3 mA. This value is marked with the green point in the graph.

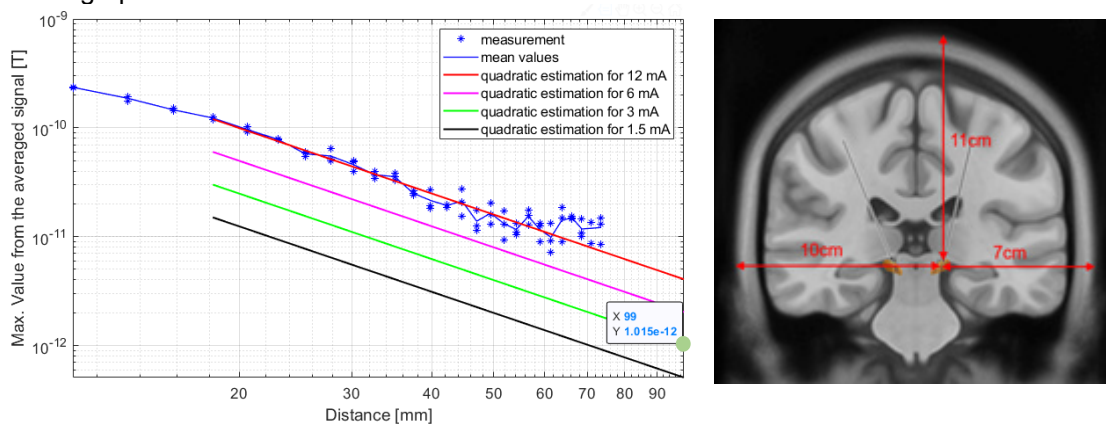


Figure T1-2: On the left side, the magnetic flux density was measured over the distance (blue line). The quadratic decrease of the magnetic field can be seen and is estimated for different stimulation amplitudes: 12 mA (red), 6 mA (pink), 3 mA (green), and 1.5 mA (black). For a real case example, the forward calculated value is 1 pT for an amplitude of 3 mA and a distance of 100 mm (thick green dot). The distances between the target in the Nucleus subthalamicus (STN) and various positions on the head surface can be seen in the right figure in a coronal view.



Figure T1-3: Vercise Cartesia™ directional lead from company Boston Scientific with eight contacts in total. Two different bipolar stimulation modes (green and red).

Nevertheless, for relatively close distances of between 11 and 40 mm we investigate the magnetic field strengths for a horizontal and vertical measurement for two bipolar electrode configurations highlighted in Fig. T1-3 in green and red. We were able to measure slight differences in the field strengths caused by the minor deviation of the bipolar modes (1.5 mm). Otherwise, this would limit the accuracy of the electrode localization.

First measurements were done with the unidirectional fluxgate magnetometer (Fluxmaster, Stefan Mayer Instruments), which can be fixed easily in the head scanner system to run the measurement. For this purpose, we use our custom-made head scanner that is continuously maintained by **Z2**. The magnetometer is rotated at each measuring point in all three orthogonal directions to get the complete magnetic information at this point. In addition, other magnetometers developed within the framework of the CRC are used for our analysis in this biomedical application. The following sensors were used:

1) Resonant ME cantilever in passive mode [Sa16] (in cooperation with **Z2**): Four sensors were combined in a double tuning fork design with an orthogonal longitudinal ME sensor location. The magnetic field generated with the monopolar electrode configuration was measured; however, the sensitivity of the sensor concept that was about 40 pT/Hz^{1/2} was insufficient for bipolar measurement without averaging. An averaging time of ten

seconds, i.e. 1600 averages at an adjusted frequency of 160 Hz, was realized to measure the magnetic field of 1 pT for the bipolar electrode configuration.

2) Electrically modulated resonant ME cantilever [Ha18] (in cooperation with **A7**): The sensor measured the magnetic field generated in monopolar stimulation and also for bipolar stimulation with the adjusted stimulation parameter 5.5 V of amplitude, 240 μ s of pulse width, and 160 Hz of frequency. The measured values were verified with a reference fluxgate measurement. The magnetic field generated by the real current-controlled stimulator could not be detected without averaging. The ME sensor has a noise level of about 25 pT/Hz^{1/2}. The magnetic field was measurable with an average of about 4 seconds, i.e. 640 averages at an adjusted frequency of 160 Hz.

3) Δ E-effect surface acoustic wave sensor [T1-8] (in cooperation with **B1** and **A8**): The sensor was able to measure the resultant magnetic field for bipolar electrode configuration with a minimum adjusted amplitude of 1 V, a pulse width of 240 μ s, and a frequency of 160 Hz. Since the noise level of the sensor decreases over the frequency [T1-4], the peaks from the third and higher harmonics can be seen in the frequency domain. Thus, this sensor system is most promising for this application because it could measure about 100 % of the signal power according to its corresponding bandwidth (see Fig. T1-5). With its noise level, it will already be possible to measure the field under monopolar stimulation with physiologically adjusted parameters in the real DBS system from Boston Scientific. This can be predicted because the real DBS system in the cylindrical head phantom was tested and analyzed under the SQUID-MEG device in cooperation with the group of Prof. Schnitzler in Düsseldorf, which will be explained next. Through intensive research on this new sensor system, it will soon have the sensitivity to enable measurement of fields of bipolar stimulation, which is sufficient for electrode localization.

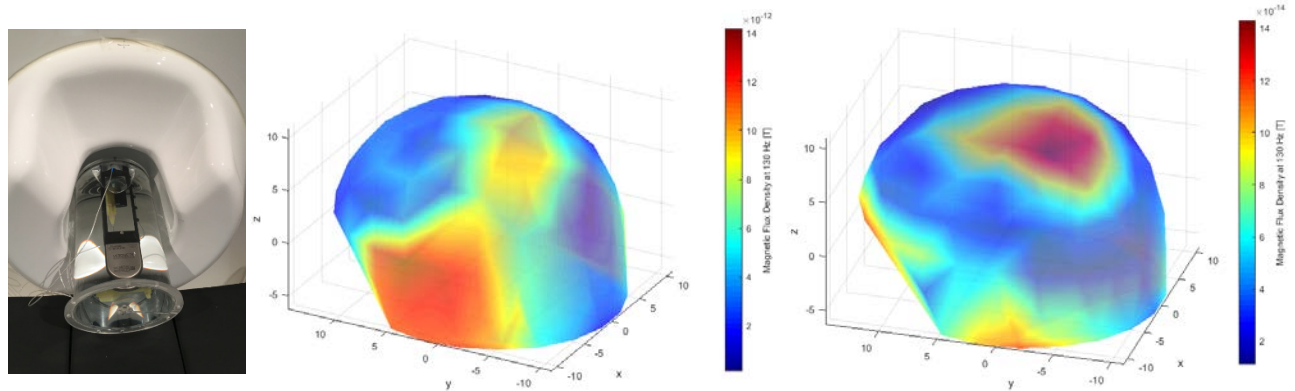


Figure T1-4: On the left, the cylindrical phantom head in the MEG system (TRIUX, Elekta Neuromag®) can be seen. The Vercise PC stimulator is placed and fixed inside the model. The middle and right figure show the measured magnetic field distribution for both monopolar and bipolar electrode configuration with 102 MEG SQUIDS. The bipolar mode (right) generates a more focused spatial distribution due to the current flowing through both activated contacts and can be used for electrode localization. The monopolar mode (middle) measures the field generated by the current flowing through the whole system, which limits the localization accuracy of the electrode.

In collaboration with Prof. Schnitzler and his group in Düsseldorf, we assessed the real DBS system inside the SQUID-MEG with a noise level of 3 fT/Hz^{1/2} as shown on the left of Fig. T1-4. For real physiological stimulation parameters (1.5 mA, 60 μ s, 130 Hz), we measured the maximum field strength at the fundamental frequency of $\sim$ 14 pT for the monopolar and $\sim$ 140 fT for the bipolar electrode configuration. This confirms once again that the field in monopolar mode is approximately 100 times greater than the field in bipolar mode. The bipolar

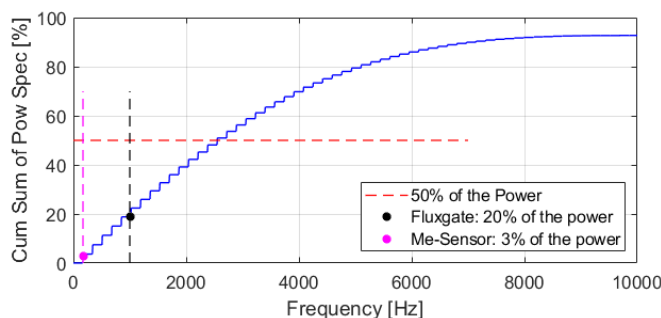


Figure T1-5: The cumulative sum of the power spectrum is shown. The fluxgate sensor (1 kHz bandwidth) measures 20 % of the signal power, the ME sensor (few Hz bandwidth) in passive mode measures only 3 %, and the SAW sensor (wide bandwidth) measures $\sim$ 100 %.

mode generated a more focused spatial magnetic field distribution, whereas the monopolar mode measured the field generated by the current flowing through the whole system (see Fig. T1-4). It was also confirmed which field strengths are to be expected in reality at a distance of about 100 mm, which was 1 pT for the

fluxgate measurement that has a bandwidth of 1 kHz and measured 20 % of the signal power (see Fig. T1-5). Since only one frequency sample point was considered in this case (3 % of the signal power), and this point is only 15 % of the predicted field for the fluxgate measurement (that is, 0.15 pT), the measured values matched approximately the forward calculated predicted values. These analyzed requirements on the sensors being developed in the framework of the CRC have been discussed.

The position of the electrode can be calculated based on the magnetic field recordings as described above in our phantom head. Afterwards, the detection of the stimulated area around the calculated position can be

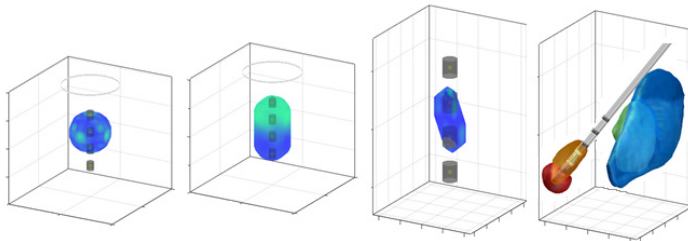


Figure T1-6: The example simulated volume of tissue activated for monopolar (first), bipolar (second) and directional (third) stimulation, and within Lead-DBS.

estimated in different ways by advanced modelling approaches and simulations. The relevant medical parameter that has been elaborated, in particular by McIntyre and colleagues, by estimating the volume of tissue activated (VTA) during stimulation can be calculated. They have developed a theoretical model based on a finite element model (FEM) assuming in each of the elements a number of axons with special excitability assumptions. This then leads to a theoretically defined VTA and represents one of the best models to explain

many of the observed clinical effects during stimulation [Bu08, Bu11]. We can calculate it for our homogeneous phantom head with a constant electrical conductivity as shown in Fig. T1-6 for monopolar, bipolar, and directional stimulation considering the activation electric field thresholds from [As15]. This model had to be extended to a real model by considering different electrical conductivities and brain characteristics, which is why we opted for the open source toolbox Lead-DBS. An example is given on the right in Fig. T1-6, in which the VTA (in red) is calculated within the brain represented by three brain structures (nucleus subthalamicus in yellow, globus pallidus internus in green, and externus in blue). Lead-DBS provides FEM-based VTA model and gives us the possibility to use subcortical atlases in MNI space and provides us with DBS relevant fiber tracts such as dentate-rubro-thalamic tract and the cortico-spinal tract [Me15, Me16]. With it, all the statistical and analytic functions of this toolbox (e.g. VTA) can be used and one's own programming code can be integrated. This topic is being further developed [Sc18, Gu18, Ho19a].

Collaboration with the research department of the company Boston Scientific within the transfer project is ideally suited for this biomedical application. Both groups are very interested in finding the optimal stimulation parameters for each individual patient to improve the therapeutic efficacy. Preliminary work by our application partner such as [T1-7] and [Ma12] shows that the company has the specific know-how in advanced anatomical and electrical modelling of DBS and has also participated in many clinical studies.

References

- [As15] M. Aström, E. Diczfalussy, H. Martens, K. Wardell: Relationship between Neural Activation and Electric Field Distribution during Deep Brain Stimulation, *IEEE Trans Bio Eng.* 62 (2015), 664-672.
- [Bu08] C. R. Butson, S. E. Cooper, J. M. Henderson, C. C. McIntyre: Patient-Specific Analysis of the Volume of Tissue Activated During Deep Brain Stimulation, *NeuroImage* 34 (2008), 661-670.
- [Bu11] C. R. Butson, S. E. Cooper, J. M. Henderson, C. C. McIntyre: Probabilistic analysis of activation volumes generated during deep brain stimulation, *NeuroImage* 54 (2011), 2096-2104.
- [De13] **G. Deuschl**, Y. Agid: Subthalamic neurostimulation for Parkinson's disease with early fluctuations: balancing the risks and benefits, *The Lancet Neurology* 12(10) (2013), 1025-1034.
- [Gu18] K. Gunalan, B. Howell, C. McIntyre: Quantifying axonal responses in patient-specific models of subthalamic deep brain stimulation, *NeuroImage* 172 (2018), 263-277.
- [Ha18] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yazar, A. Piorra, R. Knöchel, Y. Fetisov, E. Quandt: Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing, *Journal of Physics D: Applied Physics* 51 (2018).
- [Ho17] A. Horn, M. Reich, J. Vorwerk, N. Li, G. Wenzel, Q. Fang, T. Schmitz-Hübsch, R. Nickl, A. Kupsch, J. Volkmann, A. Kühn, M. Fox.: Connectivity Predicts deep brain stimulation outcome in Parkinson disease, *Ann Neurol.*, 82 (2017), 67-78.
- [Ho19] A. Horn, N. Li, T. Dembek, A. Kappel, C. Boulay, S. Ewert, A. Tietze, A. Husch, T. Perera, W. Neumann, M. Reiser, H. Si, R. Oostenveld, C. Rorden, F. Yeh, Q. Fang, T. Herrington, J. Vorwerk, A. Kühn: Lead-DBS v2: Towards a comprehensive pipeline for deep brain stimulation imaging, *NeuroImage* 184 (2019), 293-316.

- [Ho19a] B. Howell, K. Gunalan, C. McIntyre: A Driving-Force Predictor for Estimating Pathway Activation in Patient-Specific Models of Deep Brain Stimulation, *Neuromodulation: Technology at the Neural Interface* 22 (2019), 403-415.
- [Ia19] M. I. Iacano, S. R. Atefi, L. Mainardi, H. C. Walker, L. M. Angelone, G. Bonmassar: A Study on the Feasibility of the Deep Brain Stimulation (DBS) Electrode Localization Based on Scalp Electric Potential Recordings, *Front Physiol.* (2019), 9:1788.
- [Jo16] M. Joliot, G. Jobard, M. Naveau, N. Delcroix, L. Petit, L. Zago, F. Crivello, E. Mellet, B. Mazoyer, N. Tzourio-Mazoyer: AICHA: An atlas of intrinsic connectivity of homotopic areas, *Journal of Neuroscience Methods*, 254 (2015), 46-59.
- [Ko18] L. Konopleva, K. Il'yasov, H. Skibbe, V. Kiselev, E. Kellner, B. Dhital, M. Reiser: Model-free global tractography, *Neuroimage* 174 (2018), 576-586.
- [Li19] P. Limousin, T. Foltynie: Long-term outcomes of deep brain stimulation in Parkinson disease, *Nat Rev Neurol.* 15(2019), 234-342.
- [Ma12] **N. Maling**, R. Hashemiyoony, K. D. Foote, M. S. Okun, J. C. Sanchez: Increased Thalamic Gamma Band Activity Correlates with Symptom Relief following Deep Brain Stimulation in Humans with Tourette's Syndrome, 7(9) (2012).
- [Ma11] H. C. Martens, E. Toader, M. M. J. Decre, D. J. Anderson, R. Vetter, D. R. Kipke, K. B. Baker, M. D. Johnson, J. L. Vitek: Spatial steering of deep brain stimulation volumes using a novel lead design, *Clinical neurophysiology : official journal of the International Federation of Clinical Neurophysiology* 122(3) (2011), 558-566.
- [Me15] A. Meola, A. Comert, F. C. Yeh, S. Sivakanthan, J. C. Fernandez-Miranda: The nondecussating pathway of the dentatorubrothalamic tract in humans: human connectome-based tractography study and microdissection validation, *Neurosurgery* 124 (2016), 1211-1547.
- [Me16] A. Meola, F. C. Yeh, W. Fellows-Mayle, J. Weed, J. C. Fernandez-Miranda: Human Connectome-Based Tractographic Atlas of the Brainstem Connections and Surgical Approaches, *Neurosurgery* 79 (2016), 437-455.
- [Mi16] K. G. Mideksa, A. Singh, N. Hoogenboom, H. Hellriegel, H. Krause, A. Schnitzler, **G. Deuschl**, J. Raethjen, G. Schmidt, M. Muthuraman: Comparison of imaging modalities and source-localization algorithms in locating the induced activity during deep brain stimulation of the STN, *Conf Proc IEEE Eng Med Biol Soc.*, (2016), 105-108.
- [Mo14] T. Morishita, S. M. Fayad, M. A. Higuchi, K. A. Nestor, K. D. Foote: Deep brain stimulation for treatment-resistant depression: systematic review of clinical outcomes, *Neurotherapeutics : the journal of the American Society for Experimental NeuroTherapeutics* 11(3) (2014), 475-484.
- [Re11] M. Reiser, I. Mader, C. Anastasopoulos, M. Weigel, S. Schnell, V. Kiselev: Global fiber reconstruction becomes practical, *Neuroimage* 54 (2011), 955-962.
- [Re17] P. C. Reinacher, M. T. Krüger, V. A. Coenen, M. Shah, R. Roelz, C. Jenker, K. Egger: Determining the Orientation of Directional Deep Brain Stimulation Electrodes Using 3D Rotational Fluoroscopy, *Am J Neuroradiol.* 38(6) (2017), 1111-1116.
- [Sa16] S. Salzer, R. Jahns, A. Piorra, I. Teliban, J. Reermann, **M. Höft**, E. Quandt, R. Knöchel: Tuning Fork for Noise Suppression in Magnetolectric Sensors, *Sensors & Actuators: A. Phys* 237 (2016), 91-95.
- [Sc13] W. M. Schuepbach, J. Rau, K. Knudsen, J. Volkmann, P. Krack, L. Timmermann, T. D. Halbig, H. Hesekamp, S. M. Navarro, N. Meier, D. Falk, M. Mehdorn, S. Paschen, M. Maarouf, M. T. Barbe, G. R. Fink, A. Kupsch, D. Gruber, G. H. Schneider, E. Seigneuret, A. Kistner, P. Chaynes, F. Ory-Magne, C. B. Courbon, J. Vesper, A. Schnitzler, L. Wojtecki, J. L. Houeto, B. Bataille, D. Maltete, P. Damier, S. Raoul, F. Sixel-Doering, D. Hellwig, A. Gharabaghi, R. Kruger, M. O. Pinsker, F. Amtege, J. M. Regis, T. Witjas, S. Thobois, P. Mertens, M. Kloss, A. Hartmann, W. H. Oertel, B. Post, H. Speelman, Y. Agid, C. Schade-Brittinger, **G. Deuschl**: Neurostimulation for Parkinson's Disease with Early Motor Complications, *N Engl J Med* 368 (2013), 610-622.
- [Sc15] S. A. Schneider, **G. Deuschl**: Medical and surgical treatment of tremors, *Neurologic clinics* 33(1) (2015), 57-75.
- [Sc18] C. Schmidt, U. Van Rienen: Adaptive Estimation of the Neural Activation Extent in Computational Volume Conductor Models of Deep Brain Stimulation, *IEEE Trans on Biom Eng.* 65 (2018), 1828-1839.
- [Sh14] A. Shalash, A. Alexoudi, K. Knudsen, J. Volkmann, M. Mehdorn, **G. Deuschl**: The impact of age and disease duration on the long term outcome of neurostimulation of the subthalamic nucleus, *Parkinsonism & related disorders* 20(1) (2014), 47-52.
- [Vo10] J. Volkmann, C. Daniels, K. Witt: Neuropsychiatric effects of subthalamic neurostimulation in Parkinson disease, *Nat Rev Neurol* 6(9) (2010), 487-498.
- [Wi13] K. Witt, O. Granert, C. Daniels, J. Volkmann, D. Falk, T. van Eimeren, **G. Deuschl**: Relation of Lead Trajectory and Electrode Position to Neuropsychological Outcomes of Subthalamic Neurostimulation in Parkinson's Disease: Results from a Randomized Trial, *Brain* 136 (2013), 2109-2119.

- [Ye10] F. Yeh, V. Wedeen, W. Tseng: Generalized q-sampling imaging, *IEEE Trans. Med. Imag.* 29 (2010), 1626-1635.
- [Yo10] N. Yousif, N. Purswani, R. Bayford, D. Nandi, P. Bain, X. Liu: Evaluating the impact of the deep brain stimulation induced electric field on subthalamic neurons: a computational modelling study, *Journal of Neuroscience Methods*, 188 (2010), 105-112.
- [Yo12] N. Yousif, R. Borisjuk, N. Pavese, D. Nandi, P. Bain: Spatiotemporal visualization of deep brain stimulation-induced effects in the subthalamic nucleus, *Neuroscience* 36 (2012), 2252-2259.

3.3.2 Project-related publications

- [T1-1] M. M. Reich, A. Horn, F. Lange, J. Roothans, S. Paschen, J. Runge, F. Wodarg, N. G. Pozzi, K. Witt, R. C. Nickl, L. Soussand, S. Ewert, V. Maltese, M. Wittstock, G. H. Schneider, V. Coenen, P. Mahlke, W. Poewe, W. Eisner, **A.-K. Helmers**, C. Matthies, V. Sturm, I. U. Isaias, J. K. Krauss, A. A. Kuhn, **G. Deuschl**, J. Volkmann: Probabilistic mapping of the antidystonic effect of pallidal neurostimulation: a multicentre imaging study. *Brain*. 1;142(5), (2019) 1386-98.
- [T1-2] **M. Yalaz**, A. Teplyuk, M. Muthuraman, **G. Deuschl**, **M. Höft**: The Magnetic Properties of Electrical Pulses delivered by Deep Brain Stimulation Systems, *IEEE Trans on Instrumentation and Measurement*, doi:10.1109/TIM.2019.2945744 (2019).
- [T1-3] M. Jakobs, **A.-K. Helmers**, M. Synowitz, P. R. Sloty, J. M. Anthofer, J. R. Schlaier, A. W. Unterberg, K. L. Kiening: A multicentric, open-label, controlled trial on acceptance, convenience and complications of rechargeable internal pulse generators for deep brain stimulation - The Multi Recharge Trial, *JNS19* (2019), 360.
- [T1-4] P. Durdaut, A. Kittmann, E. Rubiola, J.-M. Friedt, E. Quandt, R. Knöchel, **M. Höft**: Noise Analysis and Comparison of Phase- and Frequency-Detecting Readout Systems: Application to SAW Delay Line Magnetic Field Sensor, *IEEE Sensors Journal*, 19(2019), 8000-8008
- [T1-5] S. Paschen, J. Forstenpointner, J. Becktepe, S. Heinzl, H. Hellriegel, K. Witt, **A.-K. Helmers**, **G. Deuschl**: Long-term efficacy of deep brain stimulation for essential tremor: An observer-blinded study. *Neurology*. 19;92(12) (2019) e1378-e86.
- [T1-6] P. Krack, J. Volkmann, G. Tinkhauser, **G. Deuschl**: Deep brain stimulation in movement disorders: from experimental surgery to evidence-based therapy, *Movement Disorders*, in press (2019).
- [T1-7] **N. Maling**, S. F. Lempka, Z. Blumenfeld, H. Bronte-Stewart, C.C. McIntyre: Biophysical basis of subthalamic local field potentials recorded from deep brain stimulation electrodes, *J Neurophysiology* 120(4) (2018), 1932-1944.
- [T1-8] A. Kittmann, P. Durdaut, S. Zabel, J. Reermann, J. Schmalz, B. Spetzler, D. Meyners, N. X. Sun, J. McCord, M. Gerken, G. Schmidt, **M. Höft**, R. Knöchel, F. Faupel, E. Quandt: Wide Band Low Noise Love Wave Magnetic Field Sensor System, *Scientific Reports*, 8, (2018), 278.
- [T1-9] M. Muthuraman, J. Raethjen, N. Koirala, A. R. Anwar, K. G. Mideksa, R. Elble, S. Groppe, **G. Deuschl**: Cerebello-cortical network fingerprints differ between essential, Parkinson's and mimicked tremors, *Brain*, (2018), 1770-1781.
- [T1-10] N. Koirala, V. Fleischer, M. Glaser, K. E. Zeuner, **G. Deuschl**, J. Volkmann, M. Muthuraman, S. Groppe: Frontal Lobe Connectivity and Network Community Characteristics are Associated with the Outcome of Subthalamic Nucleus Deep Brain Stimulation in Patients with Parkinson's Disease. *Brain Topogr.* Mar;31, (2018), 311-21

3.4 Project Plan

Objectives

The long-term aim of this project is (1) to develop a recording device with ME sensors to measure the topographic position of the electrode in the brain of patients reliably. The exact number and placement of the sensors will be determined. Since at the beginning of the second phase of the CRC such large arrays of sensors will not be available, scans with single sensors or small arrays of sensors will be performed. (2) The orientation of the electrode and the stimulated area with respect to the anatomical structures in the brain from these electrode artifacts shall be detected. This can currently only be derived from CT, rotational fluoroscopy, and X-ray assessments of the patient. To achieve this, the imaging data and the reconstructed position of the stimulated contact will be integrated and currently available techniques for the calculation of the stimulated field will be applied. Thus, this recording device will be able to measure, analyze, and visualize the location of the electrode and the stimulated brain areas.

Working hypotheses

1. The position of the electrodes can be detected with high precision with magnetic field measurements at the stimulation strength used in patients.
2. The orientation of the electrode can be detected by comparing the bipolar full ring electrode stimulation with the bipolar stimulation of segmented electrode contacts.
3. The magnetically determined localization (MDL) of the electrode position enables better clinical decision making, e.g. through active contact selection to predict clinical outcomes by using the threshold for capsular side effects.
4. Once the MDL system has been integrated into an image-based analysis tool to visualize the magnetically determined electrode position within individual anatomy of the patient's brain, clinical studies to establish the use of this tool can be applied.

Timetable for the different work packages:

No.	Work package	2020		2021				2022				2023				2024	
		III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP1	Sensor Characteristics																
	a Testing CRC Sensors																
	b Phantom Measurement																
WP2	Measuring the Position and Orientation of the Deep Brain Stimulation Electrode																
	a Localization Algorithm																
	b Localization using Sensor Arrays																
	c Detecting the Orientation of Directional DBS electrode																
WP3	Estimation of the Volume of Tissue Activated																
	a VTA Estimation																
	b VTA Validation in DBS Patients																
WP4	System Integration																
	a Sensor-Cap Development with ME sensors																
	b Software / Hardware Integration																
	c Testing of the Device in Patients																

Researcher
 Boston Scientific
 Physician

WP1: Sensor Characteristics

The CRC will provide this project with (newly) developed sensors. The first step is to evaluate the characteristics of these sensors for usability in this application for our research question according to a testing pipeline. The selected sensors will then be used for the required measurements in the next work packages. In cooperation with **Z2**, similar sensors will be collected and combined in a sensor array. Boston Scientific will provide us with the necessary equipment for the DBS system. At the beginning of the project, the current pacemaker (Vercise™) and the directional electrode (Vercise Cartesia™) will be provided. The electrode will then be replaced every second year. This work package requires continuous work with close communication and feedback with material scientists in project area **A**.

WP1a: Testing CRC Sensors

In this work package, we want to create a procedure pipeline that tests the sensors for their usability and practicability for our application of DBS. Mainly, the ME cantilevers with electrical frequency conversion (**A7**), the magnetoelastic surface acoustic wave delay line sensors (**A9**), and other sensors being developed within the framework of the CRC will be tested, but additional external sensors could be passed through this pipeline. We want to distinguish three different phases (of magnetic field strengths) in the pipeline after the sensor is qualified for the subsequent phantom and patient measurements. In each phase, the measured magnetic field will be analyzed with respect to its signal characteristics (noise level and frequency bandwidth) and the decrease of the magnetic field over the distances from 5 cm to 10 cm. This will be done in the first phase with our phantom model in which the voltage-controlled pacemaker (own electronics) stimulates the electrode. It will then be replaced by a real current-controlled DBS system (Vercise Gevia™ or PC) using relatively high stimulation amplitudes of 10 mA, 130 Hz of stimulation frequency, and 60 μ s of pulse width. In the third phase, the amplitude will be reduced to 2 mA, which is in the range of patient values. If the sensor delivers promising and reproducible results in the measurement analysis, it will be qualified for further measurements described in the following work packages, e.g. for head scans and patient measurements.

WP1b: Phantom Measurement

This work package deals with ME sensor measurement with our cylindrical phantom head in the head scanner (**Z2**). The distribution of the magnetic field will be measured around the phantom head to determine the required spatial sensor arrangement at the measuring surface. First, high-resolution measurements, e.g. 16 measurement points around the phantom at each of the 16 z-heights (ending up with $16 \times 16 = 256$ sensor points), will be performed in order to analyze magnetic differences with the same stimulation settings in different bipolar electrode configurations. For this, we will stimulate the electrode between two contact heights (e.g. contact 1 vs. 234 and contact 234 vs. 567, see Fig. T1-7 for contact numbering) and between two segmented contacts that lie on top of each other in the same electrode rotation (e.g. contact 2 vs. 5 and contact 3 vs. 6, see Fig. T1-7 for contact numbering). The spatial sensor resolution will then be gradually reduced, and differences will be analyzed to end up with a trade-off between the number of sensor points and the measuring quality that distinguishes different electrode configurations. The results will also be discussed with Boston Scientific and possible suitable programming of the pacemaker (frequency, pulse width, amplitude, contacts of the electrode) for magnetic measurements will be found.

WP2: Measuring the Position and Orientation of the Deep Brain Stimulation Electrode

The aim of this work package is, on the one hand, to further develop reconstruction techniques to locate the position of the DBS electrode in our existing phantom head and, on the other hand, to measure and determine the orientation of the directional DBS electrode. This will be done with magnetic field measurements. The use of ME sensor arrays is a measuring requirement that minimizes the measuring time and makes possible recording at all the desired sensor points simultaneously. This is also addressed in this work package. Basic support for all medical biomagnetic measurement applications will be given in **Z2**. A researcher from Boston Scientific will collaborate with us to determine the electrode rotation in the phantom by using magnetic field measurements and comparing them to the rotation results obtained from neuroimaging data with a clinically available software package.

WP2a: Localization Algorithm

This work package deals with measurements from single ME sensors from WP1a and the head scanner (**Z2**) for our cylindrical phantom head and real DBS patients. Since most of the measurements were performed with the fluxgate sensor in the first phase of the CRC, the applied reconstruction algorithms have to be adapted for the ME or SAW sensors, which have a larger bandwidth and thus measure an increased signal power (see Fig. T1-5). They differ by sensor characteristics, e.g. frequency bandwidth, sensor noise performance, and spatial transfer function. For best localization of the electrode, the number of measuring points of the sensors and its spatial resolution at the sensor level, the measuring time at each point, and the sensor orientation during the measurement should be well determined. The measuring requirements will be theoretically calculated and practically tested. At this point, different localization algorithms such as the dipole-fitting approach, RAP-MUSIC, and Beamformer will be tested and further improved. So far, the dipole-fit algorithm achieved the best results. In collaboration with **A8**, the localization accuracy will be further improved by using the extended sensor models and the more realistic head geometry. The analyzed results for the phantom measurements will be required for the same measuring procedure with real DBS implanted patients. The optimum number of measurement data locations for the best compromise between high resolution and short measurement time should be figured out in this work package. The movement of the patients' heads during recording has to be monitored and re-calculated in the patient data. Furthermore, there are also some limitations for measurements with patients, which will have to be developed, considering relative fixation of the head position during the scans, the stimulation parameters, or comfortable measuring procedures. The

investigated sensor localization algorithm in **B2** for the phantom head should also be tested for this application in phantoms and later in patients.

WP2b: Localization using Sensor Arrays

Measurements with small sensor element arrays are the first step toward the long-term goal of this project. We are considering a 3 x 3 ME sensor array with a symmetrical distribution (i.e. with equal distance along the perpendicular axes on a plane) and with the same sensor orientation for each sensor. After a 90° rotation of the plane along its normal vector, the same sensor location will be reached measuring the other magnetic component on a plane (orthogonal of the first measurement) ending up with a 2D measurement. Mechanical constraints due to the sizes of the sensors and electromagnetic constraints due to avoiding crosstalk would limit the total length and width of the sensor array. This project is primarily aimed at using ME sensors. Nevertheless, we have access to a high-resolution EGI EEG system with 256 channels in our department and to a SQUID-MEG system in Düsseldorf with Prof. Schnitzler for validation purposes, if necessary. There is still ongoing work with EEG [Ja19, Mi16] to locate the electrode. The sensor array will be realized in a collaboration with the development part **Z1**, **Z2**, and simulation part **A8**.

WP2c: Detecting the Orientation of Directional DBS electrode

The goal of this work package is the determination of the orientation of the directional electrode in our phantom head and in patients from magnetic field measurements. The degree of rotation varies during implantation of the electrode and can only be determined by postoperative imaging with radiation [Re17]. The knowledge of the electrode rotation is important to guide the deep brain stimulation in a desired direction to better treat the patient. For this, as a first step we want to determine the electrode z-height implanted in patients or placed in the phantom with bipolar electrode configuration. Therefore, we measure over the entire z-height and select the height value where the magnitude of the magnetic field shows the highest value. As soon as the electrode height is known, we want to measure the magnetic field in the certain z-plane along the sensor ring also with a high resolution of measuring points. We plan to investigate both monopolar and bipolar electrode

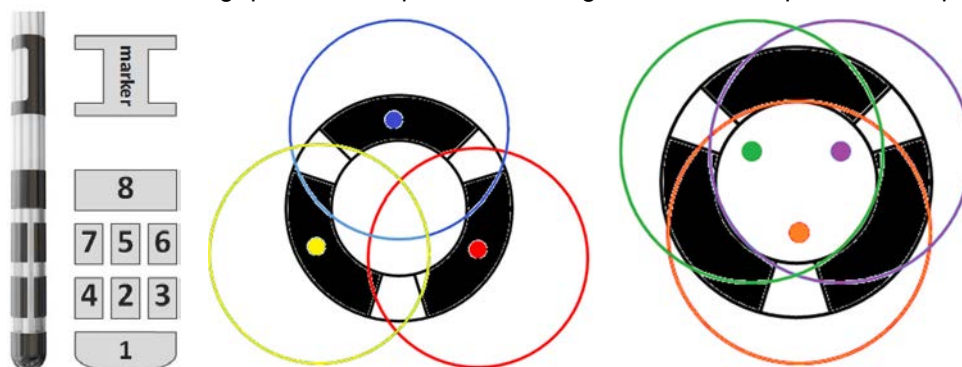


Figure T1-7: On the left side, the directional electrode with its eight contacts can be seen. The middle and right figures show qualitatively the physical mass points (red, blue, yellow thick dots) of the monopolar electrode configuration with each activated segmented contacts and of the segmented bipolar mode using each activated both neighboring segmented contacts.

configuration as shown in Fig. T1-7 with its physical mass points each set of stimulation. At the measuring points on the sensor ring that are close to these colored points, the magnetic field will be increased and the rotation can be determined. With monopolar stimulation, we want to stimulate the entire ring (e.g. by using contact 234), which can be interpreted as a reference measurement. We then want to excite the segmented contacts individually (contact 2, contact 3, contact 4) and deduce the orientation of the electrode by comparing the magnetic fields, since the corresponding physical mass point shift depending on the electrode configuration. In the bipolar mode, we want to stimulate the complete ring with the contacts 2, 3, and 4 against the ring with the upper contacts 5, 6, and 7. This measurement should again be interpreted as a reference measurement. Afterwards, we want to stimulate contact 2 against the upper contact 5, contact 3 against contact 6, and contact 4 against contact 7. The magnetic field is shifted accordingly by the shift of the mass points and thus the orientation of the electrode can be concluded. Similar to the electrode localization, it has to be examined whether the monopolar mode generating high magnetic fields but superimposed by artifacts or bipolar mode generating weak magnetic fields with no artifacts can be used. Our results will be compared with the rotation results from Boston Scientific using the Guide™ XT software and neuroimaging data from the same patient or phantom. Deviations of both results are documented and a suitable solution for both alternatives will be investigated.

WP3: Estimation of the Volume of Tissue Activated

The spatial extent of the neural response to electrical stimulation via DBS is known as the volume of tissue activated (VTA) that can be controlled with stimulation parameters such as amplitude, pulse width, and electrode configuration [Yo10, Yo12]. It is assumed that more precise modelling of the VTA could facilitate better programming of the DBS device. The main aim of this work package is to estimate the VTA for a given specific set of neuromodulation parameters, DBS electrode model, ideal or realistic assumptions of tissue properties, and individual or normalized brain structures. We will use the open-source toolbox Lead-DBS providing FEM-based VTA model [Ho17]. The VTA estimation will be compared by using anatomical electrode reconstruction based on metal artifacts in neuroimaging data and using our magnetically determined localization (MDL) algorithm. Our scientific collaborators at Boston Scientific have special experience in modelling of the stimulated area and they will mainly perform the VTA estimate through anatomic electrode reconstruction with their own commercial software GUIDE™ XT, whereby we will determine it through MDL using Lead-DBS. Both procedures will be validated with real patient data in WP3b and compared with each other.

WP3a: VTA Estimation

The aim in this work package is to estimate the volume of tissue activated surrounding the implanted electrode which has to be calculated with neurostimulation parameters such as amplitude, pulse width, and electrode contact configuration. The frequency does not influence the VTA estimation [Yo10]. In the first part of this work package, subcortical human brain atlases will be used with homogeneous and isotropic electrical conductivity available within Lead-DBS (see Fig. T1-8) [Ho19]. The result will be a high-resolution map of the stimulated area with detailed information of the relation between the shape of the stimulated area and the anatomy. The next step is to estimate the VTA in addition to neuronal fiber tracts with fiber tract-based atlases, which were created on the basis of high-spatial-resolution diffusion tensor MR imaging. The change of the shape of the stimulated area caused by the fiber tracts will be analyzed. Precision improvements on VTA that end with a more patient-specific estimation of the stimulated area is the second part of this work package. It will consider

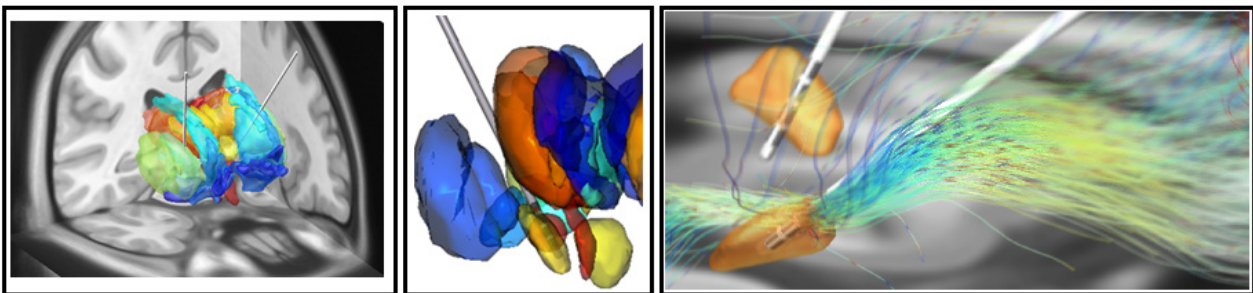


Figure T1-8: The left figure shows the ACHA atlas [Jo16] and both DBS electrodes within Lead-DBS. The middle figure presents the estimated VTA (red ball) within the ACHA atlas with homogeneous isotropic conductivities. In the right figure, the fiber tracts running through the STN (orange) and VTA (red) can be seen [own created figures].

the individual brain structures of the patient with their own segmented brain structures and reconstructed fiber tracts (see Fig. T1-8 right). The brain structures will be extracted from the collaborators. The Lead-Connectome submodule provides different tracker algorithms to estimate the whole-brain fiber tractogram based on diffusion tensor MR imaging. We will use the best available technique, choosing between the Gibbs' tracking [Re11], Mesotracker algorithm [Ko18], and the Generalized q-Sampling Imaging Approach [Ye10]. This will be crucial to gain deeper understanding of the cortical areas affected by the deep brain stimulation. Hence, when done, the single-patient imaging result can be combined with normative group connectome data to guarantee the accuracy of the result. Subsequently, the VTA can be calculated with the FEM-based model while considering the developed individual brain characteristics. At this point, we will have the fusion of the whole analysis results that consists of the measured electrode location with its mass point of stimulation (WP2), the modelled anatomical brain structures based on preoperative MR and postoperative CT images, and the location of the DBS electrode in this structures (WP3) and the estimated volumes of tissue activated for both our measured (MDL + Lead-DBS) points and the points anatomically determined (GUIDE™ XT + Lead-DBS) by Boston Scientific (WP3). These volumes will then be weighed against each other for accuracy and validation of our approach.

WP3b: VTA Validation in DBS Patients

To validate both the measured and the anatomically determined estimations of the VTA, ten Parkinsonian patients with implanted electrodes will be tested, in which the side effects of the patient caused by Capsula

interna (CI) stimulation will be summarized as a function of the stimulation amplitude. Therefore, patients with clinically well-positioned electrodes can be taken. **B9** and **T1** will recruit patients jointly and evaluate at least two patients together. The patients' stimulation area will be tested with continuously increasing stimulation strengths at neighboring electrodes, and the clinical effects will be observed and documented with standard clinical assessment. At increasing field strengths, there will be clinical side effects because the internal capsule will be activated. This can be identified with visual inspection by a clinician. The stimulated area will be calculated from the recordings at each stimulation strength and the amount of capsular involvement will be analyzed. Both estimated volumes will be compared in this work package and it is investigated which both measured and calculated physical mass points of the VTA reach the CI faster with increasing amplitude. The observed side effects of the patient during stimulation and the calculated stimulation area, including CI, lead to a better estimation of the VTA. The WP3b requires close collaboration with Boston Scientific and medical staff.

WP4: System Integration

We will develop a standard arrangement of sensors for ME sensor guided programming of patients with deep brain stimulators (e.g. sensor cap). The advantage of these sensors will be the ability to measure outside the magnetically shielded chamber, which is an important condition for other sensor types such as the commonly used SQUID sensors for the MEG. A software package (i.e. based on MATLAB) will be developed that visualizes the measured magnetic field distribution at the sensor level, the estimated volume of tissue activated for a given set of neurostimulation parameters within the individual MRI of the patient, and if desired, the activated cortical areas caused by the projection of the stimulated fiber tracts to the cortex. This can be understood as a package that can be wrapped into imaging software (Lead-DBS and GUIDE™ XT). WP4 will be mainly supported by **Z2** in the development part and by Boston Scientific with neuroimaging know-how.

WP4a: Development of a Sensor Cap with ME sensors

At the beginning of this work, research must be done and simulations must be performed to analyze how many sensors are needed with what orientations, and to determine the distribution of the sensors on the sensor cap. We anticipate constructing a stretch cap that holds the desired number of ME sensors closely to the subject's head (e.g. 16 sensors until the end of this funding period). The sensors can be pre-positioned in an international montage model (e.g. international 10/20 montage, see Fig. T1-9), so the sensor placement errors can be minimized. On the other hand, it will be examined whether a larger sensor distribution on the side of the head is more promising (see Fig. T1-10).

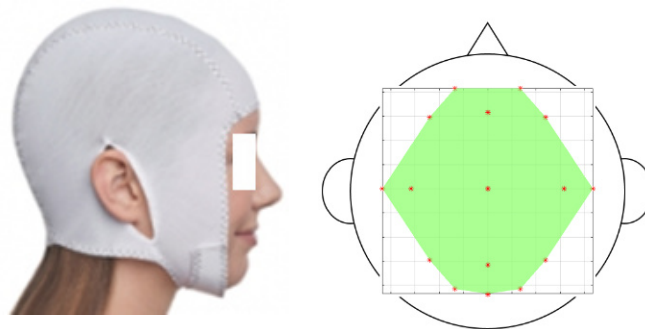


Figure T1-9: The left figure shows the intended stretch sensor cap as an example (<https://www.brainlatam.com/uploads/produto/eeg-caps-for-adults-149.png>). The right figure shows an example distribution of 16 sensor positions in the international ten-twenty electrode system. This can be applied for ME sensors.

WP4b: Software and Hardware Integration

For the realization of the desired software package, the total measured and analyzed information should be combined and displayed together. Since the analysis of the measured magnetic field distribution, the implemented electrode localization algorithms, and the estimation of the volume of tissue activated (Lead-DBS) are performed within MATLAB software, a laptop with installed software should be sufficient for this application in the beginning. A graphical user interface (GUI) will be programmed, that outputs everything important for the user. The VTA has part of a visualization system that will also allow the medical specialist to observe the brain structures that are responding directly to the electrical stimulation. The sensors on the cap are connected to an amplifier box which is connected to the laptop. Thus, this system, with intuitive software and a modular structure to suit any lab, will become a practical reality.

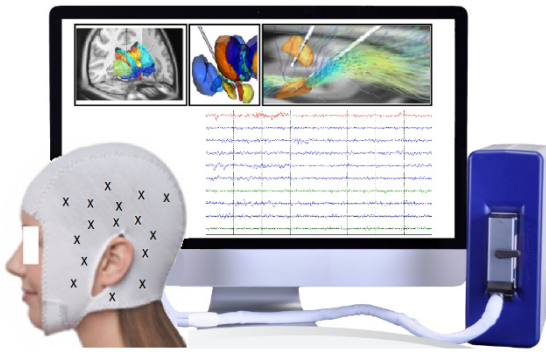


Figure T1-10: The figure shows the envisaged imaging system device with intended stretch sensor cap with example sensor positions, the amplifier box that is connected with the cap and the monitor showing the results.

WP4c: Testing of the Device in Patients

The purpose of the imaging system device is to estimate the stimulated area in individual patients. Variation in the electric stimulation parameters affect the spread of activation and can have serious consequences on therapeutic effects or induce side effects when such parameters are not carefully adjusted. This work package deals with the testing of this device by analyzing certain patient groups with side effects and comparing these patients with DBS control groups without side effects. We will include 10 more DBS Parkinsonian patients and an additional 10 essential tremor patients in this study and tested for cerebellar activity. The hypothesis then will be that the differences of the clinical symptomatology are due to differences of the stimulated area. The clinical studies will be conducted as soon as the measuring device is available and can be used for patients. Initial pilot trials will be performed with high-resolution EEG (256-channels). The studies will be supported by the **physician** with scheduling suitable patients. Boston Scientific is also interested in these studies and will support us in the research of the device software. These clinical studies will suffice to validate this new device and will underline the usefulness of this approach.

Prospects

It is expected that the project will enable the development of a device for ME sensor guided programming of patients with deep brain stimulators which can measure the stimulated area in patients outside of the magnetic chamber until the end of the funding period. This project will be further developed as a transfer project with the company Boston Scientific. Particularly, the imaging software will then need further adaptation. Clinical studies on the value of programming with the ME guided programming device will be needed. This may lead to a clinical study submitted to the clinical trials program of the DFG. Alternatively, the project will be replaced by an MEG-project during the third funding period, as we should be able by then to record the MEG with ME sensors and their value for specific questions will be explored.

3.5 Role within the Collaborative Research Centre

Collaborations are planned with the following projects:

A7	Application of electrically modulated resonant ME cantilever for DBS measurements
A8	Modelling of sensor array distribution, improvement of localization accuracy
A9	Application of SAW magnetic field sensors for DBS measurements
B1, B2	Research of the ME and SAW sensor systems and arrays, sensor localization (B2)
B9	Recruitment of Parkinsonian patients jointly and evaluation of at least two patients together
B10	The common use of all study participant management and data acquisition procedures
Z1	ME sensors for sensor systems and arrays
Z2	Support provided for Biomagnetic measurements: Construction of ME sensor systems and arrays, performing measurements with head scanner within the magnetically shielded chamber, improvement of the phantom head
Boston Scientific	This funding period of the CRC will be continuously supported by the company Boston Scientific, which is interested in these research topics

This project is an application project from the viewpoint of the sensor development. The new sensors will be tested with this paradigm and the narrow band (e.g. resonant ME cantilevers) and wide band (e.g. based on

SAW) will be specifically of interest for this project. Close feedback of the experience in patients is necessary therefore with related research on those sensors in the **A** projects. From the clinical neuroscience point of view, it is an important point within the present development of new and more customizable electrodes. It is expected that a device as planned in this project will be able to improve patient specific programming. **T1** will participate in the focus group "Biomedical Applications".

3.6 Differentiation from other funded projects

Other projects than those mentioned in 1.8.1 are clinical studies which have no overlap with the present project line. (Earlystim clinical study and follow-up studies, 'Studie zum Vergleich der Wirksamkeit der DBS auf die Lebensqualität bei Parkinson-Patienten im Vergleich zu einer optimalen medikamentösen Therapie'; BMBF 01KG050502).

3.7 Project funds

3.7.1 Funds requested

Funding for	2020 (2 nd half)		2021		2022		2023		2024 (1 st half)	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
TV E-13, 100%	0.5	34.2	1	68.4	1	68.4	1	68.4	0.5	34.2
TV-Ä1, Neurologist	0.125	12.0	0.25	23.9	0.25	23.9	0.25	23.9	0.125	12.0
Total		46.2		92.3		92.3		92.3		46.2
Direct costs	Sum		Sum		Sum		Sum		Sum	
Consumables, equipment up to 10 T€	3.00		6.00		6.00		6.00		3.00	
Total	3.00		6.00		6.00		6.00		3.00	
Total	49.2		98.3		98.3		98.3		49.2	

(All figures in T€)

3.7.2 Staff

	No	Name, academic degree, position	Field of research	Department of university or non-university institution	Commitment in hours/week	Category	Funded through:
Available							
Research staff	1	Günther Deuschl, Prof. Dr. med. Project coordinator	Neurology, Deep brain stimulation	UKSH neurology	5		University
	2	M. Höft Prof. Dr.-Ing. Project coordinator	Microwave Engineering	TF EIE	4		University
	3	Helmert, Ann-Kristin Dr. Project coordinator	Neurosurgery, Deep brain stimulation	UKSH neurosurgery	5		University
Application partner staff	4	R&D employees Project partner	Neuroscience, Deep brain stimulation	Boston Scientific Inc	4		Company
Requested							
Research staff	5	M. Sc. Mevlüt Yalaz, Doctoral Researcher	Microwave Engineering	TF EIE		TV E13	

Research staff	6	Dr. med. Jos Becktepe, Medical Doctor	Neurology, Deep brain stimulation	UKSH neuro		TV Ä1	

Job description of staff (supported through available funds):

1. **Prof. Dr. Günther Deuschl** is responsible with M. Höft and A.-K. Helmers for the coordination and scientific management of the project. He will work with the scientific staff member on all the analytic steps. He will work with the physicians and technicians to get the clinical analysis and to test patients.
2. **Prof. Dr.-Ing. Michael Höft** is responsible for the coordination and scientific management of project in agreement with G. Deuschl and A.-K. Helmers. He advises the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of the related measurement setups and procedures.
3. **Dr. Ann-Kristin Helmers** is responsible for the coordination and scientific management of project in agreement with G. Deuschl and M. Höft. She advises the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of conduction of clinical trials.
4. **R&D employees** are responsible for the coordination and scientific management of the project within Boston Scientific. They will work with the researcher on all analytical steps, mainly in WP3 for advanced computational DBS modelling, but also in WP1 and WP4. Especially, Dr. Nicholas Maling brings the required expertise in this area through his doctorate time in the laboratory of Cameron McIntyre in Cleveland.

Job description of staff (requested):

5. **M.Sc. Mevlüt Yalaz**, doctoral researcher (Ph.D. candidate), who investigates the research ideas proposed in this document.
6. **Dr. med. Jos Becktepe** is a physician, who takes care of the clinical questions and all patient assessments. He will also help with the interpretation of the experiments in work packages 2, 3, and 4.

3.7.3 Direct costs

	2020 (2 nd half)	2021	2022	2023	2024 (1 st half)
Funds available (in T€)	3.00	6.00	6.00	6.00	3.00
Funds requested (in T€)	3.00	6.00	6.00	6.00	3.00

Running costs will cover small mechanical parts and electronic equipment. For project parts WP2, WP3, and WP4, most MRI-images are available as long as these patients had the surgery in the Department of Neurosurgery at Kiel University. Special MRI-imaging will be needed for patients which were not operated on here. We estimate that 10 MRI scans will be needed per year which will be paid on the basis of fixed costs of 300 € per individual session. Running consumable costs will be paid out of research funds of the applicant.

3.7.4 Contribution of Boston Scientific

	2020 (2 nd half)	2021	2022	2023	2024 (1 st half)
Staff (in hours per week)	4	4	4	4	4
Instrumentation (in T€)	26	0	10	0	10

Boston Scientific will provide us with a complete current-controlled DBS system (rechargeable stimulator Vercise Gevia or Vercise PC, segmented electrode) at the beginning of the transfer project (~26 T€). The electrode will be replaced every other year (~10 T€ each electrode), so the sum of the monetary contribution of our industrial partner is 46 T€. The commercial GUIDE™ XT software (~500 T€) will be used by the R&D employees working 4 hours a week on the project.

3.1 General information about service project Z1

3.1.1 Project title: MEMS magnetoelectric sensor fabrication

3.1.2 Research area(s):

406-02 Synthesis and Properties of Functional Materials

3.1.3 Project leader(s)

Meyners, Dirk, Dr. rer. nat.
22.05.1973, German

Niekiel, Florian, Dr.-Ing.
01.09.1987, German

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Is the employment of the project leader(s) at the institution(s) indicated contractually fixed for the duration of the proposed funding period?

Meyners, Dirk, Dr.: yes, Niekiel, Florian, Dr.: no

Do any of the above mentioned persons hold fixed-term positions?

Meyners, Dirk, Dr.: no, Niekiel, Florian, Dr.: yes, (end date 28.02.2021)

In the case of funding, Florian Niekiel will be employed at least until the 30.06.2024 by Fraunhofer ISIT.

Funding for the project leader(s) at the institution(s) indicated is covered by core support: yes

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

The primary objective of **Z1** is the microelectromechanical systems (MEMS) fabrication of magnetoelectric (ME) sensors to enable the realization of the CRC's scientific work program and to provide the different projects with fully or partially processed sensors for their research tasks. While new sensor concepts are pioneered in the **A** projects, the **B** projects need a sufficiently large number of reliable sensors with reproducible sensor characteristics. Thus, **Z1** acts as the interface between the project areas **A** and **B**. It provides technological support to the **A** projects and makes the new findings of these projects available for the **B** projects.

To achieve this objective, **Z1** maintains a technology platform providing both full fabrication flows as well as separate process modules. **Z1** closely collaborates with the **A** projects during the technological realization of new sensor concepts, which results in separate process modules to aid the research. Upon maturity of the sensor concepts, the separate process modules are integrated to a full fabrication flow, capable of providing fully fabricated sensors for the projects of area **B**. In this way, **Z1** regularly implements new sensor concepts and technologies into the technology platform, making them accessible to all projects in the CRC.

Within the first funding period, a cross-institutional technology platform has been established. This platform combines the capabilities of CAU and ISIT in the field of bulk-micromachining (BMM) and surface-

micromachining (SMM), and in the processing of different materials. At present, the platform comprises three full process flows for various designs of resonant, ΔE -effect sensors and sensors for frequency conversion approaches. In addition, process modules are provided for fabrication of electrically modulated, piezotronic, and surface acoustic wave (SAW) sensors.

This existing technology platform will serve as a starting point for the proposed funding period. In the course of the studies, the platform will be revised, extended, and adapted to the newest findings in and needs of the research projects. The work plan focuses on technology platform revisions, fabrication of MEMS ME sensors as well as integration of new concepts and materials. The next steps for the technology platform include – but are not limited to – the integration of the separate process modules into a full flow for the fabrication of SAW sensors and the integration of a process module for powder-based permanent magnets (**A1**, **A2**).

3.2.1 Report and current state of research

Aside from biomagnetic diagnostics, there are manifold possible applications of ME composites as magnetometers, energy harvesters, tunable microwave devices such as inductors, band-pass filters, antennas, current sensors, and ME random access memories [Ch18, Tu19]. Applicability of MEMS ME structures is further increased because of miniaturization and on-chip integration with readout electronics. However, it is even more remarkable that only few research groups have reported on MEMS-fabricated ME sensors [On11, Pr11, Ma12, Ma13, Na13, Na17, Be17, Ng18, Bh19]. In these reports, BMM as well as SMM approaches are taken to create free-standing, often resonating ME structures. Besides the integration of ME materials without functional degradation, the reduction of residual mechanical stress have been identified as major issue to MEMS ME devices [On11, Ma13, Be17], which confirms our own results.

At the beginning of the first funding period, separate fabrication flows for various ME sensor concepts have been available from prior work. The project started with an intensive technological exchange for platform definition. Feasible magnetostrictive, piezoelectric materials, layer stacks, substrates, process sequences, and finally complete cross-institutional flows were identified. For the last, mutual compatibility of the different process steps is a key requirement. A cross-institutional technology platform has been established and maintained within **Z1**, relying on the combination of resources and capabilities of both institutes. The current platform comprises AlN and AlScN as piezoelectric materials as well as FeCoSiB and exchange biased FeCoSiB multilayers as magnetostrictive materials. The concentration of the process flows within the technology platform allowed focused and efficient work on the complex fabrication process for the most promising process flows as well as the fabrication of ME sensors themselves. A large number of ME sensors have been fabricated within **Z1** to serve the demands within the CRC. In addition, the research on new sensor concepts in the **A** projects has been supported with partly processed wafers.

ME sensor fabrication

Over the course of the first funding period, it has been identified that a treatment of the fabrication flows in the cross-institutional technology platform separated by technology variant is beneficial for the overall organization. At the beginning, the fabrication was implemented and organized according to a baseline flow combining BMM and SMM technology variants to benefit from common process modules. However, the strong differences in technology (compare Fig. Z1-1) demands different design rules which results in different mask sets. Furthermore, the differences in processing and process complexity result in strongly varying lead times. A temporal decoupling of the different variants was necessary, which led to a split into separate organizational entities. This does not alter the fact that the fabrication flows of the different variants are strongly linked on the technology level. Especially the functional layers, namely the piezoelectric and magnetostrictive thin films, are shared by the fabrication flows to leverage the available expertise and resources. The fabrication flows established and maintained within the technology platform to the end of the first funding period are summarized in Fig. Z1-1.

Wafer-cut ME sensors

Within the technology platform, the process flow of wafer-cut ME sensors is by far the simplest in terms of microsystem technology (compare Fig. Z1-1). It is based on double-side polished wafers with the functional piezoelectric and magnetostrictive layers being deposited on the top and bottom sides, respectively. In a final step, the wafers are cut into cantilevers using a dicing saw. Finished sensors are shown in Fig. Z1-2a. By its simplicity, the risk of degrading functional materials properties during processing is minimized. In particular, partially processed wafer-cut structures often serve as templates for materials research in the **A** projects [Z1-4, Z1-9]. **A7** demonstrated the feasibility of converse ME sensors applying wafer-cut ME structures [Ha18].

Z2 has assembled wafer-cut ME sensors forming tuning forks and used them for measurements on phantoms. In the **B** projects, this kind of sensor was used to confirm noise modelling and test read-out techniques [Z1-5 – Z1-10]. Due to their size, resonant frequencies at about 1 kHz are comparatively low and the typical achievable limit of detection (LOD) is on the order of 1 pT/Hz^{1/2} in resonance.

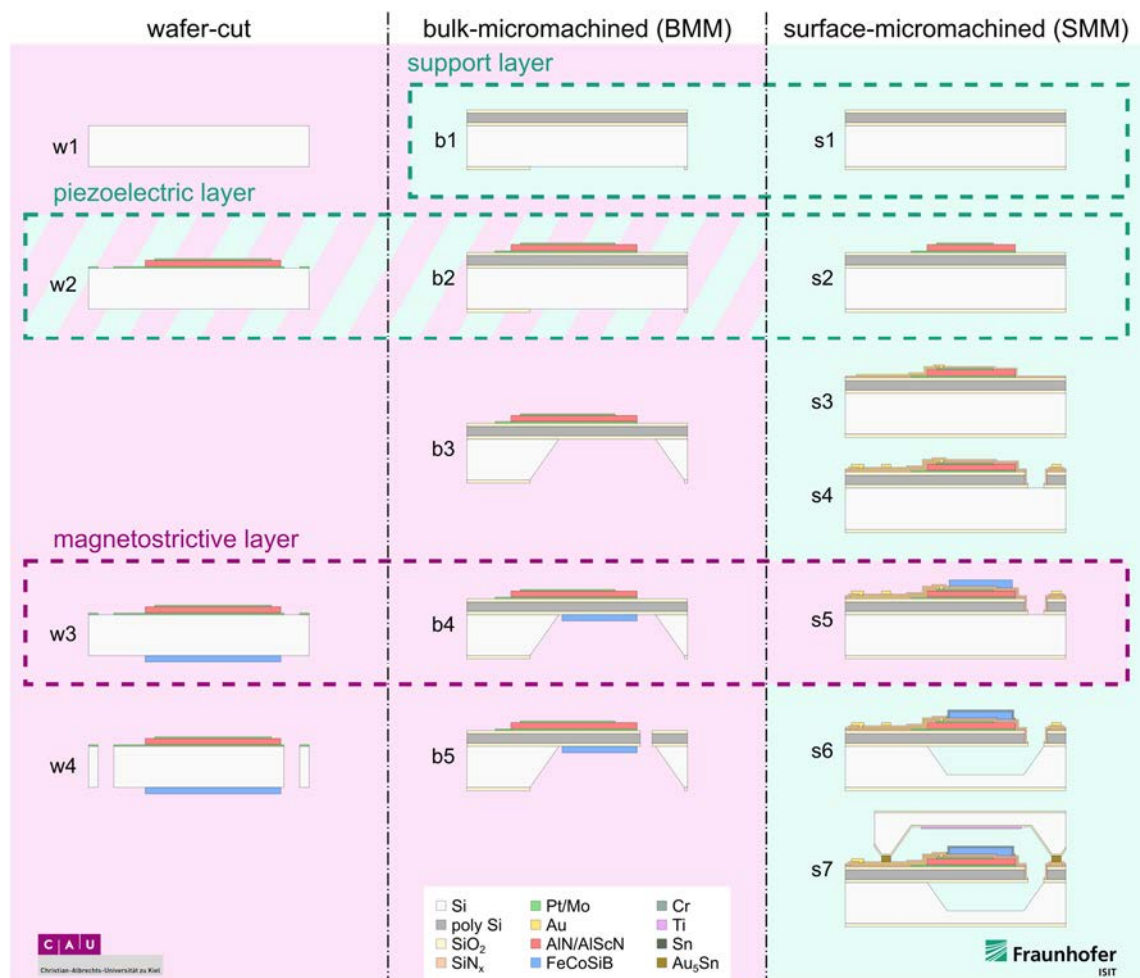


Figure Z1-1: Process flows maintained by the cross-institutional technology platform for wafer-cut, BMM, and SMM ME sensor fabrication. The background colour encodes the institute executing the process step.

Wafer-cut ME sensors (typical cantilever size 26.25 mm x 2.45 mm x 350 µm):

- w1: double-side polished Si wafer, 350 µm thickness,
- w2: sputter depos. and structuring of piezoelectric layer stack on frontside (e.g. Ta / Pt / AlN / Cr / Au),
- w3: sputter depos. and structuring (ion beam etching) of FeCoSiB-based magnetostrictive layer on backside,
- w4: dicing into cantilevers.

BMM ME sensors (typical cantilever size 3 mm x 1 mm x 50 µm):

- b1: oxidized silicon wafer with polished poly Si layer, diced into 5 x 5 cm² substrates, structuring of rear SiO₂,
- b2: sputter depos. and structuring of piezoelectric layer stack (e.g. Ta / Pt / AlN / Cr / Au),
- b3: wet etching of bulk Si by KOH or TMAH (buried SiO_x functions as etch stop),
- b4: sputter depos. and structuring (ion beam etching) of FeCoSiB-based magnetostrictive layer on backside,
- b5: cantilever release by means of deep reactive ion etching.

SMM ME sensors (typical cantilever size 1 mm x 200 µm x 12 µm):

- s1: oxidized 200 mm silicon wafer with polished poly Si layer,
- s2: sputter depos. and structuring of piezoelectric layer stack (e.g. Pt / AlN or AlScN / Mo),
- s3: low-stress PECVD SiN_x layer and sputtered Au for wiring of the piezoelectric layer,
- s4: preparation of frontside for release etch (opening poly Si, low-stress nitride and bondframe deposition),
- s5: sputter depos. and structuring (ion beam etching) of FeCoSiB-based magnetostrictive layer,
- s6: release etch from the surface in TMAH after protecting the magnetostrictive layer with a Cr thin film,
- s7: vacuum wafer-level packaging with cap wafer by Au-Sn transient liquid phase bonding and chip dicing.

Bulk-micromachined ME sensors

The flow of BMM ME sensors allows for the deposition of piezoelectric and magnetostrictive layers on opposite substrate sides, too. The major difference to wafer-cut sensors is given by the much smaller sensor size with lateral cantilever dimensions down to 1 mm x 3 mm (compare Fig. Z1-2b). The sensor outline is fabricated by means of optical lithography and wet and dry etching. The thickness of the freestanding cantilever is determined by a buried poly Si layer and amounts to either 25 μm or 50 μm . Due to their smaller dimensions, BMM ME sensors are suitable for use in sensor arrays (**B1**, **Z2**). Furthermore, this kind of sensor is investigated as ΔE -effect sensors in **A4**. In collaboration with **A4**, a redesign has been undertaken to enable investigation of torsional and bending modes of sensor operation. **B7** successfully applied BMM ME sensors for magnetic particle mapping.

Whereas highly sophisticated magnetostrictive multilayers can be integrated into wafer-cut ME sensors, the integration into the flow of BMM sensors is much more challenging (Fig. Z1-1, b4). Because of the deposition into a cavity, the flow has been revised two times (see section “Process integration and new technologies” below). For substrate thicknesses of 25 μm and 50 μm , the LOD reaches 5 to 10 $\text{pT}/\text{Hz}^{1/2}$ and 2 to 5 $\text{pT}/\text{Hz}^{1/2}$ in mechanical resonance at either 4.5 kHz or 7.5 kHz, respectively.

Surface-micromachined ME sensors

Following the flow summarized in Fig. Z1-1, SMM ME sensors have been fabricated within **Z1**. An example sensor is shown in Fig. Z1-2c. The first wafer run has been conducted in close collaboration with **A1**, **A3**, and **A4**. Several aspects of the fabrication technology have been investigated, which yielded an improvement of the overall process flow (e.g. a low-stress SiN_x protective layer, ion beam etching of FeCoSiB, and a Cr layer to protect the magnetostrictive layer). Due to the high complexity, especially related to the wafer-level vacuum packaging and the necessary experiments during fabrication, the completion of the first wafer run took 14 months. From the first run, 191 cantilever sensors were retrieved with the best ones reaching an LOD of 50 $\text{pT}/\text{Hz}^{1/2}$ in resonance for direct detection (resonance frequencies from 7 kHz to 19 kHz) for cantilevers only 1000 μm x 200 μm in size. In comparison to the best BMM ME sensors, the LOD is degrading by about one order of magnitude. This is a result of enhanced demagnetization effects and the exposure of FeCoSiB to the elevated temperature during wafer level packaging. The fabricated sensors are further studied in collaboration with **A3** (resonant sensors), **A4** (ΔE -effect sensors), **A8** (modelling), and **B7** (magnetic particle imaging). After a phase of technology and design review, a second wafer run has been started which is still ongoing. Further experiments are included to optimize the deposition of the piezoelectric layer, the surface for the deposition of the magnetostrictive layer, and the release etch. The organization of the redesign in the style of multi-project wafers adopted from foundry services has been particularly fruitful. Design rules have been distributed within the CRC together with a description of the technology and intended cross section. Together with technical support by **Z1**, several projects (**A3**, **A4**, **A8**, **B7**) have contributed to the design for the second wafer run.

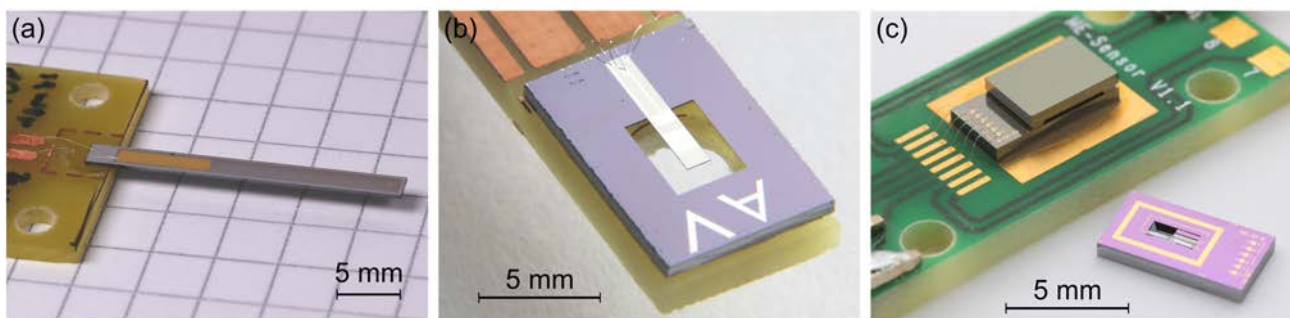


Figure Z1-2: Photographs of the fabricated wafer-cut (a), BMM (b), and SMM ME sensors (c).

Process integration and new technologies

Besides the fabrication of ME sensors, the second objective of **Z1** has been the integration of new technologies into the cross-institutional technology platform. This reflects the necessity to keep the technology platform flexible and capable of reacting to new concepts and new findings within the CRC and make them available for the research projects. As part of process integration, partial wafer processing has been offered as a service for process modules, where the first steps of integration have been overcome. This has relieved the work load in the research projects, especially in project area **A**.

Magnetostrictive layer

As one of the functional materials, the magnetostrictive phase has substantial impact on the achievable ME sensor performance. Therefore, it needs to be integrated into the process flow without degrading its magnetic and magnetoelastic properties. In close collaboration with **A1**, effects were investigated that emerged from deposition and structuring the magnetic material as well as other ME sensor fabrication steps (results of wafer mapping of magnetic anisotropies are discussed in the **A1** proposal). The lift-off technique has proven to be unsuitable for pattern transfer, as shadowing effects near the resist structures cause a significant reduction in deposition rate. Hence, multilayers exhibiting thin non-magnetic interlayers cannot be fabricated without pinholes at the boundary area. In contrast to that, a flat surface of magnetostrictive structures was achieved by a combination of UV lithography with subsequent ion beam etching. Even several micron thick magnetic layers were successfully patterned without heating them by ion bombardment to temperatures higher than 80 °C. The surface of resulting magnetic structures is smooth (see Fig. Z1-3). The edge profile flattens out and the edge angle can be tailored to between 45° and 170° by adjusting the angle of ion incidence. Flat edges can be used to reduce stray field-induced magnetization effects (**A1**).

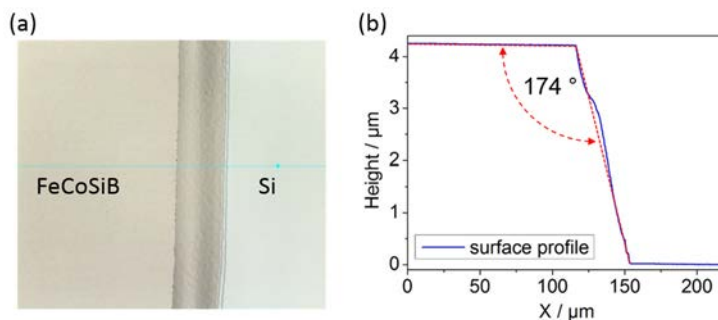


Figure Z1-3: (a) Optical micrograph captured by a confocal LASER scanning microscope at the edge of a 4 μm thick exchange biased FeCoSiB stack. Structuring was conducted by IBE with 400 eV Ar ions at an angle of incidence equal to 30°. (b) Edge profile along the line indicated in (a).

According to Fig. Z1-1, the magnetostrictive layer for BMM ME sensors must be deposited into a cavity on the wafer backside (b4 in Fig. Z1-1). In such cases, the resist is applied by spray-coating to ensure homogeneous resist coverage across the cavity. In addition, the tone of the lithography mask was inverted, which changed the lithography to negative exposure. By this, reflections from the cavity edges and undesired UV light exposure are diminished. Resulting resist profile and cross-sectional analysis of a structured magnetostrictive multilayer are shown in Fig. Z1-4. For further improvement and in collaboration with **A1**, ongoing work is considering a new process flow that enables the deposition of piezoelectric and magnetostrictive layers on one wafer side. Such a new flow includes chemical-mechanical-polishing of AlN/Cr/Au/SiO₂ to provide a smooth surface for the subsequent FeCoSiB multilayer growth.

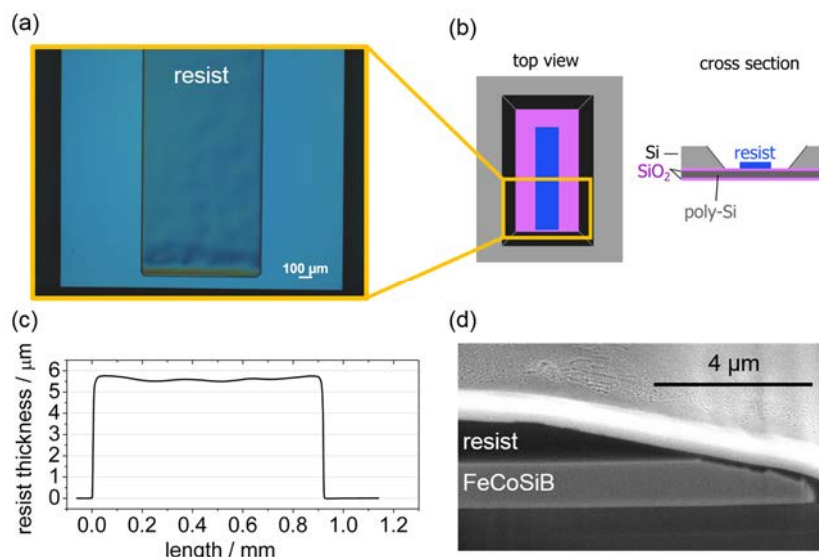


Figure Z1-4: Structuring of magnetic layers in a cavity of a BMM sensor. (a) Optical micrograph of the resist after spray-coating, exposure, and development. (b) Schematic illustration of (a) in top and cross-sectional view. (c) Surface profile measured across the resist structure displayed in (a). (d) Cross section of structured magnetic layer using spray-coating and IBE.

The integration of exchange biased magnetostrictive multilayers in the SMM fabrication flow turned out to be more challenging. To explore size effects, e.g., FeCoSiB multilayers were deposited and patterned into desired sensor structures for magneto-optical characterization in **A1**. While compatibility with the following processes (structuring, protection, and release etch) could be demonstrated, the temperatures necessary for the bonding process deteriorate the magnetic properties. The exchange biased multilayer has a significantly lower temperature budget. Work is currently ongoing to test a post-bonding magnetic annealing on wafer-level to restore the exchange bias configuration.

Piezoelectric layer

Two deposition processes for AlN were available from prior work (pulsed-DC sputtering at 200 °C (CAU) [Ya16] and pulsed-DC sputtering at 400 °C (ISIT) [Ma12]) and have been implemented in the cross-institutional technology platform. In addition, the promising novel piezoelectric material AlScN has been integrated during the first funding period [Z1-3]. It was successfully used during the first run of the SMM ME sensor fabrication flow. A direct comparison of cantilever sensors with AlN and AlScN operated in direct detection (compare report **A3**) showed higher sensitivities but also higher voltage noise densities for the AlScN variant. Ongoing investigations are focusing on the influence of a change in the piezoelectric layer on the performance of other sensor concepts. First results show an increased electromechanical coupling coefficient for AlScN, which is expected to enhance the performance of the ΔE -effect sensor concept (**A4**).

The planned variant of BMM ME sensors with sol-gel deposited PZT was dropped from the technology platform. Together with **A3**, the technological challenges have been evaluated versus the potential benefits. The high losses of PZT due to its hysteretic ferroelectric nature and the challenging integration of PZT in the complex ME sensor fabrication led to this decision. The liberated resources have been used to strengthen AlScN integration and the additional work with respect to SAW sensors.

Vacuum packaging

Vacuum packaging of ME sensors is important to increase their performance by reducing air damping as well as protect the sensitive part from environmental influences. In addition, sensitivity to shock loading is reduced by providing mechanical limits to the deflection of the movable structure. Wafer-level vacuum packaging of ME sensors fabricated using the SMM process flow (compare Fig. Z1-1) was advanced with further experiments. A Ti thin film as a getter material was added to further improve the vacuum. A full activation of the getter material requires temperatures of 400 °C, which exceeds the tolerable limit of 350 °C before degradation of the magnetostrictive material [Hr14]. Experiments were conducted with partial activation at 330 °C during bonding as well as bonding at a lower temperature and performing a post-annealing for getter activation. The investigated processes have successfully been applied during sensor fabrication following the SMM process flow, which has led to sensors with quality factors of 1500 - 3500.

Deviating from the original work plan, packaging of BMM ME sensors has not been conducted in this funding period. Instead, work on magnetostrictive layer integration and fabrication of partially processed wafers was intensified at CAU. Outside the CRC a process for encapsulation of BMM energy harvesters has been developed in cooperation between ISIT and CAU. This technology can serve as a basis for future vacuum encapsulation of BMM ME sensors fabricated within the CRC.

Vector field sensors

It was planned to study the assembly of 3D vector field ME sensors within **Z1**. To bring down complexity to a manageable amount, an assembly based on vacuum packaged ME sensors fabricated by SMM with exchange biased magnetostrictive layers was planned. The vacuum packaging is necessary for the mechanical support of the 3D assembly, and the implementation of the exchange biased magnetostrictive layer is a prerequisite to omitting biasing coils. Due to technological issues with the compatibility of exchange biased magnetostrictive layers and vacuum packaging technology (temperature sensitivity), the experiments on vector field ME sensors have not started yet. Preliminary work has been conducted on influences of neighboring cantilever sensors in collaboration with **A3** and **A8** on ME sensor arrays.

SAW guiding layer

During the investigations on SAW ME sensors by **A3**, the demand for high quality SiO₂ layers as wave guides emerged with additional requirements regarding very low surface roughness for the subsequent deposition of the magnetostrictive layer. This could be established with the resources available in the cross-institutional technology platform and resulted in a process module for the deposition and polishing of high quality SiO₂ guiding layers on 100 mm substrates. This process module has been elaborated in close collaboration with **A3** and can now be executed by **Z1**, as requested by **A9**.

The work on SAW ME sensors was not scheduled in the original project plan but is an example on how **Z1** reacts to the newest findings of the **A** projects. The collaboration has been found to be especially fruitful, promoting the initial idea of partially processed wafers provided by **Z1** to separate process modules. The gradual transition from first experiments led by **A3** to the operation of the complete process module by **Z1**

results in a relief of resources in the scientific projects, while at the same time ensuring an efficient and productive implementation.

Powder-based permanent magnets

A cleanroom compatible processing technology to integrate powder-based materials into MEMS has been developed at ISIT in collaboration with the CAU outside the CRC in a different project (BMBF 16ES0186K) focused on energy harvesting [Re16,Z1-2]. This technology allows the integration of powder-based volumetric permanent magnets fabricated from commercial NdFeB powder filled into Si cavities and solidified with an ALD layer. In this project, energy harvesters excited by magnetic interaction have been studied. Due to the similarities to resonant ME sensors, the capabilities within the CRC have been used to probe these harvesters as magnetic field sensors. Despite the fact that these devices were not optimized for sensor applications, very promising first results could be obtained (compare report **A3**) [Z1-1]. A LOD below $10 \text{ pT/Hz}^{1/2}$ has been achieved in resonance at frequencies of 2.2 kHz and 3.6 kHz. For direct detection with sensors not requiring an additionally provided DC bias magnetic field, these sensors are competitive with the best ME sensors (i.e. the BMM sensors with exchange biased magnetostrictive multilayers).

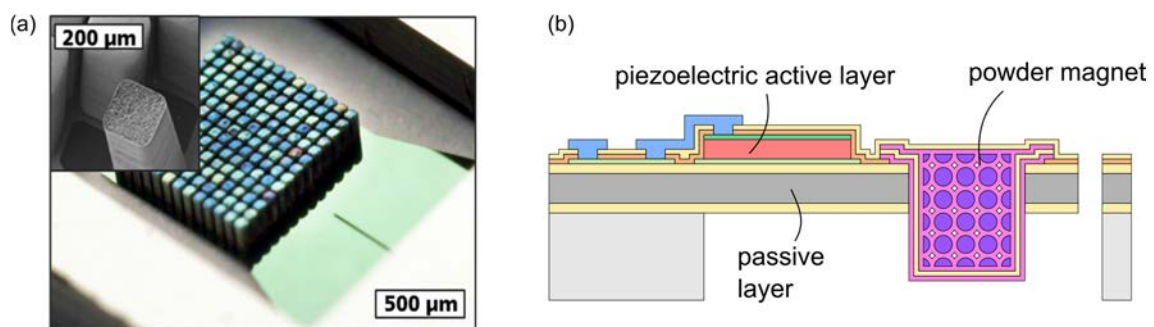


Figure Z1-5: (a) Photograph of magnets protruding through the tip of a cantilever made from polycrystalline Si and a piezoelectric AlN thin film (viewed from the backside). The inset shows an SEM image of a single magnet with broken tip revealing the solidified powder microstructure. (b) Schematic cross section of the technology used for the fabrication [Z1-1].

References

- [Be17] S. P. Bennett, J. W. Baldwin, M. Staruch, B. R. Matis, J. LaComb, O. M. J. van 't Erve, K. Bussmann, M. Metzler, N. Gottron, W. Zappone, R. LaComb, P. Finkel, Magnetic field response of doubly clamped magnetoelectric microelectromechanical AlN-FeCo resonators. *Appl. Phys. Lett.* **111**, 252903 (2017).
- [Bh19] D. Bhatia, H. Sharma, R. S. Meena, V. R. Palkar, Confirmation of spatial coexistence of magneto-electric coupling in Bi_{0.7}Dy_{0.3}FeO₃ thin films integrated with Si/ZnO film for MEMS and memory applications. *Journal of Materials Research and Technology.* **8**, 553–560 (2019).
- [Ch18] Z. Chu, M. PourhosseiniAsl, S. Dong, Review of multi-layered magnetoelectric composite materials and devices applications. *J. Phys. D: Appl. Phys.* **51**, 243001 (2018).
- [Ha18] P. Hayes, V. Schell, S. Salzer, D. Burdin, E. Yazar, A. Piorra, R. Knöchel, Y. K. Fetisov, E. Quandt, Electrically modulated magnetoelectric AlN/FeCoSiB film composites for DC magnetic field sensing. *J. Phys. D: Appl. Phys.* **51**, 354002 (2018).
- [Hr14] V. Hrkac, E. Lage, G. Köppel, J. Strobel, J. McCord, E. Quandt, D. Meyners, L. Kienle, Amorphous FeCoSiB for exchange bias coupled and decoupled magnetoelectric multilayer systems: Real-structure and magnetic properties. *J. Appl. Phys.* **116**, 134302 (2014).
- [Ma12] S. Marauska, R. Jahns, H. Greve, E. Quandt, R. Knöchel, B. Wagner, MEMS magnetic field sensor based on magnetoelectric composites. *J. Micromech. Microeng.* **22**, 65024 (2012).
- [Ma13] S. Marauska, R. Jahns, C. Kirchhof, M. Claus, E. Quandt, R. Knöchel, B. Wagner, Highly sensitive wafer-level packaged MEMS magnetic field sensor based on magnetoelectric composites. *Sens. and Actuators, A* **189**, 321–327 (2013).
- [Na13] T. Nan, Y. Hui, M. Rinaldi, N. X. Sun, Self-biased 215 MHz magnetoelectric NEMS resonator for ultra-sensitive DC magnetic field detection. *Scientific reports.* **3**, 1985 (2013).
- [Na17] T. Nan, H. Lin, Y. Gao, A. Matyushov, G. Yu, H. Chen, N. Sun, S. Wei, Z. Wang, M. Li, X. Wang, A. Belkessam, R. Guo, B. Chen, J. Zhou, Z. Qian, Y. Hui, M. Rinaldi, M. E. McConney, B. M. Howe, Z. Hu, J. G. Jones, G. J. Brown, N. X. Sun, Acoustically actuated ultra-compact NEMS magnetoelectric antennas. *Nature communications.* **8**, 296 (2017).

- [Ng18] T. N. Nguyen, Characterization and Modeling of Magnetoelectric Micro Sensor, Dissertation, Université Paris-Saclay (2018).
- [On11] T.-D. Onuta, Y. Wang, C. J. Long, I. Takeuchi, Energy harvesting properties of all-thin-film multiferroic cantilevers. *Appl. Phys. Lett.* **99**, 203506 (2011).
- [Pr11] K. Prashanthi, M. Mandal, S. P. Duttagupta, R. Pinto, V. R. Palkar, Fabrication and characterization of a novel magnetoelectric multiferroic MEMS cantilevers on Si. *Sens. Actuators, A* **166**, 83–87 (2011).
- [Re16] T. Reimer, F. Lofink, T. Lisec, C. Thede, S. Chemnitz, B. Wagner, Temperature-stable NdFeB micromagnets with high-energy density compatible with CMOS back end of line technology, *MRS Adv.* **1**, 209–213 (2016).
- [Tu19] C. Tu, Z.-Q. Chu, B. Spetzler, P. Hayes, C.-Z. Dong, X.-F. Liang, H.-H. Chen, Y.-F. He, Y.-Y. Wei, I. Lisenkov, H. Lin, Y.-H. Lin, J. McCord, F. Faupel, E. Quandt, N.-X. Sun, Mechanical-Resonance-Enhanced Thin-Film Magnetoelectric Heterostructures for Magnetometers, Mechanical Antennas, Tunable RF Inductors, and Filters. *Materials (Basel, Switzerland)*. **12** (2019).
- [Ya16] E. Yazar, V. Hrkac, C. Zamponi, A. Piorra, L. Kienle, E. Quandt, Low temperature aluminum nitride thin films for sensory applications. *AIP Advances*. **6**, 75115 (2016).

3.2.2 Project-related publications by participating researchers

a) Peer-reviewed publications and books

- [Z1-1] **F. Niekietl**, J. Su, M. T. Bodduluri, T. Lisec, L. Blohm, I. Pieper, B. Wagner, **F. Lofink**, Highly Sensitive MEMS Magnetic Field Sensors with Integrated Powder-based Permanent Magnets. *Sens. Actuators, A* **297**, 111560 (2019).
- [Z1-2] E. Yazar, S. Fichtner, P. Hayes, A. Piorra, T. Reimer, T. Lisec, P. Frank, B. Wagner, **F. Lofink**, **D. Meyners**, E. Quandt, MEMS-Based AlScN Resonating Energy Harvester With Solidified Powder Magnet. *J. Microelectromech. Syst.*, 1–13 (2019)
- [Z1-3] S. Fichtner, N. Wolff, **F. Lofink**, L. Kienle, B. Wagner, AlScN: A III-V semiconductor based ferroelectric. *J. Appl. Phys.* **125**, 114103 (2019).
- [Z1-4] M. Jovičević Klug, L. Thormählen, V. Röbisch, S. D. Toxværd, M. Höft, R. Knöchel, E. Quandt, **D. Meyners**, J. McCord, Antiparallel exchange biased multilayers for low magnetic noise magnetic field sensors. *Appl. Phys. Lett.* **114**, 192410 (2019).
- [Z1-5] S. Salzer, V. Röbisch, M. Klug, P. Durdaut, J. McCord, **D. Meyners**, J. Reermann, M. Höft, R. Knöchel, Noise Limits in Thin-Film Magnetoelectric Sensors With Magnetic Frequency Conversion. *IEEE Sensors J.* **18**, 596–604 (2018).
- [Z1-6] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, J. McCord, **D. Meyners**, E. Quandt, G. Schmidt, R. Knöchel, M. Höft, Improved Magnetic Frequency Conversion Approach for Magnetoelectric Sensors. *IEEE Sens. Lett.* **1** (2017).
- [Z1-7] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, P. Hayes, A. Piorra, **D. Meyners**, E. Quandt, G. Schmidt, R. Knöchel, M. Höft, Thermal-Mechanical Noise in Resonant Thin-Film Magnetoelectric Sensors. *IEEE Sensors J.* **17**, 2338–2348 (2017).
- [Z1-8] S. Salzer, P. Durdaut, V. Röbisch, **D. Meyners**, E. Quandt, M. Höft, R. Knöchel, Generalized Magnetic Frequency Conversion for Thin-Film Laminate Magnetoelectric Sensors. *IEEE Sensors J.* **17**, 1373–1383 (2017).
- [Z1-9] V. Röbisch, S. Salzer, N. O. Urs, J. Reermann, E. Yazar, A. Piorra, C. Kirchhof, E. Lage, M. Höft, G. U. Schmidt, R. Knöchel, J. McCord, E. Quandt, **D. Meyners**, Pushing the detection limit of thin film magnetoelectric heterostructures. *J. Mater. Res.* **32**, 1009–1019 (2017).
- [Z1-10] J. Reermann, C. Bald, S. Salzer, P. Durdaut, A. Piorra, **D. Meyners**, E. Quandt, M. Höft, G. Schmidt, Comparison of reference sensors for noise cancellation of magnetoelectric sensors. *2016 IEEE SENSORS*, 1–3 (2016).

b) Pending patents

- [Z1-P1] U. Hofmann, H. J. Quenzer, F. Niekietl: Mikromechanische Aktuatorvorrichtung und Verfahren zu dessen Herstellung, DE 10 2017 205 047

Please note that with this proposal Dr.-Ing. Florian Niekietl takes over the responsibilities of former project leader Dr. Fabian Lofink in **Z1**. Therefore, both authors have been accounted for in the above publication list.

3.3 Project plan

Objectives

The cross-institutional technology platform has been established and been proven functional within the first funding period. The primary objective of **Z1** is to provide the following services within the CRC:

- Fabrication of sensors with the full process flows maintained within the technology platform, from designs developed in the **A** projects for applications in the **B** projects,
- Support in the realization of sensor concepts from **A** projects by taking over processing tasks as process modules maintained within the technology platform,
- Technological consulting on feasibility and implementation possibilities.

Besides these services, the internal project goals of **Z1** for the second funding period focus on improvement and expansion of the technology platform to ensure efficient and up-to-date MEMS ME sensor fabrication for the CRC.

- Improving the technology covered by the platform to enhance performance, reliability, and yield,
- Integration of new technologies based on the latest results of the CRC,
- Continuing the supply of resonant ME sensors beyond the discontinuation of **A3**.

Proposed research methods

The work in **Z1** will be done at the Kieler Nanolabor (CAU) and at the Fraunhofer Institute for Silicon Technology (ISIT) in Itzehoe. The cross-institutional technology platform depends on the resources and capabilities of both institutions and cannot operate without the close collaboration of all scientists involved.

CAU

In 2017 the Kieler Nanolabor was registered by the DFG as a core facility in the category of micro- and nanotechnology. The cleanroom comprises class 100 and class 1000 areas with a total footprint of 300 m². The laboratory provides equipment for BMM of substrates with diameters up to 150 mm. In December 2017, a new magnetron sputter deposition tool (*von Ardenne* CS400) with 9 sputter sources for piezoelectric and magnetic layer growth was successfully installed. By substrate rotation, the new tool enables the deposition of complex magnetostrictive multilayers with high homogeneity across 200 mm wafers. At the Kieler Nanolabor the following techniques are available for layer deposition: magnetron sputter deposition, plasma enhanced chemical vapor deposition, pulsed laser deposition, atomic layer deposition, sol-gel, and electroplating. In addition to conventional optical lithography (up to 150 mm wafers with backside alignment), electron beam lithography and laser writing are accessible. Pattern transfer can be done by either wet chemical treatment, reactive ion etching, or ion beam etching. The last dry etching technique is essential for successful pattern transfer to magnetostrictive multilayers. A complete list of currently installed tools is given in section REF and online on the webpage of the Kieler Nanolabor (<http://www.kompetenzzentrum-nanosystemtechnik.uni-kiel.de/de/nanolabor/ausstattung>).

The highly flexible process management allows fast response to new research findings in the **A** projects so that new materials and concepts can be efficiently transferred to the technology platform. Special aspects of the work in Kiel deal with the integration of complex magnetostrictive layer systems and the low-temperature and low-stress deposition of AlN by pulsed-DC sputtering. The BMM approach to fabricate ME sensors has the advantage that processing both sides of a substrate can be performed in a straightforward manner. This possibility increases the degree of freedom of sensor design and enables the deposition of magnetostrictive and piezoelectric layers on smooth substrate surfaces without the need for stacking them (compare Fig. Z1-1). In the current funding period of the CRC 1261, various process flows for ME sensors were established in the Kieler Nanolabor.

ISIT

Fraunhofer ISIT operates a MEMS cleanroom with a footprint of 1000 m² with a variety of methods of micro- and nanotechnology in Itzehoe as well as a branch office on site with the CAU in Kiel. Extensive equipment for the deposition and patterning of thin film materials, including chemical vapor deposition, physical vapor deposition, lithography, wet and dry etching as well as wafer-level packaging is available. Basic device characterization of fabricated devices is executed at ISIT with semi-automatic electrical wafer testing. For the assembly of sensor systems, dedicated tools are available. In the ISIT MEMS cleanroom, various SMM ME

sensors were fabricated within the current phase of CRC 1261. A focal topic at ISIT is the deposition and integration of piezoelectric thin films. Two cluster tools are available with the capabilities of growing PZT, AlN, and AlScN thin films as well as the necessary metal electrodes. Advanced characterization tools are at hand for the evaluation of the piezoelectric performance. Continuous efforts are made in the improvement and reliability of the piezoelectric materials. ISIT further provides the equipment and processes necessary for the integration of powder-based permanent magnets, which will further be developed and enhanced in the following years. The process for the integration of powder-based permanent magnets is fully compatible with the fabrication of piezoelectric MEMS devices.

Both for the preparation of BMM and SMM ME sensors, thick epitaxially grown and polished polycrystalline Si on SiO₂ is used as a substrate. This substrate layer permits precise control of the substrate thickness, enables high Q-values, and gives additional design freedom, e.g. for coupled sensor structures. Silicon wafers with this layer structure are fabricated at ISIT using the established Poly-Si technology platform. SMM ME sensors are fabricated using the capabilities to release freestanding microstructures from the frontside available at ISIT. These include dry gas-phase etching using XeF₂ and wet chemical etching using Si-enriched tetramethylammonium hydroxide (TMAH) and potassium hydroxide (KOH). The frontside release is especially important to enable the hermetic wafer-level vacuum packaging in the next step. The available bonding processes include anodic, glass frit, and transient liquid phase bonding, while vacuum is ensured by the addition of metallic thin film getter material.

Workplan

The work packages within the service project **Z1** are best understood by looking at the role **Z1** plays within the CRC, schematically sketched in Fig. Z1-6. The **A** projects focus on sensor technology, conceiving and testing different physical realizations for new sensor concepts. The **B** projects integrate the sensor devices on a system level to do application-related research. The technology platform of **Z1** is at the interface between the two project areas, picking up the newest findings from the **A** projects and making them available to the **B** projects in form of sensor devices. The service project **Z2** acts as the interface between **Z1** and the **B** projects.

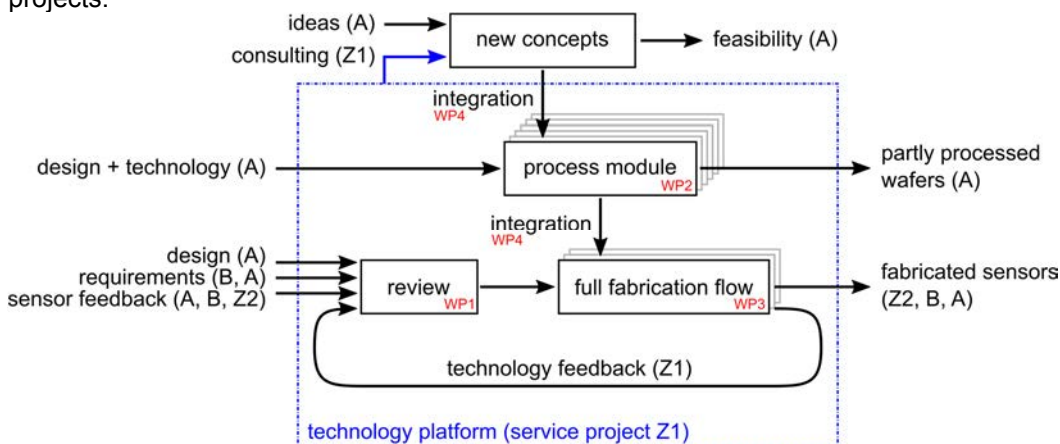


*Figure Z1-6:
Definition of the
technology platform
maintained by Z1 and its
role within the CRC.*

The transfer of new technologies conceived in the **A** projects takes place in a two-step process to ensure agility and the ability to react to the newest findings from the **A** projects or changed requirements from the **B** projects in a timely manner. With the increasing technology-readiness level of a new technology investigated in project area **A**, **Z1** starts integrating the technology or parts of it in one or more process modules (WP4). These process modules are maintained within the technology platform and can be executed by **Z1** upon request (WP2). In this way, processing load is taken over by **Z1** during the fundamental research on a sensor concept, which causes a relief of resources in the scientific projects. The experience and expertise available in the **Z1** ensures an efficient and purposeful work on the fabrication processes.

Upon maturity of the sensor concept, the second step of process integration is done (WP4), elaborating a full fabrication flow based on the separate process modules and available standard processes. The full fabrication flows are maintained and executed by **Z1** (WP3) to yield functional sensor devices for use in the **B** projects but also to create feedback for the **A** projects, e.g. in form of parameter studies. The fabrication flows are executed in a cyclic manner. Before the next cycle, the flow undergoes a phase of review and redesign (WP1) that involves the responsible **A** projects for a continuous improvement of the fabricated sensors. A special situation is given for the concept of resonant ME sensors. These have been studied in detail in **A3**. This concept has reached maturity, where a dedicated scientific project cannot be maintained. To sustain the availability of resonant ME sensors within the CRC, the service project **Z1** takes over the responsibility

(WP5). Besides the fabrication of these sensors, the work done by **Z1** will include implementation of technological improvements and the adaptation of the designs to specific requirements for applications. A chronology of the work packages is given in Tab. Z1-1. Due to the strong service nature of the work done by **Z1** and the high dynamics of the research done within the CRC, a precise temporal separation of the work packages is challenging. The aim is to provide the services as they are needed by following a priority scheme. Only the cycles of the full fabrication flows are planned on a fixed schedule.

Table Z1-1: Time schedule of work packages in Z1.

	2020		2021				2022				2023				2024	
	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2
WP1: Review of technology platform																
WP2: Process modules for fabrication of MEMS ME sensors																
WP3: Full flow fabrication of MEMS ME sensors																
WP4: Integration of new technologies																
WP5: Resonant magnetoelectric sensors																

CAU (Meyners)
 ISIT (Niekiel)

WP1: Review of the technology platform

WP1 is the work package continuously updating the definition of the cross-institutional technology platform to further improve its performance and react to new findings from within the CRC as well as from the outside. The main work in WP1 is strongly linked to the execution of the full fabrication flows (WP3). In advance of the next run, the complete fabrication flow is reviewed and adjusted to make adaptations concerning peculiarities and new findings learned from the last run. Besides feedback from the characterization of the fabricated sensors in **Z2**, test structures are included in the design to perform process control monitoring within **Z1**. The documentation is updated and distributed within the CRC, including the available materials, critical dimensions, and design rules. An iteration of the designs is organized by **Z1**, where the sensor concept specific expertise of the **A** projects and the requirements of the **B** projects are combined, resulting in a new multi-project wafer mask set for the next run. This leads to a peak activity in WP1 before the scheduled full flow fabrication runs, as shown in Tab. Z1-1. The less complex process management allows more frequent revisions of the BMM flow.

Additional work in WP1 relates to the process modules and process integration in WP2 and WP4, respectively. Within WP1 new findings and technologies are reviewed to identify the technologies which are to be integrated into the technology platform within WP4. It further is the work package where the feedback from the other projects of the CRC is collected, reviewed, and appropriate measures are derived to ensure the optimal benefit of **Z1** for the CRC. These are ongoing tasks, not captured in Tab. Z1-1. Time available to the end of the project will be used to review the technology platform in preparation of the next phase of the CRC.

WP2: Process modules for the fabrication of ME sensors

WP2 covers the work on the separate process modules maintained within the technology platform. While the initial process integration is captured in WP4, WP2 comprises the execution and further enhancement of the process modules offered to the **A** projects. The objective pursued with WP2 is to take over processing load from the scientific projects to relieve their resources. In addition, the expertise and experience combined within **Z1** ensures an efficient and productive processing. The process modules maintained in the cross-institutional technology platform also act as an intermediate step to a full fabrication flow. The research and testing performed as separate process modules are necessary steps before the integration into full fabrication flows.

The process modules currently maintained within the cross-institutional technology platform include:

- The preparation of substrates with polished, low-stress poly-Si layer of controlled thickness, acting as an elastic layer for the definition of flexible resonating structures,
- Deposition and structuring of magnetostrictive layers and multilayer stacks (FeCoSiB, exchange biased multilayers),
- Deposition and structuring of piezoelectric thin film stacks including electrodes (AlN, AlScN),
- Deposition and polishing of high quality PECVD SiO₂ guiding layers on 100 mm wafers (SAW),

- Sensor templates for the evaluation of new functional materials and sensor concepts.

The list of process modules on offer is expanded to react to the discoveries within the CRC. For the second funding period, it is planned to include a process module for the integration of permanent magnets, which is based on the recently developed fabrication technique using powder agglomeration. Besides its use for resonant sensors (compare WP5), this technology is of high interest for the **A** projects working on sensor technology. Collaboration with **A1** is planned to investigate the applicability of integrated permanent magnets as sources for bias magnetic fields controlling the magnetic orientation of magnetostrictive thin films. Together with **A2**, the use of powder-based permanent magnets in hybrid magnetoelectric sensors will be studied, e.g. for attractive and repulsive potential contributions to the energy landscape of the movable part.

WP3: Full flow fabrication of ME sensors

WP3 comprises the fabrication of ME sensors following various sensor concepts in the form of multi-project wafer runs. The full fabrication flows maintained within the technology platform build the basis for sensor fabrication in this work package. The work is not limited to the technical execution of the flows but includes the scientific work critical to successful fabrication, enhancement of the understanding of interplay between the processes, and the necessary experiments to improve the used technology.

With the experience gained over the first funding period of the CRC, the fabrication flows are treated as separate entities to ease their organization. They are inevitably linked on the technology level by sharing process steps and mutually benefit from each other (compare Fig. Z1-1). Especially the core competencies of building the functional layers, namely the piezoelectric and magnetostrictive thin films, are common in all fabrication flows. The different fabrication flows are assigned to an institution to lead its organization based on where the majority of process steps are executed. From the work of the previous funding period, the technology platform currently maintains three full fabrication flows, listed in Tab. Z1-2. The large number of flows maintained within the technology platform is necessary to serve the needs of the CRC, as they bring distinct features not possible otherwise (compare Tab. Z1-2). For the second funding period, a fabrication flow for SAW sensors based on 150 mm quartz wafers will be added. While the necessary process integration work will be done in WP4, the execution and iterative enhancement of the flow is part of WP3.

The schedule for WP3 as shown in Tab. Z1-1 represents the cycles planned for the bulk- and surface-micromachined sensor fabrication. It accounts for the time necessary for the characterization of the fabricated sensors and the increased processing time due to the complexity of the fabrication flows, as learned during the first funding period. In synchronization with the scientific projects, the cycles are aligned to the beginning of the second phase. In this way, additional time for sensor evaluation is available at the end, which will be used by **Z1** for review and to prepare the first fabrication runs of the third phase.

*Table Z1-2: Full fabrication flows maintained by **Z1** within the cross-institutional technology platform.*

Fabrication flow	wafer-cut	bulk-micromachined	surface-micromachined
Distinct features	fast processing, perfect surfaces for deposition	miniaturization	miniaturization, hermetic vacuum encapsulation
Application fields	templates for materials research & new sensor concepts, tuning fork, converse ME sensors, noise and transfer function modelling	Resonant sensors, magnetic modulation, ΔE -effect sensors	Resonant sensors, ΔE -effect sensors
Magnetostrictive materials	Advanced magnetic multilayers	Parallel exchange biased multilayers	Integration of exchange biased multilayers ongoing
Piezoelectric materials	AlN/AlScN	AlN/AlScN	AlN/AlScN
Planned cycles	continuous	6	3
ME sensors / wafer	32	60	380

WP4: Integration of new technologies

WP4 comprises the process integration work necessary to transfer the new technologies identified in WP1 to process modules (WP2) or full fabrication flows (WP3) maintained within the cross-institutional technology platform. It focuses on the initial establishment of new processes into process modules and full fabrication flows for WP3 and WP2. As process integration for new technologies is a major challenge in MEMS fabrication, it can only efficiently and purposefully be done by the experienced scientists in **Z1** who combine the

expertise and resources of both institutes. The work on integration explicitly includes the early support of the scientific projects. Technical consulting provided as part of **Z1** within WP4 helps the scientific projects to find a feasible technological realization for a sensor concept.

As seen in Tab. Z1-1, WP4 is an ongoing work package reacting to the findings of the **A** projects and the requirements of the **B** projects. The first tasks for the following funding period include a process module for the integration of powder-based permanent magnets (to become part of WP2) and the setup of a full fabrication flow for SAW sensors (to become part of WP3). Fig. Z1-7 shows the starting point for this fabrication flow on 150 mm quartz wafers. The work with respect to the integration of magnetostrictive multilayers is continued. Exchange biased multilayers with anti-parallel magnetization in adjacent magnetostrictive layers need to be integrated into BMM ME sensors as well as exchange biased multilayers into SMM ME sensors.

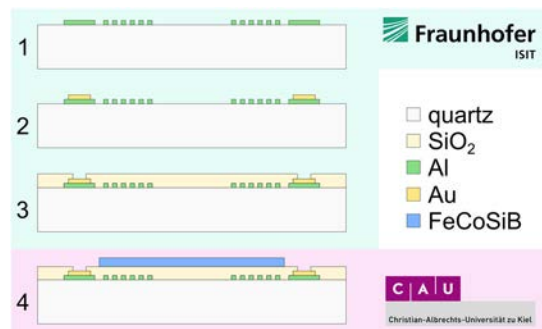


Figure Z1-7: New process flow for the fabrication of SAW magnetic field sensors based on ST-cut 150 mm quartz wafers to be included in the technology platform:

*1: deposition of Al thin film and high resolution structuring of interdigital transducer electrodes,
2: deposition and structuring of Au bond pads,
3: PECVD deposition of SiO₂ with subsequent CMP polishing and dry etching to open bond pads,
4: low temperature sputter deposition of magnetostrictive layer and structuring.*

WP5: Resonant ME sensors

Within WP5 **Z1** takes over work with respect to the resonant ME sensor concept within the CRC. This sensor concept has been studied extensively within **A3** and reached maturity. To ensure the availability of resonant ME sensors to the CRC (especially the applications in **B7** and **B9**), the following tasks are part of WP5:

- Design of resonant ME sensors with respect to requirements from **B** projects (e.g. frequency, size)
- Evaluation of the sensors fabricated as part of WP3 and characterized by **Z2** to further enhance the fabrication process and improve sensor performance, reproducibility, and reliability,
- Further research on resonant sensors excited by the interaction of powder-based magnets.

Prospects

The main objective of **Z1** will remain in the fabrication of sensors based on the findings of the **A** projects for the applications in the **B** projects as well as the technical support of the pioneering work performed within the **A** projects. The major challenge is to keep the cross-institutional technology platform maintained by **Z1** up-to-date to the newest findings in the **A** projects, while at the same time ensure a steady fabrication of sensors in sufficiently high numbers with low variance in properties. This can only be achieved by an agile approach of expanding the technology platform as needed but also keeping it focused to sustain operation. On a broader time scale, **Z1** will be challenged by technological developments which at the same time provide opportunities for further enhancement. In particular, platform integration of the concepts for hybrid and piezoelectric ME sensors (**A5**) will pose a specific challenge as these concepts involve new multifaceted materials. Underlined by the rise of the SAW ME sensor, future technological requirements will enforce the need for high resolution lithography. This will require invest in new equipment, e.g. e-beam lithography. Over the maturing of the CRC, the focus is anticipated to shift from research on sensor concepts towards applications relying on the studied sensors. **Z1** plays an important role in this development. As seen from the example of resonant sensors, **Z1** takes over the responsibility for matured sensor concepts to ensure their availability for the **B** projects beyond the point where a dedicated scientific project cannot be maintained within the CRC.

3.4 Role within the Collaborative Research Centre

The service project **Z1** plays an important role within the framework of the CRC, as – together with **Z2** – it acts as the interface between the project areas **A** and **B**. While the **A** projects pioneer new sensor concepts, the **B** projects implement the sensors in biomedical applications. The scientific work of the **B** projects relies on the availability of sufficiently large numbers of sensors with reliable and reproducible sensor characteristics. The researchers of **Z1** will participate in the focus groups “Magnetic Layers” and “ME Sensors”. Collaborations with the following projects are planned:

- A1** Providing partially-processed wafers and sensor templates for studies on magnetic multilayers; integration of new magnetic multilayers and powder-based permanent magnets.
- A2** Providing processes for piezoelectric and magnetostrictive functional layers as well as partially processed cantilevers exhibiting magnetostrictive layers and powder-based permanent magnets.
- A4** Supply of ΔE -effect sensors for comparison; technical consulting with respect to external fabrication, support in the realization of post-fabrication processes, esp. the magnetostrictive functional layer.
- A5** Providing partially-processed wafers, esp. piezoelectric and magnetostrictive functional layers for piezotronic magnetometers.
- A6** Advanced characterization of functional materials to improve fabrication technology and for identification of process real structure interrelations.
- A7** Fabrication of converse ME effect sensors; support in miniaturization of the sensor concept.
- A9** Partial processing of SAW sensor wafers as process module; implementation of full fabrication flow on 150 mm quartz wafers.
- A10** Providing ME sensor structures for research on magnetic noise modelling.
- B1** Providing ME sensors in various concepts for studies on sensor noise performance, feedback regarding sensor performance.
- B2** Providing a sufficient number of ME sensors for studies on digital signal processing, feedback regarding sensor performance.
- B7** Design and fabrication of resonant sensors for particle imaging; focus on miniaturization to improve resolution, feedback regarding sensor performance.
- B9** Design and fabrication of resonant ME sensors for movement analysis, focus on tuning adjustment of the resonance frequency, feedback regarding sensor performance.
- B10** Providing a sufficient number of ME sensors for magnetocardiography.
- Z2** Electronics assembly and characterization of ME sensors; feedback regarding sensor performance.
- T1** Fabrication of ME sensors.

3.5 Differentiation from other funded projects

The proposed project is not in conflict with any other funded projects of the principal investigators.

3.6 Project funding

3.6.1 Previous funding

Funding of this project within the Collaborative Research Centre 1261 started in July 2016.

3.6.2 Requested funding

Funding for	2020/2		2021		2020		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Postdoctoral researcher, 100 %	2	74.1	2	148.2	2	148.2	2	148.2	2	74.1
Total		74.1		148.2		148.2		148.2		74.1
Direct costs	Sum		Sum		Sum		Sum		Sum	
Equipment up to k€ 10, software, consumables CAU	8		8		9.5		12		2.5	
Equipment up to k€ 10, software, consumables ISIT	8.2		9		9.7		8.4		1.7	
Total	16.2		17		19.2		20.4		4.2	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation up to k€ 50	0		0		0		0		0	

Total	0	0	0	0	0
Grand total	90.3	165.2	167.4	168.6	78.3

(All figures in k€)

3.6.3 Requested funding for staff for the new funding period

	Se- quen- tial no.	Name, academic degree, position	Field of research	Department of university or non-university institution	Project com- mitment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1.	Meyners, Dirk, Dr., Senior Re- searcher	Functional Materials	IMS	4		Core support
	2.	Niekiel, Florian, Dr., Postdoctoral Researcher	MEMS	ISIT	8		Fraun- hofer
	3.	Lisec, Thomas, Dr., Senior Re- searcher	MEMS	ISIT	2		Fraun- hofer
	4.	Malavé, Antonio, Dr., Senior Re- searcher	Functional Materials	IMS	2		Core support
Non-research staff	5.	Metzing, Thom- as, Dipl.-Ing., Engineer		IMS	2		Core support
	6.	Pieper, Isa, Dipl.- Ing., Engineer		ISIT	4		Fraun- hofer
	7.	Heinrich, Felix, Dipl.-Ing., Engi- neer		ISIT	4		Fraun- hofer
Requested staff							
Research staff	8.	Kittmann, Anne, M.Sc., Postdoc- toral Researcher	Functional Materials	IMS		E14	
	9.	N.N., Postdoc- toral Researcher	MEMS	ISIT		E14	

Job descriptions of staff for the proposed funding period (supported through existing funds):

1. Dr. Dirk Meyners represents **Z1** with regard to wafer-cut and BMM ME sensors. He supervises the postdoctoral researcher at the CAU and supports planning and execution of ME sensor fabrication in Kiel. He coordinates the cooperation with other projects of the CRC together with Dr. Niekiel.
2. Dr. Florian Niekiel is responsible for the coordination and the scientific management of the part of **Z1** carried out at Fraunhofer ISIT. Together with Dr. Meyners, he represents the project within the CRC and externally. He supervises the postdoctoral researcher at the ISIT and supports the planning and execution of the work and evaluation of the results.
3. Dr. Thomas Lisec is the scientist in charge of the powder MEMS technology at ISIT. He supports the postdoctoral researcher in the integration of the powder-based permanent magnet process module.
4. Dr. Antonio Malave is the responsible scientist for the operation and maintenance of the Kieler Nanolabor. He will support the researcher at the CAU in the selection, planning, and execution of the MEMS processes.
5. Dipl.-Ing. Thomas Metzing will provide technical support at the CAU including maintenance of clean-room equipment.
6. Dipl.-Ing. Isa Pieper aids the postdoctoral researcher in the coordination of the fabrication in the cleanroom at ISIT (programming the MES, conducting measurements, inspecting the wafers in-between processing steps).
7. Dipl.-Ing. Felix Heinrich aids the postdoctoral researcher in the characterization of test structures and devices using electrical wafer test.

Job descriptions of staff for the proposed funding period (requested funds):

8. It is planned to employ M.Sc. Anne Kittmann as postdoctoral researcher. Since end of 2014 she investigates bulk-micromachining of ME cantilever and SAW sensors. She received her degree in materials science from CAU in June 2015. After one year parental leave, she is expected to finish her doctoral thesis "Magnetic field sensors based on Love-wave SAW devices" in April 2020. Benefitting from several years of experience, she conducts the processing of wafer-cut and bulk MEMS ME sensors as well as partly processed wafers at the Kieler Nanolabor (WP2, 3 and 5). She works on the extension of the technology platform to new bulk-micromachined sensor concepts (WP4). Because her scope of duties comprises process integration, process adaptation as well as coordinating and managing of the technology platform (WP1), a postdoc position is requested.
9. The postdoctoral researcher is in charge of the scientific work and support tasks (WP1-WP5) planned in this project taking place at ISIT. He/She will closely coordinate and collaborate with the postdoctoral researcher at CAU. As the tasks involve process integration and adaption as well as coordination and managing of the technology platform, a postdoctoral researcher is requested.

3.6.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/2
CAU: existing funds from CAU	3	6	6	6	3
Sum of existing funds	3	6	6	6	3
Sum of requested funds	16.2	17	19.2	20.4	4.2

(All figures in k€)

Equipment up to k€ 10, software, consumables for financial year 2020/2		CAU	ISIT
Si wafer, quartz wafer	k€	1.5	2.2
Lithography masks	k€	1.5	4.8
Sputter and evaporation deposition targets and materials (FeCoSiB, MnIr)	k€	3.0	3.0
Consumables for dry/wet etching, lithography, vapour deposition, assembly and packaging	k€	2.0	1.2

Equipment up to k€ 10, software, consumables for financial year 2021		CAU	ISIT
Si wafer, quartz wafer	k€	3.0	0.8
Lithography masks	k€	1.0	
Sputter and evaporation deposition targets and materials (Au, Al, Pt, AlSc, FeCoSiB)	k€	2.0	3.9
Magnetic powder (NdFeB)	k€		0.3
Consumables for dry/wet etching, lithography, vapour deposition, assembly and packaging	k€	4.0	4.0

Equipment up to k€ 10, software, consumables for financial year 2022		CAU	ISIT
Si wafer, quartz wafer	k€	1.5	2.1
Lithography masks	k€	2.0	4.8
Sputter and evaporation deposition targets and materials (FeCoSiB, Ta, Cu)	k€	2.0	
Consumables for dry/wet etching, lithography, vapour deposition, assembly and packaging	k€	4.0	2.8

Equipment up to k€ 10, software, consumables for financial year 2023		CAU	ISIT
Si wafer, quartz wafer	k€	3.0	0.6
Lithography masks	k€	2.0	
Sputter and evaporation deposition targets and materials (Au, Al, Pt, AlSc, FeCoSiB, MnIr)	k€	3.0	3.9
Magnetic powder (NdFeB)	k€		0.3
Consumables for dry/wet etching, lithography, vapour deposition, assembly and packaging	k€	4.0	3.6

Equipment up to € 10, software, consumables for financial year 2024/1		CAU	ISIT
Si wafer, quartz wafer	k€	0.5	0.3
Lithography masks	k€	0.5	
Consumables for dry/wet etching, lithography, vapour deposition, assembly and packaging	k€	1.5	1.4

3.1 General information about Project Z2

3.1.1 Project title: Magnetoelectric Sensor Characterization

3.1.2 Research areas:

408 Electrical Engineering
 408-01 Electronic Semiconductors, Components, Circuits, Systems
 408-02 Communications, High-Frequency and Network Technology, Theoretical Electrical Engineering

3.1.3 Project leaders

Höft, Michael, Prof. Dr.-Ing.
 02.07.1972

Schmidt, Gerhard, Prof. Dr.-Ing.
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Do any of the above-mentioned persons hold fixed-term positions? No

3.1.4 Legal issues

This project includes

1.	research on human subjects or human material.	no*
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

*All measurements on volunteers and human material are performed by related medical persons under responsibility of the corresponding B projects. The central project **Z2** only supports the handling of those measurements.

3.2 Summary

The aim of this central project is the functional characterization of the different magnetoelectric sensors that are investigated and manufactured in the A projects using the electronic readout circuits and signal processing methods developed in **B1** and **B2**. It includes measurements of the spectral distribution of noise, the limit of detection (measured in resonance and with frequency conversion techniques), the bandwidth of operation, the robustness against acoustic interferences, and distortions produced by neighboring sensors, to name just a few. As for the already established sensor types, the measurement procedures will be automated for the new sensor concepts and corresponding support will be provided to the researchers from the related A and B projects. Furthermore, the results will be collected to perform a meaningful comparison of the sensor concepts characterized under the same measurement conditions.

To arrive at viable systems for biomedical diagnostics, sensor arrays will be built with sensors fabricated in **Z1**. The arrays will be investigated and related limits will be analyzed. Crucially, this will be done for a sensor array system suitable for deep brain stimulation (DBS) measurements from **T1** with the final goal to get completely rid of a head scanner. This will enable confident results for patients due to much faster measurement time. Related measurements on healthy subjects and patients will be prepared and support will be given to the

medical personnel. The same holds for the movement analysis **B9**, the cardiologic project **B10**, and the 3D flux density measurements for **B7**. In addition, the hardware in terms of amplifiers, signal generators, stimulators, and interfaces will be extended and enhanced permanently in this central project.

3.3 Project progress to date

3.3.1 Report and current state of research

State of knowledge and initial questions at the last application

The complete functional characterization of magnetoelectric sensors includes the measurement of the spectral distribution of noise, the limit of detection, the operation bandwidth, the influence of acoustic interference, and directional pattern. The measurements have to be done in both magnetically shielded and unshielded environments. The measurement results are stored in a database designed for the analysis and comparison of different sensor concepts. Another task of project **Z2** is the measurement support of medical applications as well as improvement of the head phantoms, head scanner, measuring electronic components, and adaptation of the sensors developed in the **A** projects and **Z1** for the measurements with the head scanner on head phantoms and later on patients.

Results, applied and possibly newly developed methods

Functional characterization of the ME sensors [Na08, Ya11] includes resonance frequency as well as bandwidth measurements, determination of the optimum DC magnetic bias field working point, limit of detection measurements, estimating the spectral distribution of noise, analyzing magnetic frequency conversion approaches, and directional pattern measurements. All these measurement procedures, except directional pattern analysis, are described in detail in [Ja13]. The method of measuring the directivity of another type of magnetic field sensor is given in [Ya00]. As an extension of the previous research, an automatic characterization system for cantilever-based ME sensors has been designed and implemented. To measure all the quantities mentioned above, a variety of different equipment has to be used that cannot be connected in parallel to the ME sensor systems (*Figure Z2-1*).

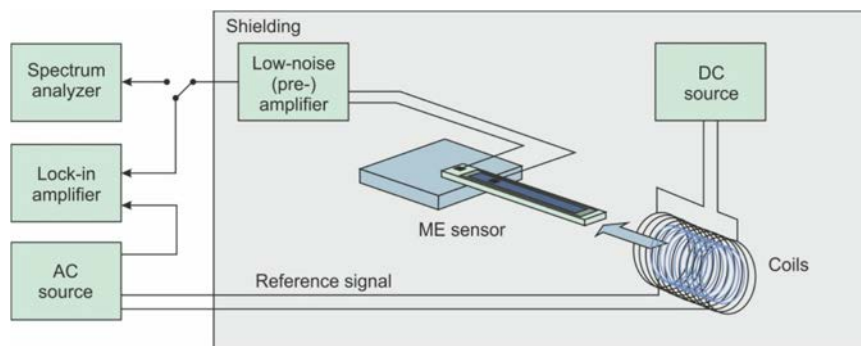


Figure Z2-1: Measurement setup diagram for ME sensor characterization. The sensor being tested along with low-noise preamplifier, battery as DC source, and testing coils are placed into electro-magnetically and acoustically shielded box for interference-free characterization. Spectrum analyzer, lock-in amplifier, and AC source, which are outside the shielding box, are used for measuring the ME sensor characteristics.

To overcome this problem, a relay switching unit has been designed (*Figure Z2-2*) for sequentially switching the signal from sensor to the required measuring instrument, and thereby avoiding mutual interference of the measuring equipment. The switching unit was tested with a calibrated magnetic field sensor to ensure that the unit does not produce additional noise or interference in the readout electronics.

The signal processing of the measured signals and their analysis are performed in a program developed in MATLAB. It contains a graphical user interface (GUI) for adjusting geometrical and physical properties of the measured sensor such as width, length, sensor material, etc., as well as parameters of the measuring equipment and low-noise amplifier. All these parameters are used for an automatically generated report after analysis of measured data. The measured sensor characteristics (by means of figures as well as recorded data) and the report file are saved on a dedicated server. Apache Subversion (SVN) was used for this purpose. Even if this is originally a version control system, the functionality of this software packages allows all CRC

members to have easy access to all measured results, to share analysis software and to be informed automatically if a new sensor was measured.

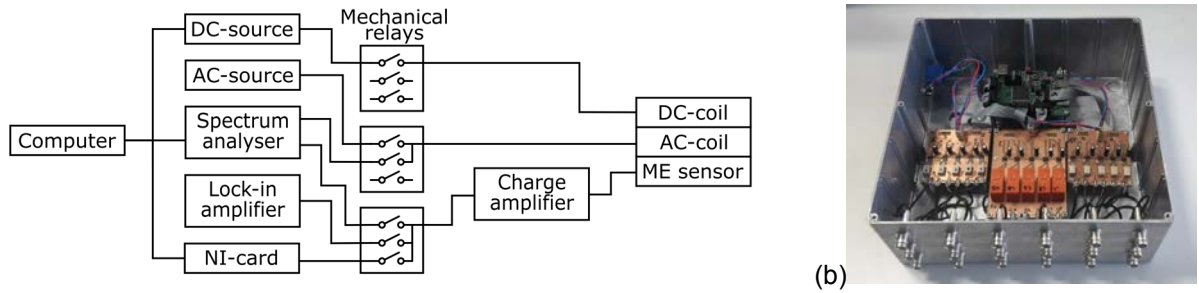


Figure Z2-2: Switching unit for the automatic measurement system: (a) switching diagram of the automatic measurement setup; (b) digitally controlled relay unit enclosed in an electrically shielded housing with microcontroller board and electro-mechanical relays ensures the interference-free operation of readout electronics during the noise-sensitive measurements.

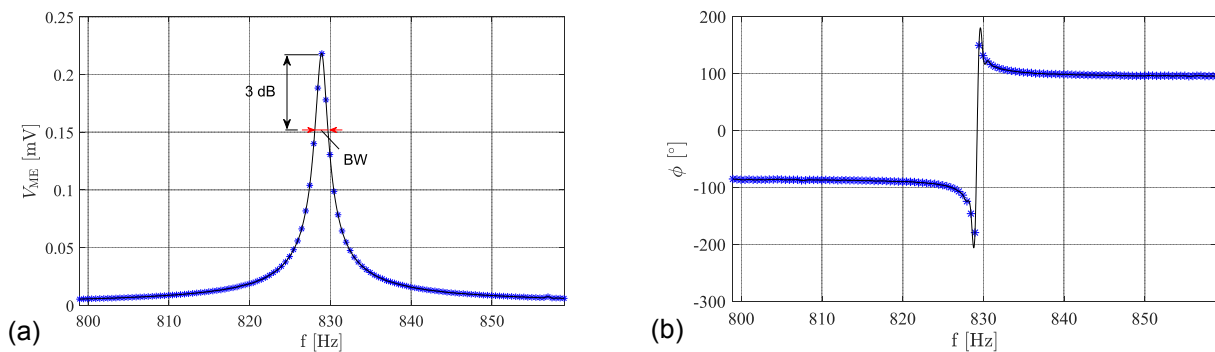


Figure Z2-3: Example frequency response of the cantilever (wafer cut) ME sensor: (a) amplitude response - the absolute value of the complex frequency response characteristic of the sensor permits defining an exact resonance frequency, bandwidth (BW), and Q-factor of the sensor; (b) phase response - the argument of the complex frequency response shows the 180-degree phase jump at the resonance frequency.

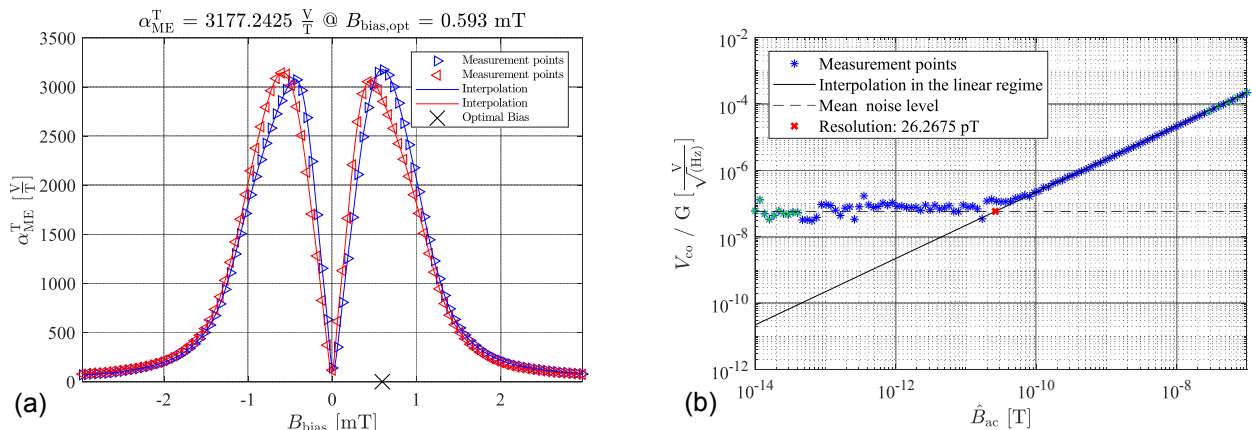


Figure Z2-4: Example DC magnetic bias curve (a) and linearity curve (b) of the cantilever (wafer cut) ME sensor measured at resonance frequency. The bias curve is measured at positive (red) and negative (blue) DC saturation with applied AC magnetic field of 100 nT amplitude. The bias curve is necessary for estimation of the optimal DC magnetic bias working point. The linearity measurement permits estimating the limit of detection (LOD), noise floor, and dynamic range of the sensor. The vertical axis in graph (b) represents the voltage across sensor electrodes without the low noise amplifier gain G .

As an example, Figures Z2-3 and Z2-4 represent the conventional measurement results of a standard ME cantilever sensor. For optimizing the measurement procedure, an algorithm that decreases the measurement time was implemented in the developed program. The measurement of the linearity curve of the cantilever sensors takes a long time because of the large number of measured points. However, it turned out that it was not necessary to perform measurements at every point of the range when the form of the characteristic is known (in our case – it is linear). Only a few measurements are needed in the range where the level of the

exciting magnetic field is large, and the same holds for ranges where the level is small and only the noise floor is measured, where the signal has a constant value on average. Then, by linearly extrapolating both measurement ranges on the whole measurement range, the intersection point of those two lines shows the limit of detection (LOD) of the measured sensor (Figure Z2-4b). The automatic measuring system also contains a function for characterizing ME sensors that utilizes magnetic frequency conversion (MFC) schemes, which are described in detail in [Ja12, Sa18].

The measurement function of the directional pattern of ME sensors has not been implemented into the automatic measurement system since a different measurement setup consisting of three mutually perpendicular Helmholtz coils (Figure Z2-5a) is required. The sensor to be investigated is located in the center of this setup. It is exposed to a homogeneous magnetic field which can be rotated in its orientation by proper excitation of the three coils. As a result, the directional pattern of the sensor (Figure Z2-5b) is measured. This measurement can be interpreted as the sensor's directional pattern in the far field, when the sensor size is much smaller than the distance to the measured source of the magnetic field.

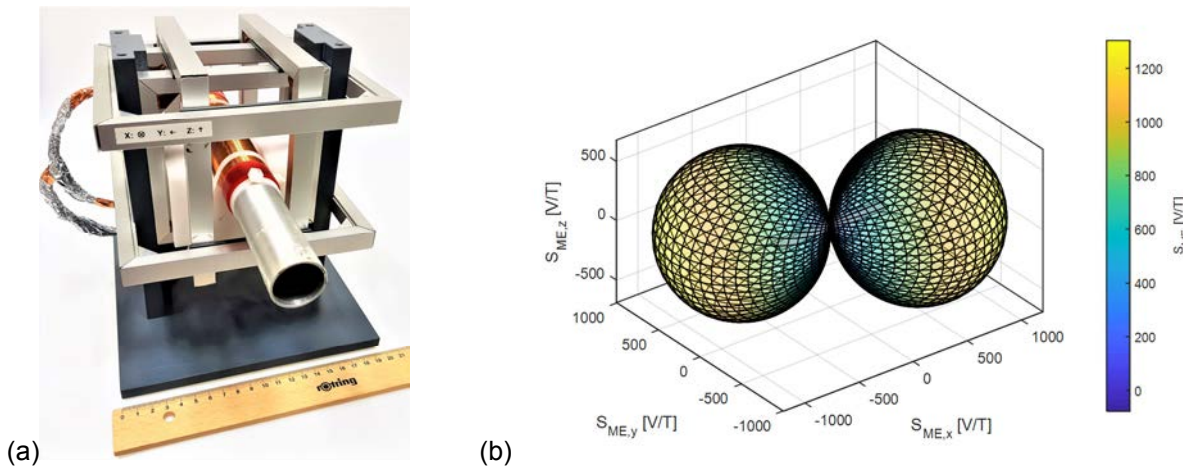


Figure Z2-5: (a) Measurement setup for directional characterization of magnetic field sensors. The setup consists of 3 mutually perpendicular Helmholtz coils that provide homogeneous rotating magnetic fields in the central area of the setup by manipulating AC currents in the coils. (b) 3D directional diagram of the wafer cut ME-sensor forms a dipole-like pattern.

However, the magnetic fields to be measured in biomedical applications usually have very low amplitude. Therefore, magnetic sensors have to be located close to the signal source. In this case, the detected fields cannot be considered homogeneous anymore, especially when relatively large sensors are used. That is why it is necessary to define the so-called “transfer function” of the sensor, in other words, the sensor sensitivity distribution along the longitudinal axis of the sensor. The “transfer function” of the ME cantilever sensor can be measured in the developed measuring setup (Figure Z2-6) which permits excitation of a local AC magnetic field by a single-loop coil that can be moved to arbitrary points along the longitudinal axis of the sensor.

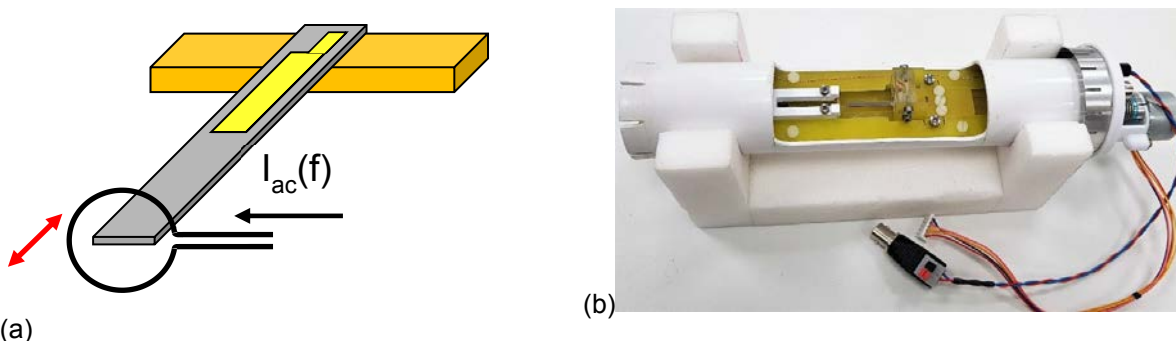


Figure Z2-6: Measurement setup for characterization of ME-sensor's “transfer function”. (a) Test signal $I_{ac}(f)$ with constant amplitude and sweeping frequency drives single-loop excitation coil which moves along the sensor. (b) Position of the single-loop coil is controlled by stepper motor with $10\ \mu\text{m}$ positioning accuracy. The measurement setup is used as part of the standard characterization system of ME sensors (Figure Z2-2).

Figure Z2-7 illustrates the complex-valued frequency response function (“transfer function”) along the longitudinal axis of the ME cantilever sensor measured in the setup described above (Figure Z2-6). The absolute value of the function represents the amplitude response (Figure Z2-7(a)) and the argument is the phase response of the “transfer function” (Figure Z2-7(b)). From the results presented in the figure, one can define the resonance frequency profile along the sensor for estimating the position of the most sensitive point along the sensor. The resonance interference effect in the form of a valley in the frequency range below the resonance, the so-called Fano resonance [Ge13], depends on the position of the local excitation source and causes the 180-degree phase jump in the region between the minima and the resonance. The positions of the minima depend on the sensor geometry and the properties of the magnetostrictive layer of the sensor. This measurement gives a deeper understanding of the sensor behavior and, hence, can theoretically help to optimize the sensor design to achieve better sensor characteristics. The “transfer function” is extremely important for developing and validating theoretical models of cantilever ME sensors developed in project **A8**, for studying U-modes of converse ME sensors designed in project **A7** [Z2-2, Z2-10] as well as for studying magnetic nanoparticles (project **B7**) [Fr19 and Z2-8]. Moreover, the estimated position of maximum sensitivity can be used for building ME sensor arrays and for solving the magnetic source localization problem studied in projects **B3** and **B5** [Z2-1 and Ha13].

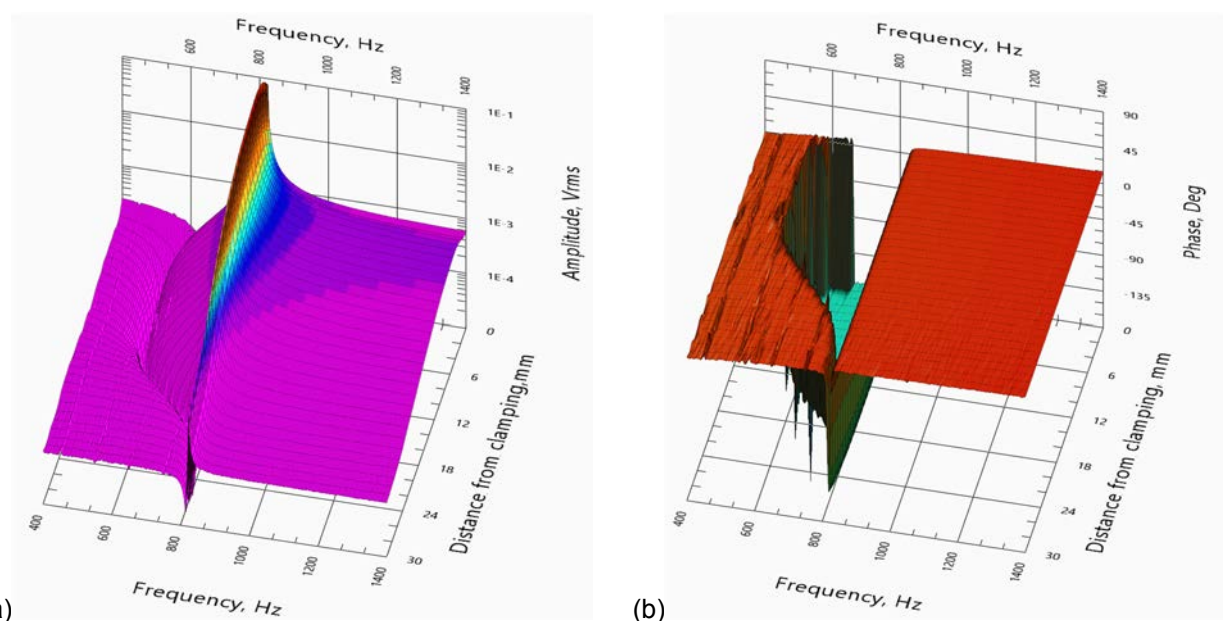


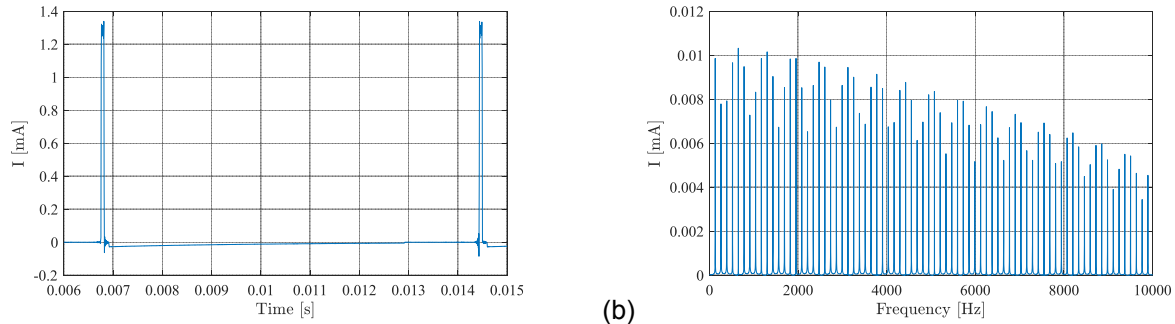
Figure Z2-7: Measured “transfer function” of the cantilever (wafer cut) ME sensor. (a) 3D representation of the amplitude response or absolute value of the complex-valued “transfer function” measured along the sensor shows the sensor sensitivity distribution along the sensor longitudinal axis and Fano resonance effect in form of a valley in frequency range between 600 Hz and 800 Hz. (b) 3D Phase response or the argument of the “transfer function” illustrates the 180-degree phase jump in the area enclosed by Fano effect and the fundamental resonance mode at 824 Hz.

One of the suitable biomedical applications which can be taken into consideration in the context of using the ME sensors invented and developed in the framework of the current CRC project is the measurement of real deep brain stimulation (DBS) signals (**B5**). Taking into account the fact that the magnetic fields generated by DBS electrodes have a broadband periodic frequency response [Z2-1] as indicated in Figure Z2-8 and very low amplitude (about 10 - 50 pT), a magnetic field sensor must meet certain requirements, namely sufficiently low detection limit, suitable operating frequency band, and interference-free operation.

At the beginning of CRC 1261, the most suitable magnetic field sensor for DBS measurements among the sensors invented and developed in the framework of the CRC project was the ME cantilever sensor with DC bias produced in projects **A3** and **Z1** [Ya16] that was expected to have an LOD of less than $10 \text{ pT/Hz}^{1/2}$ in resonance with a resonance frequency of about 850 Hz. The sensor is sensitive enough for detecting DBS magnetic fields and can measure one harmonic component of the complex DBS signal (Figure Z2-8b). However, it must be ensured that this frequency matches with the resonance frequency of the sensor.

Due to strong influence of vibrational and acoustic interference, the ME cantilever sensor cannot be used for the measurements of DBS signals (**B5**) as it is. One of the methods to suppress the interference is the combination of two identical ME cantilever sensors to a tuning fork as described in [Sa16]. The piezoelectric layer of the ME sensor is sensitive to electric fields generated by the DBS electrode and the electrode cable, as well

as ambient electromagnetic interference (50 Hz + harmonics). To overcome this problem, the sensor and the low-noise amplifier (LNA) must be electrically shielded, and the best solution for that is the integration of the sensor and the LNA into a single shielded sensor housing.



(a) (b)
Figure Z2-8: Measured waveform of the Boston Scientific DBS system with implementable current-controlled pulse generator. (a) In time domain the real DBS signal has form of a modified pulse train with pulse width of 60 – 120 μ s and pulse repetition frequency of 130 – 170 Hz. (b) Spectral representation of the DBS signal has multiple harmonics in increments equal to the pulse repetition rate.

Taking into account the above mentioned considerations and recommendations given in [Z2-4, Z2-7], some tuning fork constructions consisting of different ME sensors have been designed and fabricated along with the LNA [Z2-5] studied in project B1 and realized in compact form (Figure Z2-9, Z2-10).

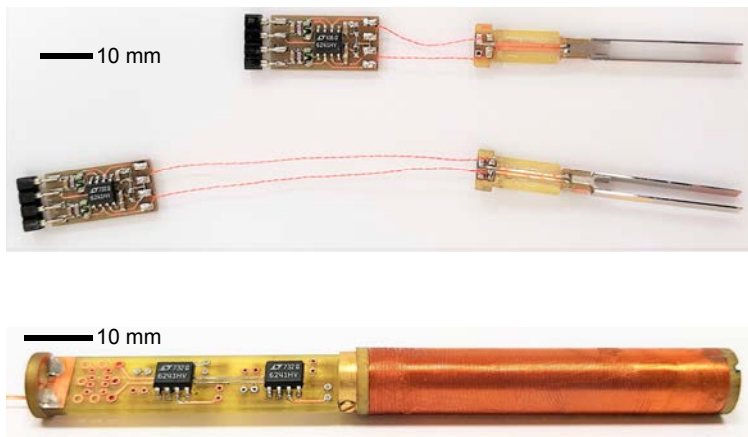


Figure Z2-9: Tuning forks with low-noise amplifier (LNA) boards for installing into shielded housing. The tuning forks consist of wafer cut cantilever ME composites comprising 300 μ m silicon substrate, 2 μ m AlN, and 2 μ m FeCoSiB. Every sensor has a charge amplifier based on a low noise operational amplifier LTC6241.

Figure Z2-10: Tuning fork with LNA board and DC bias coil driven with 30 mA current for generating optimal bias field of 0.35 mT.

A problem that occurred during the measurements with the developed ME tuning forks in the magnetically shielded chamber was the strong influence of acoustical and vibrational interference. The method of acoustical interference compensation used for the tuning fork design [Sa16] does not provide the required level of interference compensation. Originally, the method had been tested in an acoustically shielded environment by adding a stationary white noise acoustic signal as the source of interference. On the one hand, only a very small portion of interfering signal is being detected by the sensor due to its narrow bandwidths caused by the high value of the quality factor of the tuning fork resonator. Hence, even a quite high-energy, broadband, white noise, interfering signal induces a relatively small response of the sensor. On the other hand, the white noise signal is stationary, which means it has no amplitude spikes so that the tuning fork resonator does not enter the transient state. In other words, due to the relatively large relaxation time of the resonator, the measured amplitude of the white noise signal remains constant in time. The method works fine only for stationary interference, which is not the case under realistic measurement conditions.

One of the possible reasons for insufficient interference compensation was found to be a design feature of the tuning fork resonator, namely, that the cantilevers of the tuning fork are also sensitive to longitudinal component of the interference which cannot be compensated by the interference compensation concept, as reported in [Sa16]. To overcome this problem, we proposed the double tuning fork concept consisting of two identical tuning forks directed towards each other in such a manner that the maximum sensitivity of the individual tuning forks (see Figure Z2-7) coincide in space. The main idea was that the same longitudinal component of the acoustical interference should be detected by two individual tuning forks. This “double fork” setup generates two sensor response signals which have a 180° phase difference that can be compensated by further signal processing.

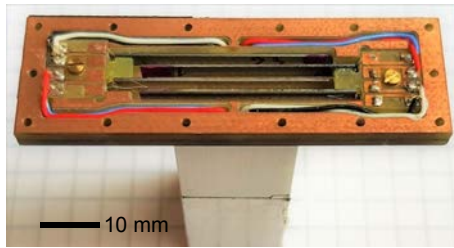


Figure Z2-11: Double tuning fork ME sensor with exchange bias ME composites enclosed in the electrically shielded housing.

Several double tuning fork designs (*Figure Z2-11, Z2-12*) have been investigated and the corresponding electronics have been designed, which includes multichannel LNA and DC low noise current sources in the case of biased sensors along with data processing software.

The evaluation of the presented sensor assemblies showed that the double-fork concept does not solve the problem of interference compensation to the necessary extent. A number of reasons may be the cause. The tuning forks are not exactly the same in terms of resonance frequencies, masses of the oscillating parts, clamping forces etc., which could cause a disbal-

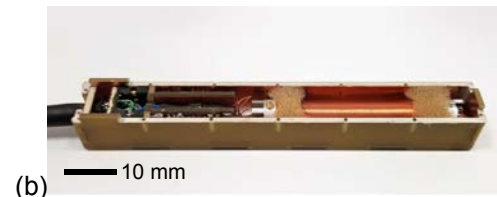
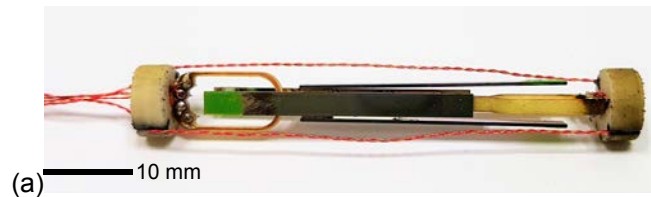


Figure Z2-12: Double tuning fork ME sensor assemblies with DC biased ME sensors. (a) Double tuning fork with mechanical coupling between tuning forks. (b) Double tuning fork design with damping mechanism for suppressing unwanted resonance modes enclosed in electrically shielded housing together with low noise amplifiers.

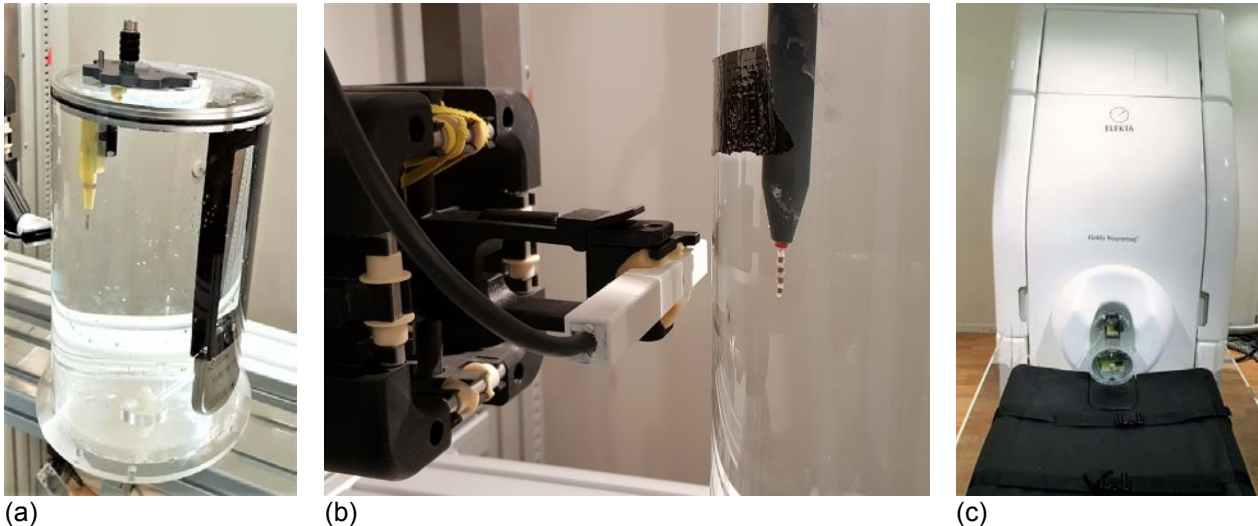


Figure Z2-13: (a) Pneumatically driven head scanner with telescopic arm for the measurement on phantoms and patients. The scanner is made of non-magnetic materials for operation in a magnetically shielded chamber. (b) Rack with laboratory equipment for generating test signals for the phantoms, multichannel data acquisition hardware (2 professional sound cards RME Fireface UFX+), and powerful workstation for digital signal processing.

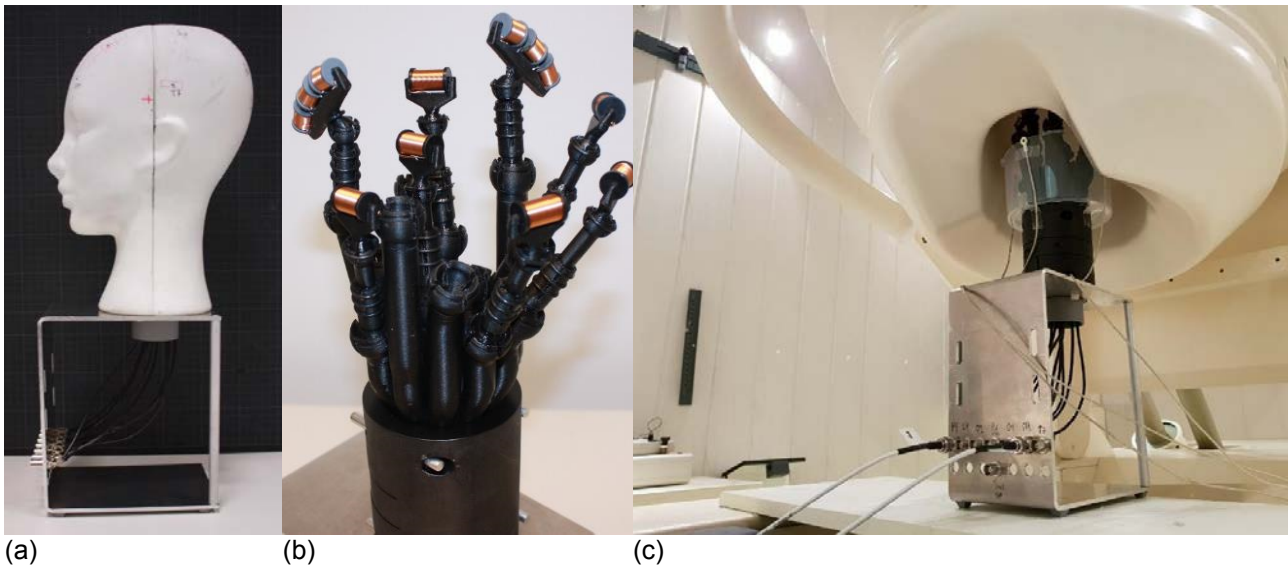
ance of the entire mechanical oscillating system and thus ineffective interference compensation, especially at the resonance frequency. Another reason could be the mutual coupling of individual ME sensors over air, which can also violate the proposed concept of acoustic interference compensation. However, the digital compensation approaches of **B2** showed very promising results [Z2-3, Z2-6, Z2-9] since a digital compensation can overcome such disbalances. However, the drawback of such approaches is that the AD conversion process has to be done prior to the subtraction of the disturbing components, which results in a very large dynamical range of the AD converters (18 bits and more). In any case, the study of the abovementioned method of acoustical interference suppression will be extended in the next funding period with theoretical approaches of research projects **A8** and **B2**.

The measurements for localizing the sources of biomedical signals were carried out in the magnetically shielded chamber utilizing a head scanner constructed for the measurements on phantoms and patients. During the current project, the head scanner (*Figure Z2-13a*) has been upgraded with a new telescopic arm for

avoiding the dead zones during the measurements, an armchair with neck support for the measurements on patients and healthy controls, and bigger channels for signal cables to enable the multichannel measurements with sensor arrays. The measurement instruments have been combined into a movable rack including a PC for data analysis (*Figure Z2-13b*). The new software for controlling the scanner and measuring DBS signals has been developed in a LabVIEW environment that allows multichannel real-time measurement and data acquisition.



(a) (b) (c)
 Figure Z2-14: "Wet" head phantom for DBS measurements. (a) The "wet" phantom is made of acrylic glass and filled with saline solution which has nearly the same conductivity as brain tissue. The real DBS electrode with pacemaker can be built into the phantom for testing real DBS signals. The position of the electrode can be estimated with sub-millimeter accuracy, which is of great importance for solving localization problems. The measurements with commercially available fluxgate sensors have been performed in a magnetically shielded chamber at CAU. (b) The measurements with sensor assemblies designed in project Z2 in magnetically shielded chamber of CAU. (c) SQUID-MEG measurements of the phantom with real DBS system at Düsseldorf University Hospital. The noise floor of the system is $3 \text{ fT/Hz}^{1/2}$, the measurements were conducted with real physiological stimulation parameters (signal amplitude: 1.5 mA, pulse width: 60 μs , and pulse rate: 130 Hz).



(a) (b) (c)
 Figure Z2-15: "Dry" head phantom. (a) The phantom is an anatomically correct model of the human head that is made of nonmagnetic material to allow measurements in the magnetically shielded chamber (b) Inner structure of the phantom permits installation of up to 24 coils into the phantom for modelling complex brain activity. (c) Measurements of the "dry" phantom at the Medical Faculty of the University of Münster with 275-channel cortical CTF MEG system.

The two different head phantoms have been designed and fabricated for measurements with the head scanner. The "wet" phantom for the measurements of DBS signals (Figure Z2-14) is in the form of an acrylic glass cylinder filled with saline water. This ensures a conductivity that is close to that of a human brain. The phantom is equipped with a mechanism for adjustment of the DBS electrode position with millimeter accuracy, which affords the opportunity of providing accurate validation of localization algorithms developed and implemented in B5. The "dry" phantom (Figure Z2-15) was specially designed for B3 for modelling different types of brain activity by means of multiple magnetic sources in the form of individually or mutually driven coils (Figure Z2-15b). The coils of the "dry" phantom can be driven directly by a multitude of available DA converter cards and

generate magnetic fields which are strong enough to be detected by the available ME sensors. Both phantoms are made out of nonmagnetic materials and can be used in the magnetically shielded chamber.

The designed head phantoms have been used for measurements with different types of sensors including the tuning forks designed within **Z2** (Figure Z2-14b), commercially available fluxgate sensors in the magnetic shielded chamber (Figure Z2-14a) as well as by professional SQUID magnetometers (Figure Z2-14c Z2-15c) in cooperation with external institutions. In each case, the measurement support provided by project **Z2** included optimization of the data acquisition software, hardware for the generation of test signals, and adjustment of the measurement setup and phantom configuration.

The MySQL database mentioned in the previous project application was supposed to be utilized for storing the measurement data of different sensors fabricated and studied in all CRC research projects for analysis and comparison of different sensor concepts. The database was not implemented as planned because a better (easier) alternative was found: the professionally developed so-called software versioning and revision control system (SVN) with a free software license, which has been used for storing, updating, and comparing the measurement data instead of the MySQL database.

References to and cooperation with other work in the Collaborative Research Centre

The main tasks of the **Z2** project were functional characterization of ME sensors developed in research projects (**A**) and measurement support of medical projects (**B**). Moreover, a particularly productive cooperation was carried out with **Z1**, which supplied the sensors that were characterized in this project and then used in assemblies for biomedical measurements (**B3**, **B5**). The hardware concepts for ME sensor characterization and related front ends for biomedical applications have been taken over from **B1**. **B2** supported the current project with the digital signal processing routine for ME sensor characterization and for biomedical applications. The measurements of the bias curve of the sensor, LOD, spectral noise density, frequency response, and magnetic frequency conversion measurements for **A1** have been running constantly throughout the project. Hardware support in terms of LNA, signal acquisition equipment, power amplifiers, etc., has been given to **A5**, **A7**, **B2**, and **B7**. Measurements of the transfer function of the cantilever ME sensors have been done for **A7**, **A8**, and **B7**.

Z2 participated in the focus group **F2** "Sensor Concepts", focus group **F3** "Biomagnetic Signal Analysis", and later on in the rearranged focus groups "Comparison of Sensor Concepts" and "Array and Phantom Measurements".

References

- [Fr19] R.-M. Friedrich, S. Zabel, A. Galka, N. Lukat, J.-M. Wagner, C. Kirchhof, E. Quandt, J. McCord, C. Selhuber-Unkel, M. Siniatchkin, F. Faupel, Magnetic particle mapping using magnetoelectric sensors as an imaging modality. *Scientific Reports* **9**, 2086 (2019).
- [Ge13] M. Gerken, Resonance line shape, strain and electric potential distributions of composite magnetoelectric sensors. *AIP Advances* **3**, 062115 (2013).
- [Ha13] L. Hamid, U. Aydin, C. Wolters, U. Stephani, M. Siniatchkin, A. Galka, MEG-EEG fusion by Kalman filtering within a source analysis framework. *Conf. Proc. IEEE. Eng. Med. Biol. Soc.*, 4819-4822, (2013).
- [Ja12] R. Jahns, H. Greve, E. Woltermann, E. Quandt, R. Knöchel, Sensitivity enhancement of magnetoelectric sensors through frequency-conversion. *Sensors and Actuators A: Physical* **183**, 16-21 (2012).
- [Ja13] R. Jahns, A. Piorra, E. Lage, C. Kirchhof, D. Meyners, J. L. Gugat, M. Krantz, M. Gerken, R. Knöchel, E. Quandt, Giant Magnetoelectric Effect in Thin-film Composites. *Journal of the American Ceramic Society* **96** (6), 1673-1681 (2013).
- [Na08] C. Nan, M. I. Bichurin, S. Dong, D. Viehland, G. Srinivasan, Multiferroic magnetoelectric composites: Historical perspective, status and future directions, *J. Appl. Phys.* **103**, 031101 (2008).
- [Sa16] S. Salzer, R. Jahns, A. Piorra, I. Teliban, J. Reermann, M. Höft, E. Quandt, R. Knöchel, Tuning Fork for Noise Suppression in Magnetoelectric Sensors. *Sensors and Actuators A: Physical* **237**, 91-95 (2016).
- [Sa18] S. Salzer, Readout Methods for Magnetoelectric Sensors, (Diss., Kiel University, 2018).
- [Ya00] M. Yamaguchi, M. Takezawa, H. Ohdaira, K.I. Arai, A. Haga, Directivity and sensitivity of high-frequency carrier type thin-film magnetic field sensor. *Sensors and Actuators* **81**, 102-105, (2000).
- [Ya11] R. Jahns, H. Greve, E. Woltermann, E. Quandt, R. Knöchel, Noise Performance of Magnetometers with Resonant Thin-Film Magnetoelectric Sensors. *IEEE Trans. on Instrumentation and Measurement* **60** (8), (2011).
- [Ya16] E. Yarar, V. Hrkac, C. Zamponi, A. Piorra, L. Kienle, E. Quandt, Low temperature aluminum nitride thin films for sensory applications. *AIP Advances* **6**, 75115 (2016).

3.3.2 Project-related publications by participating researchers

- [Z2-1] M. Yalaz, **A. Teplyuk**, M. Muthuraman, G. Deuschl, **M. Höft**, The Magnetic Properties of Electrical Pulses delivered by Deep Brain Stimulation Systems. *IEEE Trans on Instrumentation and Measurement*, doi:10.1109/TIM.2019.2945744 (2019).
- [Z2-2] P. Hayes, M. J. Klug, S. Toxvaerd, P. Durdaut, V. Schell, **A. Teplyuk**, D. Burdin, A. Winkler, R. Weser, Y. Fetisov, **M. Höft**, R. Knöchel, J. McCord, Converse Magnetolectric Composite Resonator for Sensing Small Magnetic Fields. *Scientific reports*. 9, 16355 (2019), doi:10.1038/s41598-019-52657-w.
- [Z2-3] J. Reermann, E. Elzenheimer, **G. Schmidt**, Real-time Biomagnetic Signal Processing for Uncooled Magnetometers in Cardiology. *IEEE Sensors Journal* **15** (10), 4237-4249, (2019).
- [Z2-4] S. Salzer, V. Röbisch, M. Klug, P. Durdaut, J. McCord, D. Meyners, J. Reermann, **M. Höft**, R. Knöchel, Noise Limits in Thin-Film Magnetolectric Sensors with Magnetic Frequency Conversion. *IEEE Sensors Journal* **18** (2), (2018).
- [Z2-5] P. Durdaut, V. Penner, C. Kirchhof, E. Quandt, R. Knöchel, **M. Höft**, Noise of a JFET Charge Amplifier for Piezoelectric Sensors. *IEEE Sensors Journal*, 17, (2017), 22.
- [Z2-6] J. Reermann, P. Durdaut, S. Salzer, T. Demming, A. Piorra, E. Quandt, N. Frey, **M. Höft**, **G. Schmidt**, Evaluation of Magnetolectric Sensor Systems for Cardiological Applications. *Measurement (Elsevier)*, ISSN 0263-2241, (2017)
- [Z2-7] P. Durdaut, S. Salzer, J. Reermann, V. Röbisch, P. Hayes, A. Piorra, D. Meyners, E. Quandt, **G. Schmidt**, R. Knöchel, **M. Höft**, Thermal-Mechanical Noise in Resonant Thin-Film Magnetolectric Sensors. *IEEE Sensors Journal* **17** (8), (2017).
- [Z2-8] P. Durdaut, J. Reermann, S. Zabel, C. Kirchhof, E. Quandt, F. Faupel, **G. Schmidt**, R. Knöchel, **M. Höft**, Modeling and Analysis of Noise Sources for Thin-Film Magnetolectric Sensors Based on the Delta-E Effect. *IEEE Transactions on Instrumentation and Measurement* **66** (10), (2017).
- [Z2-9] J. Reermann, C. Bald, S. Salzer, P. Durdaut, A. Piorra, D. Meyners, E. Quandt, **M. Höft**, **G. Schmidt**, Comparison of Reference Sensors for Noise Cancellation of Magnetolectric Sensors. *2016 IEEE Sensors*, 1-3 (2016).
- [Z2-10] P. Hayes, S. Salzer, J. Reermann, E. Yarar, V. Röbisch, A. Piorra, D. Meyners, **M. Höft**, R. Knöchel, **G. Schmidt**, E. Quandt, Electrically Modulated Magnetolectric Sensors. *Applied Physics Letters* **108**, (2016).

3.4 Project plan

Objectives

The essential goals of this project are functional characterization of the different magnetolectric sensors that are investigated and manufactured in the **A** projects and that include the analogous electronic readout usually provided by project **B1**, and support for the biomedical applications in the corresponding **B** projects.

The functional characterization includes the determination of the spectral distribution of the noise, the limit of detection (measured in resonance and with frequency conversion techniques), the bandwidth of operation, the interference immunity, and the directional characterization of the ME sensors. The obtained results have to be evaluated in cooperation with the corresponding projects and serve to help understand and improve the sensor parameters important for practical use. To get meaningful data for evaluation of the different sensor concepts, the functional characterization of the magnetic sensors has to be conducted under the same measurement conditions, namely, with the same shielding box and measurement instruments as well as calibrated coils for test signals. The technical support of the biomedical applications includes:

- the construction or improvement of the already existing measurement hardware, e.g. low-noise amplifiers, special waveform generators, phantoms, sensor holders, head scanner, etc.;
- the extension, enhancement, and automation of measurement procedures in term of software setup for measurements with various sensor concepts;
- measurement support on patients and biological samples.

The functional characterization and the benchmarks for the individual sensor concepts focused on medical applications are producing valuable research results that serve as initial data for the corresponding projects. Thus, the measurement data of each sensor will be stored in a database which allows direct comparison of different sensors and measuring techniques.

Proposed research methods

For the characterization of different ME sensor types, the concept of a shielded box will be used. The outer surface of the box is covered by electrically conductive material that provides electrical insulation of the characterized sensors. Vibrational and acoustical insulation are achieved with damping supports and an acoustic absorber inside the box. External magnetic fields are shielded by a 10-layer μ -metal cylinder. To eliminate the interference caused by switching power supplies, a battery-powered low noise preamplifier is used inside the box (*Figure Z2-1*). As a DC source for the magnetic bias field, a DC source (KEPCO BOP20-10ML) is used. A precision current source Keithley 6221 serves as the magnetic AC signal generator. The measurement of the noise spectra and signal amplitudes are conducted with help of a spectrum analyser SR785 and a lock-in amplifier SR830 from Stanford Research Systems. To perform the measurements on patients or phantoms, a magnetically shielded measurement chamber is used, which was built by the company Vacuumschmelze GmbH.

One of the ambitious tasks of this project is the creation of a viable system for biomedical diagnosis, namely, a portable neuroimaging device based on ME sensor arrays that eliminate the head scanner. One problem among many appears to be the multichannel signal processing approaches that require special data acquisition hardware with synchronized channels. Professional sound cards, such as RME Fireface UFX + (*Figure Z2-13*) which have been used for data acquisition with the double tuning fork design described above, can be used with relatively small sensor arrays (up to 36 sensors) providing synchronous data acquisition and data recording.

Work Plan

In order to achieve the goals mentioned above, two work packages are required. Very close cooperation with virtually all other projects is inherent in this project. The two work packages will extend over the entire project period. For a better overview, all work packages are depicted in the following timetable.

Table Z2-1: Work schedule

No.	Work package		2020		2021				2022				2023				2024	
			III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP1	Sensor characterization																	
	a	Automatic functional characterization of magnetic field sensors																
	b	Directional characterization of magnetic field sensors																
WP2	Medical applications																	
	a	Conditioning of individual sensors																
	b	Sensor arrays																
	c	Measurement setups																
	d	Camera-based co-registration system																
	e	Measurement support on phantoms and patients																

WP 1: Functional characterization of the ME sensors

Using the measurement equipment described above, corresponding research projects themselves should carry out the characterization of noise and sensitivity for new ME sensors. However, several adaptations or extensions of test setups may be necessary for new sensor types or if novel readout principles are researched (as described in the **A** projects and **B1**). Furthermore, the analysis procedures have to be refined if the LOD lowers (as to be expected in the next four years). Such extensions are performed in this work package. The sensor improvements require adaptation of the related electronics (mainly the low-noise amplifiers). Research on the improvement of the readout electronics is carried out in projects **B1** (analogue part) and **B2** (digital part). The electronics need to be adapted to the ME sensor to be measured. Also in project **B1**, a mathematical relationship for noise prediction is provided for the ME sensor systems, which will allow a comparison of the measurement results with theory.

Thus, based on measurements and theory, it will be possible to perform detailed noise and sensitivity analyses for a plurality of different ME sensors with support of **Z2**. The results will be made available to other projects of the CRC and will allow comparison with other concepts.

- **WP 1a: Automatic functional characterization of magnetic field sensors**

The existing automatic measurement system will be further used for functional characterization of ME sensors. A number of projects require measurement support with sensor characterization. Magnetic layers studied in project **A1** will be characterized using the automatic measuring system, namely the measurement of bias curve, LOD, noise amplitude spectral density (in the following abbreviated as “noise density”), and frequency conversion characteristics will be performed. Projects **A2**, **A7**, and **A10** will be provided with basic functional characterization of their sensors, such as LOD and noise density. Electrical characterization and noise density measurements of SAW sensors studied in project **A9** will be conducted in collaboration with project **B1**. The sensors fabricated in project **Z1** will be characterized using the automatic measurement system to further enhance the fabrication technology and to improve sensor performance, reproducibility, and reliability. Promising sensor candidates will be characterized and preselected for projects **B7** and **T1** to satisfy the requirements of corresponding applications. The abovementioned existing measurement routines as well as necessary measurement hardware will be adapted to new sensor concepts. Furthermore, measurement routines will be designed and implemented within an automatic measurement software framework. New suitable hardware, such as low-noise amplifiers, waveform generators, demodulators, etc., will be designed in order to complete the measurement environment for the new sensor concepts. Besides the software routines, the measurement hardware must be continually updated with suggestions from **B1** and related **A** projects. The measurement results as well as the corresponding analyses scripts will be stored in the already existing SVN database for the analysis and comparison with other sensor concepts.

- **WP 1b: Directional characterization of vector field sensors**

Measurement of the directional patterns of the sensors as well as the transfer function will be performed for vector fields sensors or sensors intended to be used in sensor arrays. Moreover, whole sensor arrays can be characterized to be optimally used (e.g. calibrated) for array processing algorithms (e.g. beamforming or minimum norm approaches) following the suggestions from **B2**. Measurement support with directional characterization of ME sensors is planned for project **A7** to estimate the orientation of the magnetic easy axis of converse ME sensors to optimize the pickup coil configuration. The measurement of the transfer function is necessary for validation of theoretical sensor models investigated in **A8**. *Figure Z2-16* shows the extended approach for measuring the transfer function of the ME cantilever sensor. The improvement compared to the measurement setup reported above (*Figure Z2-6*) consists in the ability to change the direction of the magnetic vector field in the plane of the sensor using two mutually orthogonal loops and also in the possibility of measuring the transfer function not only along the longitudinal axis of the sensor but also on the entire plane of the magnetostrictive layer of the ME sensor. The proposed measurement approach can also be used for estimating the transfer function of the converse ME sensors (**A7**) which is used to study the behavior of the magnetic domains at so-called U mechanical resonance modes. In this measurement configuration, the mutually orthogonal loops (*Figure Z2-16*) detect the magnetic vector field excited by the domains of the magnetostrictive layer when mechanical oscillation of the cantilever is driven by piezoelectric phase of the ME sensor.

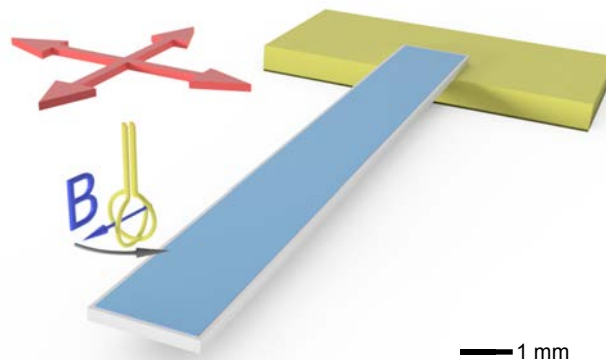


Figure Z2-16: 2D measurement configuration of the transfer function of ME sensor - the magnetic vector field B of any orientation in the plane of the sensor can be excited or detected by two mutually orthogonal loops at an arbitrary point of the ME sensor surface.

WP2: Technical support of medical applications

Technical support for the biomedical applications (**B7**, **B9**, **B10**, and **T1**) is a very important task in the project **Z2**. This work serves as a bridge between theoretical research and practical applications. The main objective of this activity is the assembly of measurement systems based on the sensors developed in the individual

research projects (**A** or **Z1**) to enable their use in real biomedical applications. Namely, this activity requires equipping the sensors with appropriate electrically shielded housing, low-noise pre-amplification as well as low-noise DC current sources (for bias adjustment) if needed. Furthermore, combining the sensors into a sensor array, setting up the readout hardware, and establishing the measurement routines are required.

- **WP 2a: Conditioning individual sensors for measuring biomedical signals**

The sensors developed in the **A** projects and in **Z1** will be equipped with analogue front ends, the concepts for which will be provided by **B1** as well as with DC-bias (modulation or pickup) coils. To reduce the influence of interference caused by electrical fields, the ME sensors with DC-bias (modulation or pickup) coils and low-noise amplification hardware will be built in electrically shielded housings. Depending on the sensor type, either compact, low-noise, digitally controlled DC current sources or low-noise generators for appropriate excitation signals that drive DC-bias or modulation coils, respectively, will be designed. The operation frequency of the sensors will be tuned, if necessary, to match the frequency of the deep brain stimulation signal in **T1**. Along with the developed hardware, the corresponding data acquisition and processing software (from **B2**) will be adapted to the specific measurement setup and conditions defined by **T1**.

Furthermore, technical support will be provided to the movement analysis project **B9** and the cardiology project **B10** with necessary electronic hardware, e.g. power amplifiers for driving signal coils, low noise amplifiers, etc. Other **B** projects will also be supported in a similar manner.

- **WP 2b: Sensor arrays for biomedical applications**

The sensors modified in WP 2a will be combined into arrays which will be used for measuring DBS signals in collaboration with **T1**. For the combination of the sensors into arrays of appropriate apertures, project-specific sensor holders which guarantee correct orientation of the individual sensors will be constructed. Developed in WP 2a, the compact DC current sources and/or the excitation signal generators will be combined into compact modules connected to multichannel synchronous data acquisition hardware (up to 3 professional sound cards, RME Fireface UFX+, can be synchronized to provide 36 synchronous channels). If more sensor elements or additional measurement channels are required, hardware from **B2** can be utilized which allows for systems with up to 256 channels. Multichannel signal processing algorithms provided by **B2** will be used for evaluation of the sensor arrays. Similar cooperation are planned with other **B** projects. An overview for delivering the project specific hardware is depicted in *Table Z2-2*. The plans are to provide each of the application projects with at least two sets of hardware for appropriate multi-channel / array processing. Please note that *Table Z2-2* is only a basic plan which might be adjusted to the needs of the individual projects and their corresponding progress.

Table Z2-2: ME sensor arrays for application projects

Project	Sensor/array type	2020		2021				2022				2023				2024	
		III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
B7	4 ... 8 ΔE sensors																
B9	16 ... 32 resonant ME sensors																
B10	16 ... 32 ΔE and electrically mod. ME sensors																
T1	16 ... 32 SAW and electrically mod. ME sens.																

- **WP 2c: Construction or adjustment of measurement setups for biomedical measurements**

The measurement setup for the collaboration with project **T1** is the head scanner shown in *Figure Z2-13a*. In the first half of the second funding period of CRC 1261, the head scanner is planned to be used for the measurements with single sensors and sensor arrays. The scanner will be upgraded with an additional degree of freedom for tilting a sensor array during the measurement. Originally developed in LabVIEW, measurement software for the measurement with the head scanner will be set up for a particular measurement task with the digital signal processing algorithms provided by project **B2**. In the second half of the project, the specially designed flexible cap with built-in sensor array will be used for the measurements instead of the head scanner. Similar technical support will also be provided to projects **B9** and **B10** with sensor holders and altered mechanical constructions. Project **B7** will receive support with constructing and controlling non-magnetic motor concepts, which were previously used in the head scanner.

- **WP 2d: Design of camera-based co-registration system**

The system is intended to be used for measurements on phantoms or patients planned in project **T1** to determine relative position of the sensor and measured object (head phantom or patient's head). The system consists of multi-camera setup by which a 3D model of the measured object can be created. Using sophisticated video signal processing, the facial landmarks or prominent points of the object can be detected and used for estimating the object's position. On the other hand, the coordinates of the sensor or sensor array with special digital markers (*Figure Z2-17*) on its surface can be also determined by the system, and hence the relative position of the measured object and the sensor can be estimated with sub-millimeter accuracy.



Figure Z2-17: Head phantom with “ArUco” digital markers for position estimation

- **WP 2e: Measurement support by measurements on phantoms and patients**

In order to carry out full and high-quality measurements in collaboration with project **T1**, the individually developed hardware components such as head scanner or “sensor cap” (see **T1** for details), head phantom, readout electronic module for individual sensors or sensor array, data acquisition module, camera-based co-registration system, etc., and software modules such as sensor or sensor array data processing software, head scanner controlling software, video data processing software for co-registration system, etc. will be combined into a viable system for biomedical diagnosis. The system will be tested on head phantoms first and on patients later. The measurements on patients will be conducted only by specially educated medical personnel.

Prospects

In the next phases of the CRC, arrays with growing numbers of sensors and more complex sub-arrays will be required. In this project, plans are to focus on miniaturization, further improvement of the required readout hardware, and improve software based on sophisticated analogue and digital signal processing. This makes achieving highly sensitive biomagnetic sensor systems possible. The main tasks of this central project will remain the measurement support for the sensor characterization and the support for the (bio-) medical application projects.

Role within the Collaborative Research Centre

The project **Z2** will participate in the focus groups “Comparison of Sensor Concepts” and “Biomedical Applications”.

Specifically, this project will collaborate closely with all sensor-producing projects in terms of characterization of different types of ME sensors. In particular, collaborations with the following projects are planned:

- A1:** ME sensor characterization
- A2:** Support with sensor characterization
- A5:** Support with sensor characterization
- A7:** Functional and directional characterization of ME sensors
- A8:** Transfer function measurements
- A9:** SAW sensor characterization at carrier frequencies up to the GHz range
- A10:** Conduction of noise density measurement
- B1:** Takeover of analogue hardware concepts of individual sensors for ME and SAW sensor characterization and related front ends for biomedical applications
- B2:** Takeover of digital signal processing routines for ME and SAW sensor characterization and for biomedical applications
- B7:** Support with sensor characterization and non-magnetic motor concepts
- B9:** Hardware support
- B10:** Hardware support
- T1:** Support for biomagnetic measurements and related data acquisition
- Z1:** ME sensor characterization

3.5 Differentiation from other funded projects

None.

3.6 Project funding

3.6.1 Previous funding

Funding for this project within the Collaborative Research Centre started in 07/2016.

3.6.2 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Postdoc, 100%	1	37.05	1	74.1	1	74.1	1	74.1	1	37.05
Total		37.05		74.1		74.1		74.1		37.05
Direct costs	Sum		Sum		Sum		Sum		Sum	
Consumables	6.0		10.0		10.0		10.0		4.0	
Equipment up to €10.000	0.0		0.0		0.0		0.0		0.0	
Total	6.0		10.0		10.0		10.0		4.0	
Instrumentation	Sum		Sum		Sum		Sum		Sum	
Instrumentation up to k€ 50	0.0		0.0		0.0		0.0		0.0	
Total	0.0		0.0		0.0		0.0		0.0	
Grand total	43.05		84.1		84.1		84.1		41.05	

(All figures in k€)

3.6.3 Requested funding for staff for the new funding period

	Se- quen- tial no.	Name, academic degree, position	Field of re- search	Department of university or non-university institution	Project commit- ment in hours per week	Cate- gory	Funding source
Existing staff							
Research staff	1	Höft, Michael, Prof. Dr.-Ing., Professor	Microwave Engineering	TF EIE	4		Core support
	2	Schmidt, Gerhard, Prof. Dr.-Ing., Professor	System Theory	TF EIE	4		Core support
Non-research staff	3	Taute, Wolfgang, Dipl.-Ing., Technician		TF EIE	4		Core support
Non-research staff	4	Prehn, Kevin, Lab Engineer		TF EIE	4		Core support
Requested staff							
Research staff	5	Teplyuk, Alexander, Dr.-Ing., Postdoc	Microwave Engineering / System Theory	TF EIE		E14	

Job description of staff (supported through available funds):

1. Prof. Dr.-Ing. Michael Höft is responsible for the coordination and scientific management of the central project Z2 in agreement with Prof. Schmidt. He advises the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of analogue system design, analogue filter technology, and related measurement setups.

2. Prof. Dr.-Ing. Gerhard Schmidt is also responsible for the coordination and scientific management of the central project Z2 in agreement with Prof. Höft. He advises the scientific employees with respect to planning, execution, and evaluation of the tasks, in particular in matters of digital system design as well as the IT infrastructure and database.
3. Dipl.-Ing. Wolfgang Taute supports the development of analogue circuits and measurement setups.
4. Kevin Prehn supports with IT infrastructure.

Job description of staff (requested):

5. The postdoctoral researcher Dr.-Ing. Alexander Teplyuk will mainly handle the tasks in this project as described in the work packages. Since the work in the central project requires knowledge from a multitude of disciplines (materials science, electrical engineering, medicine) an experienced post doc is requested.

3.6.4 Requested funding for direct costs for the new funding period

	2020/2	2021	2022	2023	2024/1
Funds available	1.5	3.0	3.0	3.0	1.5
Funds requested	6.0	10.0	10.0	10.0	4.0

(All figures in k€)

Equipment up to k€ 10, software, consumables for 2020/2

Hardware for the low-noise amplifiers and similar readout electronics	k€	3.5
Cables for the measurement chamber	k€	1.0
Mechanical components for measurement setups	k€	1.5

Equipment up to k€ 10, software, consumables for 2021

Hardware for the low-noise amplifiers and similar readout electronics	k€	3.0
Cameras for the camera-based co-registration system	k€	4.0
Mechanical components for measurement setups	k€	3.0

Equipment up to k€ 10, software, consumables for 2022

Hardware for the low-noise amplifiers and similar readout electronics	k€	4.5
Cables for the measurement chamber	k€	2.0
Mechanical components for measurement setups	k€	3.5

Equipment up to k€ 10, software, consumables for 2023

Hardware for the low-noise amplifiers and similar readout electronics	k€	4.5
Cables for the measurement chamber	k€	2.0
Mechanical components for measurement setups	k€	3.5

Equipment up to k€ 10, software, consumables for 2024/1

Hardware for the low-noise amplifiers and similar readout electronics	k€	2.0
Mechanical components for sensor arrays	k€	2.0

Justification:

For the electrical characterization of the ME sensors, individually adapted electronic circuits and mechanical setups are required. Therefore, the components such as transistors, op-amps, printed circuit boards, cables, and connectors are regularly needed for building new low-noise amplifiers, analogue frequency filters, and oscillators. The remaining hardware is described in the work packages.

3.6.5 Requested funding for instrumentation for the new funding period

None.

3.1 General information about Project MGK

3.1.1 Project title: Integrated Research Training Group

3.1.2 Project leader(s)

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None of the abovementioned persons holds a fixed-term position.

3.2 Summary

The Collaborative Research Centre (CRC) 1261 pursues two main objectives: the realization of excellent scientific research and the provision of an exceptional educational experience for young researchers which will prepare them for their next career steps. To achieve the latter, the Integrated Research Training Group (IRTG) promotes scientific independence and interdisciplinary training of all early stage researchers including post-doctoral researchers within the CRC. The IRTG education program further fosters key qualifications, including the competencies required in today's scientific communities. It imparts knowledge beyond the general approach of the CRC.

Given the highly interdisciplinary research objectives, one central aim of the IRTG is to support the direct communication between the projects of the CRC at the doctoral researcher level. By providing all relevant scientific, methodical, and organizational background right from the start, the IRTG members quickly get acquainted with their individual projects and the topic of the CRC with the IRTG supporting them in the timely completion of their projects and theses. Team-based supervision of the doctoral researcher guarantees a targeted interdisciplinary education.

The objectives are further pursued with activities for peer-based knowledge transfer, regular interdisciplinary student-only seminars, lab visits at the different research groups involved in the CRC, field trips to other research institutions, the invitation of guest scientists, participation at conferences and summer schools, regularly scheduled retreats as well as participation in public outreach activities as an integral part of the IRTG. The doctoral researchers are responsible for the planning and organization of these important activities. Moreover, compulsory external research stays are a key element of the educational measures of the CRC.

Furthermore, skills and knowledge to improve the abilities of the doctoral researchers to meet future opportunities not only in the academic sector but also on the non-academic job market are provided within the IRTG. For this, the existing institutions at Kiel University offer a large variety of lectures, workshops, and general courses. IRTG members can further broaden their knowledge by means of special courses arranged and organized by the IRTG. As gender equality measures, a mix of CRC-organized and existing University courses is offered.

As an important element, together with the Scientific Outreach Project (SOP) of the CRC, a formal evaluation process is used for continually monitoring and steering the measures of the IRTG.

Supporting the doctoral researchers to achieve their scientific research goals, the provision of an exceptional educational experience for young researchers and preparing them for their next career steps is at the heart of the IRTG.

3.3 Tabular report

In the first funding period, 30 doctoral researchers and 4 postdoctoral researchers in total participated in the IRTG. At the moment 23 doctoral researchers are members of the IRTG. During the ongoing first funding period, 8 doctoral researchers have already finished their doctorate. 9 doctoral researchers have finished or will soon finish their work and are expected to finish their doctorate within the first funding period. Table 1 lists the funding sources for the IRTG participants. The majority of the IRTG members was funded by CRC project positions. Other funding sources included, e.g., state-funded positions. For doctoral researchers on CRC positions, the participation in the IRTG is mandatory. Early-career researchers not funded by the CRC can apply for participation in the IRTG, if at least 50% of their research work lies within the scope of the CRC.

Table IRTG-1: Number of doctoral and postdoctoral researchers in the CRC and funding of their positions

Category	Funding	Total Number	Number of Women	Duration of contract / months
Doctoral Researchers	CRC project position	29	7	6 to 48, average 38
	other funding	1	0	
Total		30	7	
Postdoctoral Researchers	CRC project position	3	1	5 to 48, average 33
	other funding	1	1	30
Total		4	2	

The IRTG manager, Dr.-Ing. Julia Jedtberg was funded with a 50% E14 position during the first funding period. The activities within the IRTG qualification program that are coordinated by her are described in detail in the next section.

3.4 Qualification program

In the first funding period, the qualification program for young researchers in the CRC 1261 was established within the framework of the Integrated Research Training Group (Modul Graduiertenkolleg MGK). The program of the IRTG focuses on four action areas: *A. Supervision*, *B. Competence Development*, *C. Interdisciplinary Exchange* and *D. International Experience* (Figure IRTG-1). In the following sections, we report on the activities in these action areas and on the credit point system that has been established. In cooperation with the **SOP**, the IRTG activities were regularly reviewed: In 10/2016 a SWOT (Strengths, Weaknesses, Opportunities, and Threats) analysis and group discussion with the young researchers was conducted. In 02/2018 a short survey and group discussion were carried out in a student-only workshop. The summer school was evaluated separately in 07/2017 and 07/2018. In 02/2019 and 03/2019 a summative detailed evaluation of the different IRTG measures was conducted in a survey and in a workshop to plan the IRTG program for the second funding period. While the initial IRTG program was established by the PIs, the IRTG is characterized by a bottom-up approach for implementing changes driven by the young researchers. Many of the identified needs were already realized in the first funding period. Smaller changes to the different elements are discussed below.

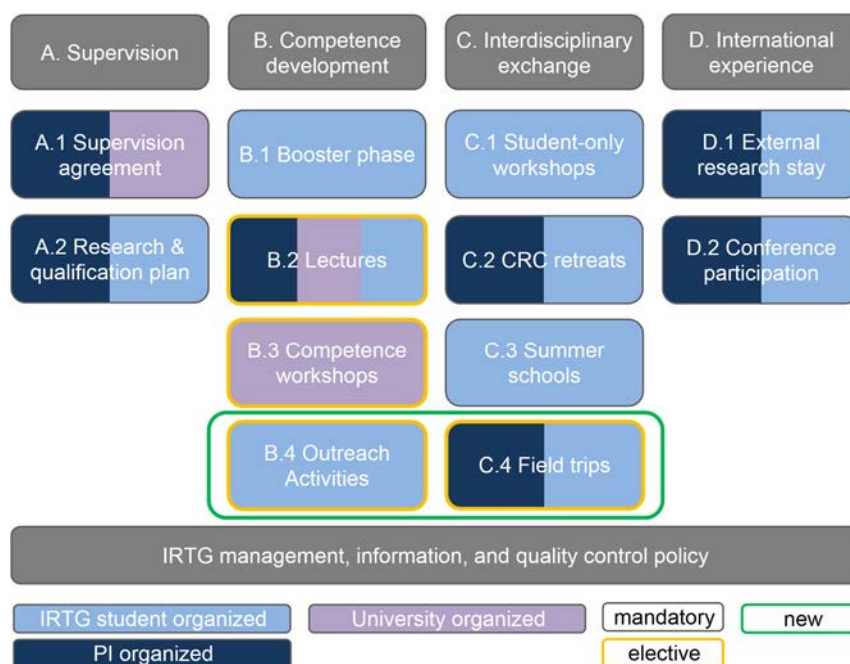


Figure IRTG-1: The Integrated Research Training Group (IRTG) encompasses four action areas A to D.

A. Supervision

A.1 Supervision agreement

Each doctoral researcher within the CRC 1261 signed a supervision agreement (A.1) in the beginning of her / his doctoral research that clarifies the responsibilities and rights of the doctoral researcher and the supervisor. More details on this are given in chapter 1.5. In the 02/2019 survey, 88% of the doctoral researchers voted to keep the supervision agreement as is. Suggestions for improvement were related to reducing bureaucracy.

A.2 Research and qualification (R&Q) plan

After the first six months of the doctorate, a research and qualification plan (A.2) was submitted, including short-term objectives and a long-term perspective for the time of the doctoral research. Subsequently, research and qualification plans were prepared and agreed on with the two supervisors every six months. More details on the supervision concept are presented in section 1.5. In the 02/2019 survey, 67% of the students voted to keep this area in its current form, 33% voted for changes. Hence, most doctoral researchers rated the R&Q plans as a good measure to reflect on their thesis project – particularly on training modules. A point of criticism related to the R&Q plan was that plans change over time and the related documentation is time-consuming. Overall, we realized that we need to raise the awareness of the R&Q plans as a planning and reflection tool and integrated this aspect into the IRTG guide handed out to new IRTG young researchers.

B. Competence development

B.1 Booster phase

For the first six months of the doctoral research, an IRTG-specific mandatory booster phase was established. It aimed at efficiently integrating new doctoral and postdoctoral researchers into the CRC by teaching them the basics of scientific work and making them acquainted with the different entities that offer competence development measures at Kiel University. The booster phase was organized by the IRTG members, supported by the IRTG manager. Each new IRTG member was assigned one advanced member of the IRTG as a mentor who assisted in organizing the booster phase of the new member. During the booster phase, the doctoral researchers also took part in a course on good scientific practice at the Graduate Center of Kiel University to prepare them for their scientific work. Components of the booster phase for doctoral researchers were:

- Introductions to relevant researchers in the CRC
- Reading an interdisciplinary compilation of 10 must-read scientific publications on CRC topics
- Lab visits, organized during student-only workshops
- “Getting Started with the Doctorate: Setting the Compass” workshop at the Graduate Center
- “Good scientific practice and management of research data” workshop at the Graduate Center
- “Academic writing” workshop at the Graduate Center
- Technical skills workshops, e.g. MATLAB

- Regular meetings with the first advisor
- Help in choosing a second advisor

The peer-to-peer knowledge transfer efficiently provided new IRTG members with the necessary information and connections in the CRC for an optimal start to their scientific work. At the same time, it provides an extra opportunity for developing strong interactions between the individual research projects. Overall, the booster phase was reviewed as a highly efficient measure. For example, most of the young researchers voted to keep the introductions to relevant researchers (88%) and the lab visits (95%) as they are. The 10 must-read scientific publications were considered useful, but the selection process of the publications needed changes. In 2019 the IRTG young researchers established a new set of publications and decided on a procedure where each year the new IRTG Board members review the paper selection at a CRC retreat meeting (IRTG management structure depicted in Figure IRTG-3 and described in section 1.5).

B.2 Lectures

CRC-specific lectures by external scientists were organized at least four times a year. The invitations were organized by the IRTG members and the CRC PIs. Attendance at guest lectures was mandatory for the early career researchers. This resulted in a rate of participation of up to 90% and never below 60%. During the first funding period the lectures listed in Table 2 were held by external guests.

Table IRTG-2: Lectures by external scientists for the IRTG members until 12/2019 (during CRC summer schools).*

Date	Name	Institute	Title of Lecture
29.11.2016	Enzo Tagliazucchi	Goethe-Universität Frankfurt am Main	The Physics of Complexity and the Healthy and Diseased Human Brain
08.12.2016	Greg Carman	University of California Los Angeles	Magnetics + Mechanics + Nanoscale = Electromagnetics Future
08.12.2016	Ion Tiginyanu	Academy of Sciences of Moldova	New Exceptional Take Off of Gallium Nitride
09.03.2017	Meinhard Schilling	TU Braunschweig	Bioelektrische und biomagnetische Messungen am Menschen: Stand und Perspektiven
30.05.2017	Dwight Viehland	Virginia Tech	Magnetoelectric Gytrators for I-V Conversion
03.07.2017*	Jens Hauelsen	TU Ilmenau	Bioelektrische und biomagnetische Signale des Gehirns: von der Messtechnik zur Quellenrekonstruktion
01.09.2017	Bharat Jalan	University of Minnesota	Novel Molecular Beam Epitaxy Approach for High Quality Complex Oxide Films
14.09.2017	Wilhelm Schulte-Mattler	University Regensburg	Physiology of Peripheral Nerve Conduction from a Signal Analysis Point of View
12.10.2017	Myriam Pannetier-Lecoeur	French Alternative Energies and Atomic Energy Commission (CEA)	Spin electronics for biomagnetic recordings
09.11.2017	Stefan Jurga	Adam Mickiewicz University	Multimodal Nanomaterials for Biomedicine
14.12.2017	Nicole Pamme	University of Hull	Magnetic forces in lab-on-a-chip for life sciences applications
11.01.2018	Sebastiaan van Dijken	Aalto University	Electric-field Control of Magnetism in Multiferroic Heterostructures
08.02.2018	Oskar Paris	University Leoben	Small Angle Scattering from Nanoporous Materials for Actuation and Energy Applications
19.04.2018	Jörg Wrachtrup	University of Stuttgart	Applying Quantum Sensors
23.04.2018	Tilman Sander-Thömmes	Physikalisch-Technische Bundesanstalt, Berlin	Biomagnetic Sensing and Processing – Progress Using a Modular Approach
28.05.2018	Richard Fu	University of Northumbria at Newcastle	Acoustic wave lab-on-chip is now flexible, bendable and potentially wearable!
10.06.2018	Giselher Herzer	VAC GmbH & Co. KG, Hanau	To catch a thief
14.06.2018	Andreas Winkler	IFW Dresden	Surface acoustic wave (SAW) sensor and actuator devices and issues in their realization
18.06.2018	Nian X. Sun	Northeastern University, Boston	RF NEMS Magnetoelectric Sensors
06.09.2018	Ursula van Rienen	University of Rostock	Computational Studies on the Volume of Activated Tissue in Deep Brain Stimulation

19.12.2018	Elizaveta V. Golubeva	Ural Federal University, Ekaterinburg	Applications of the giant magnetoimpedance effect for biosensing
04.02.2019	Leonhard Reindl	Albert-Ludwigs-Universität Freiburg	Power supply for wireless sensors systems
05.02.2019	Dave C. Johnson	University of Oregon	Synthesis and Properties of Heterostructures with Designed Nanoarchitecture
14.02.2019	Paulo Freitas	International Iberian Nanotechnology Laboratory	Spintronic sensors: fundamentals and applications
19.08.2019*	Carsten Wolters	University of Münster	Reconstruction and manipulation of neuronal networks in the human brain
19.08.2019*	Enno Lage	Analog Devices Inc.	Magnetic Sensors in the Eye of the Industry
20.08.2019*	Thorsten Buzug	University of Lübeck	Magnetic Particle Imaging
20.08.2019*	Joshua Engels	Biomagnetik Park GmbH, Hamburg	Magnetocardiography at Biomagnetik Park GmbH
21.08.2019*	Tilman Sander-Thömmes	PTB, Berlin	Optically pumped magnetometers as sensors for bi-magnetic applications
24.10.2019	Galina Kuryandskaya	University of the Basque Country UPV-EHU	Materials for magnetic sensing: focus on giant magnetoimpedance
07.11.2019	Katja Tonisch	TU Ilmenau	Scandiumaluminumnitride – an emerging material for sensing applications
14.11.2019	Ulrike Wallrabe	University of Freiburg	Coils and transformers on-chip
12.12.2019	Nicholas Maling	Boston Scientific	DBS Mechanisms, Models, and Visualization Tools

In the 02/2019 survey, 69% of IRTG members voted to keep the colloquia as is. A point of criticism was the mandatory attendance on topics not seen as relevant for their own research as well as an apparent focus on topics from materials science. Since the CRC fosters interdisciplinary research, Pls and IRTG members jointly agreed to keep mandatory attendance but to increase the number of invitations by the IRTG members.

Additionally, the doctoral researchers can choose lectures from the curriculum of Kiel University. Depending on their previous experiences, the IRTG members attended a wide range of lectures listed in Table 3. Since half of the young researchers voted to change this element, it was agreed that the option should be kept only for students who enjoy taking lectures and that beneficial lectures should be suggested to new IRTG members.

Table IRTG-3: Participation of IRTG members in elective lectures related to CRC topics.

Discipline	Lecture	Lecturer
Mat. Sci.	Engineering Aspects of Medical Technology	Enno Lage
Mat. Sci.	Cell Mechanics	Christine Selhuber-Unkel
Mat. Sci.	Magnetic Materials	Jeffrey McCord
Computer Science	Introduction of Image Processing	Sandro Esquivel
Medicine	Fundamentals of Neurosciences	Janka Held-Feindt
Electr. Engineering	Integrated Circuit Design for Medical Applications	Andreas Bahr
Electr. Engineering	Digital Signal Processing	Gerhard Schmidt
Electr. Engineering	Adaptive Filters	Gerhard Schmidt
Electr. Engineering	Numerical Calculation of Electromagnetic Fields	Ludger Klinkenbusch
Electr. Engineering	Electromagnetic Fields I and II	Ludger Klinkenbusch
Electr. Engineering	Fields and Waves in Biological Systems	Ludger Klinkenbusch
Electr. Engineering	Noise in communication and measurement systems	Michael Höft
Physics	Theoretical Mechanics	Stefan Heinze
Physics	Theoretical Electrodynamics	Stefan Heinze

B.3 Competence workshops

The Graduate Center, the Continuing Professional Development Center, the International Center, the Computer Center, and the Center for Entrepreneurship of Kiel University offered a wide range of workshops open to IRTG members. The extensive program included courses on technical and cross-curricular skills as well as advice on career planning for doctoral researchers and measures shaping the personal profile. The IRTG members took part in various cross-disciplinary courses listed in Table 4 below.

Table IRTG-4: Courses attended by IRTG members offered at Kiel University (no CRC funding)

Course	Duration / days	Institution
Project Management & Leadership	2	Graduate Center

Speaking clearly	1	Graduate Center
Develop your intercultural and study skills	1.5	International Center
Negotiation skills	2	Graduate Center
Presentation skills	1	Graduate Center
How to apply in Germany	3	Career Center
Project management	2	Graduate Center
Management Kompakt	2	Graduate Center
Agiles Projektmanagement	1	Continuing Professional Development Center
Personal Kanban - eine Methode des agilen Projektmanagements	1	Continuing Professional Development Center
Find a job in Germany's industry	1	Career Center
Critical reasoning and logic	2	Graduate Center
Writing Scientific English	1.5	Graduate Center
Slidewriting & Storytelling	1	Graduate Center
Communication in Research Projects	2	Continuing Professional Development Center
Intellectual property	1	Graduate Center
Gut abgesichert in den Berufseinstieg	0.5	Career Center
Die Bewerbungsmappe	0.5	Career Center
Assessment center	0.5	Career Center
Jobrecherche	0.5	Career Center
Promotion reloaded	1	Graduate Center
Kreativität im Forschungsprozess	1	Graduate Center
Problem solving in Industry	5	Faculty of Engineering, Service Center Education
Bewerben in der Industrie	2	Graduate Center
Designing effective academic posters with Powerpoint	1	Graduate Center
Projektbasierte Lehre lernen	2	Faculty of Engineering
Presentation skills – Managing Audiences effectively	2	Graduate Center
Strategien für effizientes Schreiben	1	Graduate Center
Kollegiales Führen im agilen Zeitalter	1	Continuing Professional Development Center
Multikulturelle Teams erfolgreich führen	1	Continuing Professional Development Center
Professionelle Gesprächsführung in herausfordernden Situationen	1	Continuing Professional Development Centre

In addition, the IRTG organized CRC-specific courses on a demand-driven basis for IRTG members (Table 5). Inventor as well as MATLAB courses were offered twice, because many of the doctoral researchers demanded these courses. In the case of the MATLAB course, the second course consisted of an introductory part and a follow-up to the first course. In the evaluation, these CRC-specific courses got an excellent rating (95% voted to keep it unchanged). 75% of the doctoral researchers voted to keep the Graduate Center courses as is. In particular, the Graduate Center course “good scientific practice and data management” was considered as too general. Here we agreed with the Graduate Center to improve this course. Starting in 2020, the course will be split up into two separate courses, “Management of Research Data” and “Good Scientific Practice”. Otherwise, we plan to continue this successful measure.

Table IRTG-5: Technical (T) and cross-disciplinary (CD) courses organized by the IRTG

Course	Date and duration	Attendees from the IRTG
COMSOL course (T)	26 October 2016, 0.5 days	14
Inventor course (T)	31 October – 03 November 2016, 4 days	12
Communication and Conflict Management (CD)	10 – 11 October 2017, 2 days	12
MATLAB course (T)	21 – 23 August 2018, 3 days	14
Inventor course (T)	23 – 24 May, 3 June 2019, 3 days	10
MATLAB course (T)	10 – 12 September 2019, 3 days	8

B.4 Outreach Activities

During the first funding period, the scientific outreach project organized several events such as exhibitions and fairs. The doctoral researchers designed the exhibition or single parts of it and also represented the CRC 1261 at several events. Details on the outreach concept and its evaluation are presented in the project description of the **SOP**.

C. Interdisciplinary exchange

C.1 Student-only workshops

For internal networking among IRTG members, mandatory student-only workshops were conducted approximately every two weeks as one- to two-hour self-organized events. The workshops were also open to BSc and MSc students writing their theses on a CRC-related topic. Due to the strong interdisciplinary nature of the CRC, naturally one focus of the workshops was on promoting the ability of early stage researchers to present results of their own scientific work to an interdisciplinary audience in an appealing and understandable manner. A second emphasis was on the knowledge transfer within the CRC. Therefore, the contributions consisted of a mixture of an introduction to a CRC project and a section dealing with current issues of research within the individual projects. The third aim was to develop a constructive culture of discussion among the members of the CRC. During the workshops, the IRTG members presented their topics and research issues in regular intervals to their peers. The working climate was very positive, enabling impartial discussions in the student-only format. Besides the presentations, the doctoral researchers organized lab visits, where one or two doctoral researchers of one working group gave insight into their lab to the other IRTG members. The planning of the student-only workshops was completely in the hands of the doctoral researchers and was organized by the doctoral researcher members of the IRTG Board. In the evaluation, this measure got an excellent rating (95% of the IRTG members voted to keep it without change).

C.2 CRC retreats

Semi-annual retreats were established as the major research and networking event for all CRC members. Going “into retreat” helped to enhance collaborations between the groups and take stock of the status of research. The focus was on discussing the latest research developments within the CRC. This ensured continuous improvement of research quality and the aspects of supervision and training. During extended discussion sections, interdisciplinary exchange was promoted. As all PIs participated at the retreats, broad input for each research project was given. Furthermore, during each retreat the IRTG members had a regular meeting to discuss the next events and upcoming issues with the IRTG manager. The CRC retreats were planned and organized by the IRTG manager together with the IRTG Board and the board of the CRC. During the first funding period the following retreats were organized:

- 12-13 September 2016, Retreat, Nordseeakademie, Leck
- 04-05 April 2017, Retreat, Akademie Sankelmark
- 04-05 October 2017, Retreat, Akademie Sankelmark
- 20-21 March 2018, Retreat, Akademie Sankelmark
- 11-12 September 2018, Retreat, Nordseeakademie, Leck
- 26-28 March 2019, Retreat, Akademie Sankelmark
- 03-04 September 2019, Retreat, Akademie Sankelmark

In the beginning, the program of the retreat was designed in such a way that each research project of the CRC was discussed, one at a time. After an evaluation by the SOP, the program was adapted by grouping the talks into different topical areas across the research projects. In this way the cooperation between the projects of the CRC was further promoted. The retreat meetings were evaluated with short questionnaires in 2017 and 2018. The overall satisfaction was high and could even be increased through further adapting the meeting to the needs of the participants.



Figure IRTG-2: Retreat at the “Nordseeakademie Leck” in fall 2018. Left: CRC members during the sessions. Right: Group picture of the IRTG members.

C.3 Summer schools

Each year the IRTG members organized a summer school with content highly relevant to the IRTG members. Additionally, the IRTG members gained project management skills during the organization of these events. The organization was assisted by the IRTG manager. During the first funding period, the following summer schools were organized:

- 03-04 July 2017, Summer School, Schloss Noer

- 24-25 July 2018, Summer School, Jugendherberge Eckernförde
- 19-21 August 2019, International Summer School, Wissenschaftszentrum Kiel
- Planned for 12-14 May 2020, Summer School, Villa Ulenspiegel, Schülp b. Nortorf

The focus of the first summer school was on basic knowledge of the CRC topics with PI talks about basics of materials science, sensor production, signal processing, and medical topics supplemented by one external speaker. A science slam introductory was organized to enhance the ability of the IRTG members to give brief presentations on their research topics that were easy to understand. The summer school also included a team building element. In the second year, the focus was on advanced medial topics in the areas of neurology and cardiology as well as on specific modelling approaches of sensor systems and on the basics of magnetism. Communication abilities were further trained in a science communication workshop on designing special give-aways for outreach events of the CRC 1261. The international summer school in 2019 was focused on the interdisciplinary exchange and networking of the IRTG members with external participants and invited speakers. In the evaluation, the summer schools were rated especially useful by the doctoral researchers, emphasizing the positive effect for interdisciplinary team building and communication (94% voted to keep this measure unchanged).



Figure IRTG-3: Left: Team communication training event at the summer school 2018 in Eckernförde, right: Participants of the international summer school 2019 at the Wissenschaftszentrum Kiel.

C.4 Field trips

To promote networking with other research groups working on CRC related topics, field trips were organized:

- 22 November 2016, DESY, Hamburg
- 21-22 February 2018, PTB Berlin
- 05 December 2018, Fraunhofer ISIT, Itzehoe
- 21-22 May 2019, University of Rostock, CRC 1270
- 18-21 September 2019, Deutsches Museum, Munich



Figure IRTG-4: Left: Visit of IRTG members at DESY in Hamburg in November 2016. Right: Visit at the CRC 1270 ELAINE in Rostock in May 2019.

During these field trips, the CRC members visited laboratories at other institutions and were introduced to the research of external scientists with talks and poster sessions. 100% of the IRTG members voted to keep the field trips as a tool to build networks, especially with other research groups.

D. International experience

D.1 External research stay

The IRTG concept was complemented by a component providing the IRTG members with the international experience necessary in the competitive environments of research and industry. Doctoral researchers conducted a 4 to 12 week research stay (average, 8 weeks) in laboratories outside Germany. These stays were funded by the IRTG budget. The doctoral researchers planned the research stay and wrote a proposal to the IRTG Board for evaluation. The proposals were reviewed with regard to the research and the financial plan. If necessary, changes were requested from the doctoral researchers. During the first funding period, 12 doctoral researchers carried out their external research stay. 4 more already have approval for their stay (see table 7).

Table IRTG-6: List of doctoral researcher of the CRC 1261, who went on an external research stay during the first funding period of the CRC 1261

Doctoral researcher	Visiting institution	Period
Sebastian Toxværd geb. Salzer	Universidad Politécnica de Madrid (UPM), Prof. José Ignacio Izpura Torres	September – November 2016
Stefan Schröder	Massachusetts Institute of Technology (MIT), Prof. Karen K. Gleason	February – April 2017
Niklas Wolff	University of Oregon, Eugene, Prof. David C. Johnson	September – October 2017
Patrick Hayes	Moscow Technological University (MIREA), Prof. Yuri Fetisov	September – November 2017
Philipp Jordt	University of California, San Diego, Prof. Oleg Shpyrko	October – December 2017
Julius Schmalz	Institute of Mechanics and Mechatronics of the Vienna University of Technology, Austria, Prof. Kaltenbacher	November – December 2017
Matic Klug	Institute Neél – CNRS, Prof. Stefania Pizzini	January – February 2018
Nils Lukat	University of South Australia, Adelaide, Australia, Prof. Benjamin Thierry	March – May 2018
Ron-Marco Friedrich	DTU in Denmark, Lyngby near Copenhagen, Prof. Hansen	March – May 2018
Phillip Durdaut	FEMTO-ST Institute, Besançon, France, Enrico Rubiola, Jean-Michel Friedt	August – September 2018
Marleen Schweichel	Chinese Academy of Science, Prof. Zhong-Lin Wang	September – December 2019
Christin Bald	University of Leuven, Prof. Sabine Van Huffel	November 2019
Mevlüt Yalaz	Case Western Reserve University (CWRU), Cleveland, Ohio, Prof. Cameron McIntyre	January – March 2020
Jingxiang Su	Northeastern University, Boston, Prof. Nian X. Sun	April – May 2020
Lars Thormählen	Northeastern University, Boston, Prof. Nian X. Sun	April – June 2020
Viktor Schell	International Iberian Nanotechnology Laboratory, Portugal, Prof. Paulo Freitas	

The doctoral researchers reported that they profited immensely from the scientific as well as personal exchange with international leading scientists, with a chance to acquire additional methodological skills. The research stays broadened the scientific horizon of the doctoral researchers and provided a first step towards building a personal, professional network. The external research stays led to joint developments of new concepts and joint publications. For example, Patrick Hayes visited the Moscow Technological University (MIREA) and published together with the group of Prof. Dr. Yuri Fetisov [see A7-6, A7-7], and Stefan Schröder visited the Massachusetts Institute of Technology (MIT) and published together with the group of Prof. Karen K. Gleason [see A2-4, A2-6]. The IRTG members wrote short reports on their experiences, which are summarized on our CRC website (<http://sfb1261.de/index.php/en/blog-en/research-stays-abroad>). All of the IRTG members voted to keep the research stays as an IRTG measure.

D.2 Conference participations

At least one presentation at an international conference, symposium, or summer school was mandatory for the IRTG members and funded by the IRTG. The participation in such events should promote the students' scientific self-independence, improve presentation skills, provide external feedback on their research, and create a personal, international network. Specialized summer schools provided a platform for interdisciplinary and intercultural exchange and offered an additional opportunity to get in touch with renowned experts from science and industrial research. IRTG members wrote a short proposal for conference participation with a financial plan and a description of their own conference contribution to the IRTG Board for approval. During the first funding period, 26 conference participations were funded by the IRTG.

Credit Point System

The IRTG was planned such that IRTG measures encompassed 10% of the working time of doctoral researchers and the young researchers had 90% of their time for independent research. The IRTG participation was based on a credit system for all activities within the IRTG. Assuming 220 working days per year, one day equaling one IRTG credit point, the doctoral researchers should achieve 66 points within their three-year doctoral work. The activities of the IRTG were divided into three groups: CRC-related, technical, and cross-disciplinary measures. A minimum of 30 points had to be achieved by CRC-related activities, 15 points by technical activities, and 8 points by cross-disciplinary activities. For lectures, the semester week hours (Semesterwochenstunden, SWS) were transferred into IRTG points (1 SWS = 1 IRTG point). For participation in the IRTG Board or planning of the summer school, etc., a fixed number of points, in these cases 10 or 4 points, respectively, was credited.

An exemplary timeline of a doctorate

Here, we want to give an example of how the IRTG activities were scheduled by a doctoral researcher (Matic Klug (A1)), throughout the three years of his doctorate (see Fig. IRTG-5). At the beginning, Matic Klug and his first advisor signed the supervision agreement (A.1). The first six months of IRTG membership formed the booster phase (B.1). During this time, Matic Klug had two student mentors, was introduced to the other IRTG members and visited different labs. Besides getting started on his research project, he visited mandatory courses on the basics of performing research, worked through a peer-chosen literature syllabus, and finally chose a second advisor. Throughout his time as an IRTG member, Matic Klug participated in the regular student-only workshops (C.1), meetings with his two advisors (A.2), CRC retreats (C.2), as well as the yearly summer school (C.3).

Based on his personal interests, he visited a range of elective workshops (B.3) and participated in an international summer school in 2017 (D.2). He conducted his mandatory research stay (D.1) at the Institut Néel – CNRS, France, in the beginning of 2018 and gave presentations at four international conferences (D.2) between 2017 and 2019. He submitted his thesis in June of 2019 and successfully defended his thesis in September of 2019.

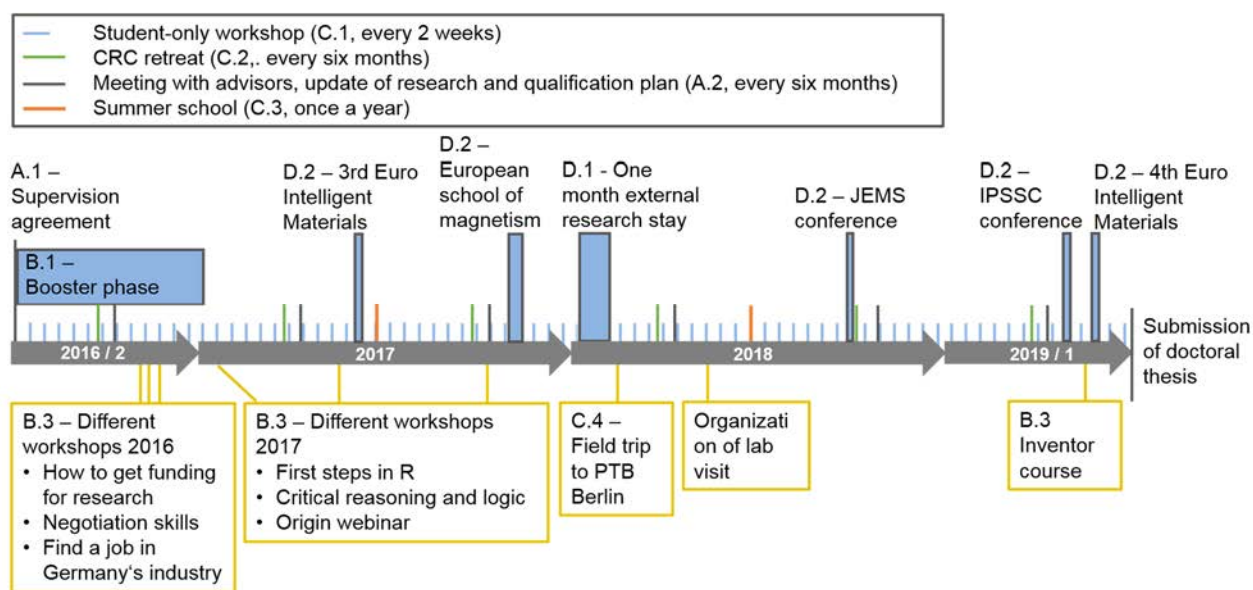


Figure IRTG-5: Example timeline from Matic Klug, a doctoral researcher within the CRC1261, who submitted his thesis after 3 years and participated in the IRTG training program.

3.5 Management and supervision

This section describes the recruitment strategy of the IRTG, the management, the action area A. *Supervision*, the information strategy, and measures for gender equality, a family-friendly workplace, and quality control.

Recruitment

Before the start of the CRC 1261, our research on magnetoelectric sensors was funded in the PAK 902 program, which ran for 1.5 years. Due to the previous funding, at the beginning of the first funding period of the CRC 1261 a large number of positions were already designated to doctoral and postdoctoral researchers, who

had been previously employed within the PAK 902 program for 1.5 years. Therefore, only a small number of open positions were announced. Due to the different starting times of the doctoral researchers and different durations of their doctoral research, the establishment of doctoral researcher cohorts was not possible. Open doctoral researcher positions were then individually filled by the respective PIs. In order to recruit potential doctoral and postdoctoral researchers from abroad, IRTG fellowships were announced in 2018 and 2019. The fellowships gave interested candidates the opportunity to come to Kiel and get to know the CRC research and the IRTG with its scientific network before starting doctoral research. Twelve such fellowships were funded. The fellowships also provided the opportunity to let new IRTG members have some temporal overlap with existing IRTG members, which guaranteed efficient knowledge transfer. This was the case for Lars Thormählen, who got a fellowship before he started his doctorate on a CRC position.

In the next funding period, 13 out of 23 doctoral researcher positions will be vacant at the beginning. All these positions will be announced in a common advertisement targeting national and international applicants. Criteria for the selection of candidates will be scientific excellence and motivation to work on an interdisciplinary project. As women are in the minority in engineering, women will be preferred in the case of equal qualifications.

IRTG management

The IRTG was governed by the IRTG Board consisting of three project leaders, the IRTG manager, and three doctoral researchers. The three doctoral researcher board members were elected by the assembly of the IRTG for one year. They were responsible for representing the doctoral researchers in the CRC 1261, supporting the organization of the IRTG, organizing student only workshops and assisting in organizing various other activities. Input from all IRTG members was obtained by regular evaluation workshops at the retreats and in the student-only workshops. The evaluation results were discussed in the IRTG Board and action was taken based on these. The IRTG Board members of the first funding period are listed in table IRTG-7:

Table IRTG-7: Doctoral researcher members of the IRTG Board during the first funding period.

	Materials Science	Electrical Engineering	Medicine / Applications
until October 2016	Patrick Hayes	Sebastian Salzer	Adrian Zaman
until October 2017	Anne Kittmann	Phillip Durdaut	Eric Elzenheimer
until October 2018	Mona Mintken	Ömür Özden	Nils Lukat
until October 2019	Marleen Schweichel, Lars Thormählen	Christin Bald	-
since November 2019	Viktor Schell	Patrick Wiegand	Mevlüt Yalaz

One of the IRTG member representatives and one representative of the PIs of the IRTG represent the IRTG in the Board of the CRC. The IRTG and the SOP worked together closely. Carolin Enzingmüller from the SOP was a permanent guest during the meetings of the IRTG Board (no voting-rights). The IRTG manager was the IRTG contact person and responsible for introducing new members of the IRTG into the organizational details and into the qualification program of the IRTG. In this way, it was ensured that new doctoral researchers were acquainted with the IRTG network. The IRTG manager furthermore organized internal workshops, field trips, and CRC lectures and supported the doctoral researchers in organizing the summer school. The general organization structure of the IRTG is depicted in Fig. IRTG-4.

The organization structure enables strong involvement of the doctoral researchers in the organization of the IRTG. The IRTG Board meets every three to four month and decides on financial and organizational issues of the IRTG. The meetings are scheduled and organized by the IRTG manager. As laid out above, responsibilities of each participant in the organization are well defined. The organization scheme with interaction on many levels facilitates efficient operation of the IRTG, allows for continuous improvement of the IRTG, and provides flexibility to respond to the needs of the participants.

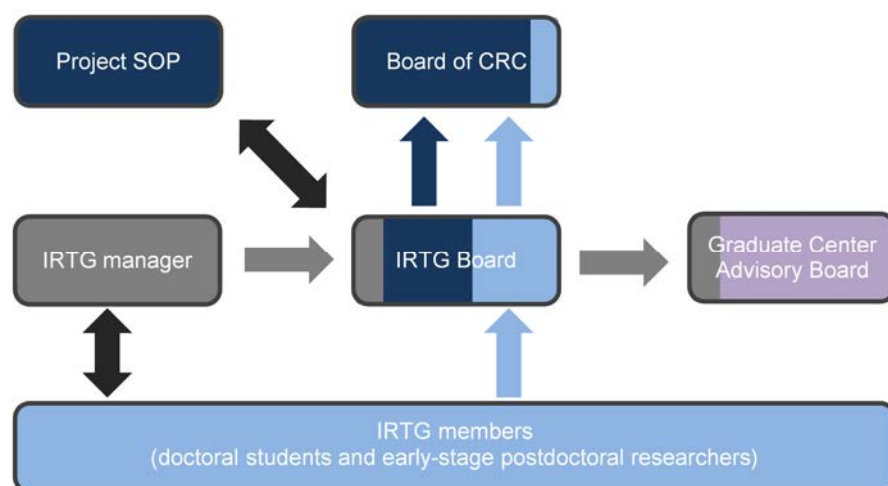


Figure IRTG-6: Organization structure of the IRTG.

Information policy

Providing all the relevant information to the IRTG members and the CRC PIs and staff was and is the responsibility of the IRTG manager. The IRTG manager informs the CRC members on upcoming events, such as retreats, guest talks, summer schools, and workshops. Organizational details for internal events are also distributed to the CRC members by the IRTG manager. For new members of the IRTG and for interested master students, an IRTG guide was developed by the doctoral researchers of the IRTG Board, the SOP, and the IRTG manager. The guide includes general information on the CRC and informs new members about the opportunities, rights, and rules within the framework of the IRTG. Email notification on CRC-relevant talks at Kiel University are periodically sent.

Gender equality

During the first funding period, gender equality measures within the CRC 1261 and the RTG 2154 were coordinated by Tina Kerby. She organized joint workshops and other measures on gender equality that are listed in table IRTG-8.

Table IRTG-8: Workshops and seminars for early career researchers in the area of Gender Equality during the first funding period

Motive analysis seminar for female Master students with Stefanie Schönbach-Fuleda	2016
Workshop on "Confident Demeanor in Challenging Situations" with Stefan Spies.	2016
Seminar on gender equality measures for female researchers with Prof. Ursula van Rienen	2018
Workshop on how to start with a family during the doctorate by the family service of Kiel University	2018
Workshop on professional track of female researchers after the dissertation by Ulrike Struwe	2018
Seminar talk on "unconscious bias" for all CRC 1261 members by Nicola Byok	2019

During the first funding period, three early career researchers, two doctoral researchers, and one postdoctoral researcher became pregnant. During the pregnancy, the doctoral researchers were supported in their work by student assistants, who helped them carrying out the necessary lab work, as they weren't allowed to work in the lab anymore. After their parental leave, the doctoral researchers were given the opportunity to reintegrate on a part-time position.

Organization of doctoral program

Details on the IRTG program components are given in section 1.4. Here, details on the supervision agreement and the research and qualification plan are summarized.

A.1 Supervision agreement

During the first funding period, a supervision agreement was developed for the IRTG of the CRC. At the beginning of their participation in the IRTG, all IRTG members and their supervisors signed this document laying out the individual rights and responsibilities of both parties. The formal agreement defines the supervision concept with two supervisors. The first supervisor is the principle investigator of the project the doctoral researcher is working on. The second supervisor should be named after the first six months and should be another principle investigator of the CRC, preferably from another discipline. The supervision agreement also

regulates the responsibilities of the doctoral researcher and the supervisor. The supervisor and doctoral researcher determine the theoretical and technical requirements and preconditions of the thesis project. The supervisor advises on the elaboration of a project outline and an accompanying timetable.

The supervision agreement includes the mandatory participation of doctoral researchers in the IRTG and states that the doctoral researcher is responsible for the documentation of the project progress in the semi-annual research and qualification plans, which are developed together with the supervisors. With the signature of the supervision agreement, the doctoral researcher and the supervision team commit themselves to follow the DFG rules on good scientific practice.

During the first funding period, the faculty established a mandatory supervision agreement for all doctoral researchers. For the CRC, our specially designed form will be used in addition to the one of the faculty in the second funding period as it is more detailed and contains regulations about the participation in the IRTG.

A.2 Research and qualification plan

The central document of the supervision concept is the research and qualification plan. With the help of the supervisor and the two peer mentors (see B.1), each doctoral researcher drafted a first version of the research and qualification plan within the first six months. The plan included research work packages, a timeline, planned competence development, and international participation as well as the individual contributions to the IRTG. The manager of the IRTG assisted the doctoral researchers in drafting the research and qualification plan. Every six months, the research and qualification plan was presented to the two supervisors and discussed and modified in mutual agreement. The final version was sent to the IRTG manager for documentation. The progress report meetings needed to be scheduled by the doctoral researchers themselves. The IRTG manager made sure that the research and qualification plans were handed in every six months.

Quality control – Evaluation of the IRTG program

The IRTG program was evaluated by the Scientific Outreach Project (**SOP**) (see WP 5 of project **SOP**). To monitor and improve the program, the **SOP** conducted a formative and a summative evaluation:

Table IRTG-9. Evaluation concept for the IRTG program accompanied by the SOP.

Evaluation	formative	summative
Goal	Quality monitoring and control regarding the IRTG program in the process	Evaluating the benefits of the IRTG program at the end of the funding period
Constructs	- Junior researchers' expectations and perceptions of the quantity and quality of interdisciplinary communication - Needs and demands for support measures - Suggestions for improving measures in the first funding period	- Junior researchers' perspectives on the perceived usefulness of IRTG measures, retrospectively - Suggestions for improving measures for the second funding phase - New ideas and additions for the second funding phase
Methods	Questionnaires, SWOT analyses, regular retreat and SOW meeting evaluations, summer school evaluation, workshop evaluations, observations, group discussions	Questionnaire, structured reflection workshop

Questionnaires were analyzed using summary descriptive statistics, such as frequency distributions, means, and standard deviations. Open answers were analyzed using content analysis identifying typical answers. Group discussions were protocolled, analyzed, and categorized. Data were collected anonymously to encourage honest and open answers. Results of the formative assessment were discussed at the student-only workshops and suggestions for adaptations were collected. Suggestions were reported to and reviewed by the IRTG Board and measures were adjusted accordingly to continuously improve the quality of the IRTG.

3.6 Environment of the Integrated Research Training Group

As a full university with around 27,000 students and 2.700 doctoral researchers, four research foci and two clusters of excellence, Kiel University provides a complete infrastructure and thereby an excellent environment for the success of the IRTG. The IRTG strongly benefits in many ways from existing structures at Kiel University that are committed to strengthen the overall graduate education.

Professional Development at Kiel University

Kiel University established a Graduate Center (<https://www.gz.uni-kiel.de/en>) as a central service unit for support of doctoral researchers in 2010. The Graduate Center provides numerous facilities for a structured doctoral program and offers an extensive and very valuable program to complement the training program of the IRTG. The IRTG manager represents the IRTG in the Graduate Center Advisory Board. Additionally, the network "Postgraduate support" (<https://www.gz.uni-kiel.de/en/info/program-coordinators>) was established, where the program coordinators of the coordinated doctoral programs meet and discuss current issues of relevance. The IRTG manager is a member of this network.

The Graduate Center and International Center at Kiel University run a comprehensive, joint support program especially designed for doctoral candidates from abroad: The program "*docs build bridges*" includes individual help during the starting period of the doctorate by experienced doctoral candidates as tutors and help in dealing with organizational issues like finding a flat or visiting government authorities or offices. Moreover, workshops on intercultural communication and language skills are offered. The support includes professional advice and orientation guidance, the offer of accommodations in guest houses, or practical help regarding integration issues. Also, knowledge of different cultures, conventions, and cultural habits is exchanged, which strengthens the personal skills of young researchers and thus prepares them for global career opportunities.

The transferable skills program of the Graduate Center is complemented by the Continuing Professional Development Centre of Kiel University (www.weiterbildung.uni-kiel.de). It serves as an additional provider of more general courses with a non-scientific focus, such as courses on time or conflict management, negotiation and communication skills, as well as university teaching and leadership course packages. Within the Continuing Professional Development Centre, additional courses and services are provided by the Career Center and the International Center of Kiel University. These institutions provide general information and advice, regarding career planning and stays abroad. Additional specialized support is offered to foreign students, doctoral candidates, and guest scientists.

In 2018 the Postdoc Center of Kiel University (<https://www.postdocs.uni-kiel.de/en>) was established. It offers specific measures for postdoctoral researchers to promote their professional career. The Postdoc Center is a trans-faculty structure whose services are aimed at researchers directly after completing their doctorate but also at experienced postdoctoral researchers on their way to becoming eligible for appointment to a professorship. By providing information and bundling offers for career advancement, the center provides the foundation for good working conditions at Kiel University that allow excellent research and teaching. Individual career advice available from the center and co-designing transferable skills trainings and further support together with the Continuing Professional Development Center and the Personnel Development Unit help empower gifted young researchers to successfully pursue career paths inside and outside of academia.

In addition to the Graduate Center, various doctoral programs exist at Kiel University. These programs are mostly centered in the topic of life and marine science, agriculture, but also medicine. Due to the greater engineering focus of the IRTG, the closest match in terms of science is the RTG 2154 "Materials for Brain". During the first funding period, we already cooperated in general non-disciplinary subjects. This will be continued within the next funding period.

Principles for Doctoral Degree Regulations at Kiel University

As described in the initial proposal, Kiel University issued the Principles for Doctoral Degree Regulations (see <http://www.gz.uni-kiel.de/en/de/doc/principles-for-doctoral-degree-regulations-at-kiel-university>) to be adopted into the doctoral degree regulations of all faculties. These principles prescribe that a binding, written supervision agreement is concluded between the doctoral advisor and the doctoral candidate. This strategy was adopted by the CRC 1261 as well. As the supervision agreement of the IRTG was specially designed for our program, we will continue the program with this document in addition to the one of the faculty. Kiel University has further established procedures for cross-faculty doctoral degrees, which facilitate doctorates in the interdisciplinary research projects of the CRC. Most relevant for the IRTG are the existing common doctoral degree regulations of the Faculty of Engineering, including the Department of Materials Science and the Department of Electrical Engineering, and the Faculty of Mathematics and Natural Sciences, including the Department of Physics.

3.7 Interim assessment and outlook

The activities of the IRTG constitute an important factor within the collaborative activities of our CRC. Due to the strong interdisciplinarity of the CRC, the IRTG measures were specially developed to increase the interdisciplinary networking and scientific activities between the different research areas. The first funding period of the CRC1261 has created highly motivated and scientifically determined doctoral researchers. From the beginning of the first funding period, interaction of doctoral researchers within and across disciplines was fostered, which led to the establishment of a closely collaborating group of people. Furthermore, with the help of the IRTG, the members identify themselves fully with the scientific goals of the CRC 1261. The interdisciplinary group forms the basis for the success of the CRC.

Overall, the training program offered by the IRTG during the first funding period has provided a balanced selection of compulsory and non-compulsory qualification measures. These measures, including scientific, technical, and cross-disciplinary training, have found strong support by the members of the IRTG. Both research-related and transferable skills training have been well received by the doctoral researchers. This is evident from the very positive evaluation of the IRTG measures conducted through **SOP**. Overall, all actions of the IRTG were met with wide appreciation by the IRTG members. This includes the external research stays, the field trips, the lab visits, the student-only meetings and the summer schools, the technical skill workshops, and workshops offered by the Graduate Center. Supported by the IRTG network, several IRTG members have obtained their doctoral degree or are close to completing their doctorate.

Based on the experience gained and the results of the evaluation from the first funding period, the majority of the existing graduate education concepts will be continued in the second funding period. Yet, minor amendments to the program will continue throughout the second funding period. One example of the adjustments is the restructuring of the retreat meetings that was already initiated during the last funding period. Planned adaptations in the initial booster phase are in constant adjustment, for example with regard to the introductory 10-paper list for new doctoral researchers. To further improve the experience of the doctoral researchers with the offered courses, through the IRTG manager we will seek active influence on the course selection in the University's Graduate Center. To ease starting in the CRC and to establish another route of interdisciplinary integration from the beginning, each new IRTG member will pair with a "buddy" from another discipline, who is also at the start of her or his doctoral research. For the invited guest program, the doctoral researchers will get more involved in the selection and invitation of the external speakers for the CRC colloquium. They will now invite guests on their own to get into contact with external research groups. This will also support all measures related to the outside scientific community, like the external research stay program.

In the first funding period several outreach activities were organized and carried out by the **SOP** with the help and participation of IRTG members. This was initially not planned as a specific measure of the IRTG. It was very well received by the IRTG members. The participation in outreach activities will be implemented as a regular IRTG measure into the qualification program (see **SOP**). Also, field trips to other institutions and research groups that were not an original measure but were introduced during the first funding period are now incorporated as a new element of the IRTG program. They provide networking opportunities with external scientists and are a way to get insight into related fields of research. During the first funding period, only doctoral researchers participated in the activities of the IRTG, because the postdoctoral researchers in the CRC were already experienced postdoctoral researchers and did not belong to the target group. In the second funding period, we will analyze the needs of potential early career postdoctoral researchers and integrate special qualification elements for them.

We regard the IRTG as a success story which supports our early-career researchers on many levels. The IRTG will remain a vibrant measure that regularly adjusts to the actual needs of the doctoral researchers and the CRC.

3.8 Project funding

3.8.1 Previous funding

The project has been funded within the Collaborative Research Centre since July 2016.

3.8.2 Existing funds for the new funding period

Available staff	No	Name, academic degree, position	Field of research	Department of university or non-university institution	Funded through:	Commitment in hours/ week
Research staff	1	McCord, Jeffrey, Prof. Dr.-Ing., Professor	Magnetic Materials	IMS	Core support	3
	2	Gerken, Martina, Prof. Dr., Professor	Theoretical Electrical Engineering	EIE	Core support	2
	3	Maetzler, Walter, Prof. Dr. med., Professor	Neurology	UKSH neuro	Core support	2
	4	Schmidt, Gerhard, Prof. Dr.-Ing., Professor	System Theory	EIE	Core support	1
	5	Parchmann, Ilka, Prof. Dr., Professor	Science and Mathematics Education	IPN	Core support	1
Non-research staff	6	Milde, Sabine, Dr., Head of GC		Graduate Center (GC)	Core support	1

Job description of staff (supported through available funds):

Due to the strongly interdisciplinary character of the CRC and the different disciplinary cultures of the involved disciplines, the IRTG is headed jointly by three project leaders from the three disciplines.

- 1.-3. Prof. McCord, Prof. Gerken, and Prof. Walter Maetzler are co-heading the project and coordinate the project. They are part of the IRTG Board. Together with the IRTG Board they decide on the IRTG program and the allocations of funds for stipends. Moreover, they will support the manager of the IRTG with the organization and coordination of the training activities.
4. Prof. Dr.-Ing. Gerhard Schmidt is responsible for the hosting and the completeness of the contents of the IRTG website. He is responsible for keeping the contents up-to-date.
5. Prof. Dr. Ilka Parchmann is head of the Chemistry Education department of the IPN. She will review the training program of the IRTG on a regular basis and will give advice for readjustment of the training measures to constantly improve the overall quality of the IRTG.
6. Dr. Sabine Milde heads the Graduate Center at Kiel University. She will help the manager of the IRTG with coordination of the activities of the IRTG regarding interdisciplinary qualifications.

Funds available for direct costs (CAU)	2016/2	2017	2018	2019	2020/1
	4.00	8.00	8.00	8.00	4.00

3.8.3 Requested funding

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Julia Jedtberg (Postdoc, 50% E14)	1	18.00	1	36.00	1	36.00	1	36.00	1	18.00
Direct costs	Sum		Sum		Sum		Sum		Sum	
Recruitment	3.00		6.00		6.00		6.00		3.00	
Research training abroad	14.00		30.00		30.00		30.00		14.00	
Total	17.00		36.00		36.00		36.00		17.00	
Fellowships	11.30		22.50		22.50		22.50		11.30	
Global funds	Sum		Sum		Sum		Sum		Sum	

summer schools	-	6.00	16.00	11.00	6.00
Project related workshops	2.50	5.00	5.00	5.00	2.50
Conference participations	7.50	15.00	15.00	15.00	7.50
Field trips	-	2.50	2.50	2.50	-
Grand total	56.30	123.00	133.00	128.00	62.30

(All figures in k€)

3.8.4 Requested funding for staff

The IRTG manager is responsible for the implementation of the program described above. Dr.-Ing. Julia Jedtberg is intended for this position. She managed the IRTG during the first funding period and knows and understands the contributing organizations of Kiel University and the role of the IRTG within a CRC. Dr.-Ing. Julia Jedtberg has professional training in the field of scientific management. She has already gained experience in the management and coordination of scientific projects and the research focus Kiel Nano, Surface and Interface Science (KiNSIS) at Kiel University.

Fundamental tasks of the IRTG manager:

- Overseeing the scientific and cross-curricular training program for the members of the IRTG.
- Review of the mentoring reports to tailor individual training measures in accordance with the identified needs for the doctoral researchers' development.
- Organizing and guiding of the recruitment measures.
- Organization of the internal and external lecturers (together with the IRTG Board).
- Supporting the IRTG Board with organizational and administrative tasks.
- Co-organization of activities like summer schools and retreats of the IRTG at external locations.
- Organizing the cooperation between the Graduate Center of Kiel University and the graduate schools of the existing Research Training Networks at Kiel University.
- Overseeing the external training program.
- Alumni management.

Staff: IRTG manager in 2020/2	k€	18.00
Staff: IRTG manager in 2021	k€	36.00
Staff: IRTG manager in 2022	k€	36.00
Staff: IRTG manager in 2023	k€	36.00
Staff: IRTG manager in 2024/1	k€	18.00

3.8.5 Requested funding for direct costs

The doctoral researchers conduct a part of their research in international research groups and laboratories outside the CRC. The **external research visits** are an essential part of the scientific and non-scientific education provided through the IRTG. The research stays provide an invaluable chance to become acquainted with other methodological skills and to broaden scientific knowledge. Visits will be financially supported by the IRTG for up to three months. The budget accommodates about seven to eight research visits per year. The selection is carried out by the IRTG Board based on short proposals. We assume an average cost of EUR 4,000 per research visit.

Research training abroad for 3 to 4 doctoral students in 2020/2	k€	14.00
Research training abroad for 7 to 8 doctoral students in 2021	k€	30.00
Research training abroad for 7 to 8 doctoral students in 2022	k€	30.00
Research training abroad for 7 to 8 doctoral students in 2023	k€	30.00
Research training abroad for 3 to 4 doctoral students in 2024/2	k€	14.00

3.8.6 Requested funding for fellowships

Fellowships for doctoral researchers and master students on their way to starting their doctoral research are financially supported by the IRTG for three to six months in length. The fellowships allow for the early integration of early stage researchers in the CRC network. They also help to obtain an early commitment from

the best researchers before regular positions within the CRC projects are available. Furthermore, the fellowship give the opportunity to attract potential doctoral researchers from other countries. Possible candidates for a doctoral research can come to Kiel for one to six months in advance get to know their potential working place and research area. About 5 doctoral researchers per year will be supported. We assume an average fellowship duration of 4 months and an average cost of EUR 1,125 for a fellowship per month.

Student fellowships for 2 to 3 students in 2020/2	k€	11.30
Student fellowships for 4 to 6 students in 2021	k€	22.50
Student fellowships for 4 to 6 students in 2022	k€	22.50
Student fellowships for 4 to 6 students in 2023	k€	22.50
Student fellowships for 2 to 3 students in 2024/1	k€	11.30

3.8.7 Requested global funds

Internal and international summer schools are an essential ingredient for imparting the interdisciplinary goals of the CRC. From a scientific point of view, the training activities are important to consolidate the scientific foundations within the interdisciplinary network. The events also help to establish and to deepen the relationships between the research groups of the CRC. Furthermore, the events help IRTG members to identify with the overall research goals. The budget supports one summer school per year, including an international summer school with external lecturers in 2022 as well as a summer school at the Deutsches Museum in Munich in 2023. We assume an average cost of EUR 6,000 for each of the internal summer school periods, a cost of EUR 16,000 for the international summer school and EUR 11,000 for the summer school at the Deutsches Museum in Munich.

Internal summer school in 2021	k€	6.00
International summer school in 2022	k€	16.00
Summer school at the Deutsches Museum in Munich in 2023	k€	11.00
Internal summer school in 2024/1	k€	6.00

The IRTG will organize **project relevant workshops** on topics that are important for most of the IRTG members, as the graduate center and other institutions of Kiel University cannot offer all courses needed. Therefore, special technical skill courses are directly offered by the IRTG. We assume an average cost of EUR 2,500 per workshop and one to two workshops per year.

Project related workshops in 2020/2	k€	2.50
Project related workshops in 2021	k€	5.00
Project related workshops in 2022	k€	5.00
Project related workshops in 2023	k€	5.00
Project related workshops in 2024/1	k€	2.50

Participation and presentations at international conferences are an essential part of the training of early career researchers. Based on a selection process by the IRTG Board, the participation at an international conference is funded for those IRTG members who present. The budget supports about seven to eight conference participations per year. We assume an average cost of EUR 2,000 per person for one conference participation.

Conference participation of 3 to 4 students in 2020/2	k€	7.50
Conference participation of 7 to 8 students in 2021	k€	15.00
Conference participation of 7 to 8 students in 2022	k€	15.00
Conference participation of 7 to 8 students in 2023	k€	15.00
Conference participation of 3 to 4 students in 2024/1	k€	7.50

During the first funding period, several **field trips to other research institutions** were conducted. This will be continued in the second funding period. We assume an average cost of EUR 2,500 per field trip.

Field trips to other research groups in 2021	k€	3.00
Field trips to other research groups in 2022	k€	3.00
Field trips to other research groups in 2023	k€	3.00

3.1 General information about the Scientific Outreach Project

3.1.1 Project title: Communicating Biomagnetic Sensing

3.1.2 Project leaders

Enzingmüller, Carolin, Dr.
17.03.1984, German

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Parchmann, Ilka, Prof. Dr. Dr. h.c.
11.06.1969, German

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Fax: +49 (0) 431 880 5352
E-Mail: parchmann@ipn.uni-kiel.de

Is the employment of the project leaders at the institution indicated contractually fixed for the duration of the proposed funding period? no

Do any of the abovementioned persons hold fixed-term positions? Carolin Enzingmüller holds a fixed-term position (end date 30.06.2020). In the case of funding, Carolin Enzingmüller will be employed at least until the 30.06.2024 by IPN.

3.1.3 Legal issues

This project includes

1.	research on human subjects or human material.	no
2.	clinical trials.	no
3.	experiments involving vertebrates.	no
4.	experiments involving recombinant DNA.	no
5.	research involving human embryonic stem cells.	no
6.	research concerning the Convention on Biological Diversity.	no
7.	investigations involving dual use research of concern.	no

3.2 Summary

The scientific outreach project (SOP) has built a substantial evidence-based outreach program that communicates CRC research to different target groups and strategically involved CRC researchers. The SOP will build on these approaches and achievements by collaborating with established and new partners in Kiel and beyond. The main target groups of the communication activities will be public audiences and stakeholders as well as educational institutions. We will engage the interested public and stakeholders in CRC research with motivating digital media that will be incorporated in the existing exhibition framework and that show different areas of the CRC and their interconnectivity. A first virtual reality (VR) video was a huge success with regard to visitor attraction and stakeholder involvement. We plan to evaluate how VR videos can be used to attract visitors and raise the interest of potential stakeholders in outreach settings. The SOP will benefit from the close cooperation with the *Deutsches Museum* in Munich, who share experiences and expertise in designing digital interactive exhibitions and VR experiences in large scale science outreach programs. With regard to educational institutions, design-based research in the previous funding period has shown that the interdisciplinary CRC research can be successfully transformed into learning environments, in-school as well as out-of-school. In this funding period, we will derive a comprehensive model of efficacy for interdisciplinary school outreach measures with regard to students' interest development and career orientation in STEM (science, technology, engineering, and math) to maximize engagement of different subgroups of students and their teachers. We will strongly collaborate with two out-of-school science education institutions in Kiel: the *Kieler Forschungswerkstatt*, an established player in the field with over 150 visiting school classes per year, and the *Schülerforschungszentren Schleswig-Holstein*, a new and growing network for talent and interest development. To

expand the reach of the outreach activities, the SOP will collaborate closely with the University Office for Press, Communication and Marketing Services for disseminating activities through various communication channels. Developed outreach materials will be disseminated through two new national science education platforms and results will be presented in scientific journals, at conferences and outreach symposia. Furthermore, an accompanying science communication program for doctoral researchers will enhance the quality of the outreach measures and ensure the active involvement of CRC doctoral researchers from all projects in public outreach as well as school outreach. The training will be formally implemented in the IRTG credit point scheme. We will evaluate how these institutional training courses prepare early career researchers for future communication tasks and may influence the quality of outreach activities. This area of training and support will be strengthened by embedding this program in the *Graduate Center* at the CAU, as well as in the *Kiel Science Outreach Campus*, a Leibniz ScienceCampus located in Kiel that specializes in the evidence-based co-design of outreach measures.

3.3 Project progress to date

To date, the SOP has designed, implemented, and improved different outreach formats and has planned, organized, and carried out a broad range of outreach activities. As a first step, important ideas and products of the CRC that are especially suitable for presentation to laypersons were identified in close collaboration with CRC researchers, for example at retreats and IRTG meetings (for details, see the following chapters). The foundation for the content specification of the SOP project was the *Model of Educational Reconstruction* [Du12], which systematically combines the researchers' expertise with research on learners and laypeople and thereby designs outreach approaches that connect to goals and pre-conditions of both target groups. Within the SOP, researchers from different research groups and science education research have cooperated in the design of and reflection on outreach measures by adapting a co-designed framework developed in the *Kiel Science Outreach Campus* (<http://www.kisoc.de/en/>) to meet the needs of the CRC. In the following, we will present the milestones reached in the first funding period.

Design of the hands-on and digital exhibition for public audiences and stakeholders

The aim of the exhibition framework is to engage public audiences in CRC research. To date, two exhibition formats have been developed to present CRC research as well as outcomes of the CRC: A hands-on exhibition and a digital exhibition. One goal was to visualize the process of biomagnetic sensing in a flexible and modular way so that CRC exhibitions can be easily adapted to different settings and target groups.

The hands-on exhibition showed the basic concepts of CRC research (Fig. SOP-1). To highlight the relevance of the CRC research for societal demands and to raise interest, two life-size person cut-outs provide information about possible fields of applications, namely measuring heart activity (**B10**) and improving deep brain stimulation (**B5/T1**). In addition, a group of sensor chain exhibits visualizes the course of the signals, from the biological source (in this case a heart depicted by a 3D model) to an amplifier & D/A converter to signal processing to a final presentation at a „medical monitor“, where visitors can see a post-processed signal (**B1**, **B2**). The sensor chain exhibits are connected through LED strips to visualize the passing signal. A sensor demo exhibit lets visitors investigate for themselves the responses of a CRC sensor to a magnetic field. Another exhibit provides additional information about the composite materials that are used in project area **A** to build the CRC sensors, for example to highlight the influence of material and geometry on sensor properties.

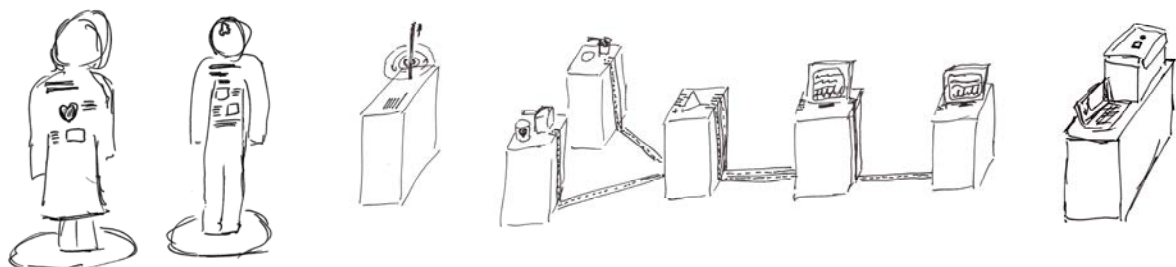




Fig. SOP-1: Schematics of the hands-on exhibit overall and a selection of finished exhibits, including the life-size person cut-outs providing medical information and the sensor chain exhibits showing the different aspects of biomedical sensing.

Digital exhibits allow for presentations in small spaces and are easy to update, transport and set up. We developed an interactive touch screen with information about the goals and the research program of the CRC (Fig. SOP-2). It serves two purposes: It supports scientists who want to introduce interested visitors and stakeholders to the CRC; and it can also serve as an information point for visitors without a scientist present, since the navigation is intuitive. To really catch the visitors' attention, a special 360°-virtual lab tour (Fig. SOP-2) was developed, showing the different steps of a CRC sensor production in the Kiel Nanolab (<https://www.tf.uni-kiel.de/matwis/afm/en/nanolab>). This is highly interesting for visitors from the public, as access to the lab is restricted. The goal was to give public audiences access to this setting via virtual reality. The VR tour was the main attraction at several events. It not only caught the attention of visitors but also served as a starting point to talk about CRC research at the hands-on exhibitions (e.g. at the Kieler Woche) or to get in dialogue with industry stakeholders (e.g. at the Hannover Messe). Furthermore, the CRC was actively invited by the DFG to present the CRC via the interactive touch screen and the VR tour at their "Research in Germany" event and invited by the organizers of the GATE conference, a congress for higher education marketing, to give a talk about the development and production of the VR tour.



Fig. SOP-2: Digital exhibition elements: Interactive touch screen (left) and VR-glasses with the virtual lab tour through the Kiel Nanolab (right).

To present the work of the CRC to the public, three exhibition presentations had been planned for each year. We not only met but even exceeded the annual quota (Tab. SOP-1). In such events for the interested public, the CRC presented itself, for example at the festival *Kieler Woche* and at the *Hannover Messe*, as well as at specialized events for stakeholders.

Table SOP-1. Presentation of CRC exhibition elements at different outreach events.

Date	Event	Target Group
02.-03.10.2019	CAU festivities for "Tag der Deutschen Einheit", Kiel	Interested public
27.09.2019	European Researchers' Night, Kiel	Interested public
04.-05.07.2019	GATE international marketing congress, Bonn	Representatives from higher education
17.-19.06.2019	4 th Euro Intelligent Materials, Kiel	Scientists
10.04.2019	Parliamentary Evening Nanotechnology, Berlin	Guests from politics, business, and science
13.-14.11.2018	Visit CRC 1270, Kiel	Scientists
25.-27.09.2018	DFG-Event "Research in Germany" at the Materials Science and Engineering Congress, Darmstadt	Scientists, representatives from funding organisations
28.09.2018	European Researchers' Night, Kiel	Interested public
16.-18.06.2018	Kieler Woche Uni live, Kiel	Interested public
25.05.2018	Meeting with representatives of the European Regional Development Fund (EFRE)	Representatives from politics
23.-27.04.2018	Hannover Messe, Hannover	Representatives from industry, scientists, interested public
08.03.2018	Student information days at CAU, Kiel	Future students
02.-03.07.2018	Nano Summer School, Kiel	Teachers
29.09.2017	European Researchers' Night, Plön	Interested public
24.-28.04.2017	Hannover Messe, Hannover	Representatives from industry, scientists, interested public
07.-09.06.2017	3 rd Euro Intelligent Materials, Kiel	Scientists

Design of the CRC teaching unit and the out-of-school project day for school students

The context of medical and applied science research is known to be highly interesting for school students and is an innovative field for context-based in-school and out-of-school learning [Ho07] [SOP-4]. The interdisciplinary structure of the CRC offers an excellent thematic foundation for the required cooperation between school subjects in the structure of the "Profiloberstufe" (upper secondary education with emphasis on specific subjects) or the "Wahlpflichtbereich" (optional courses), echoing the interdisciplinary research environment. The research within the CRC provides the opportunity to include topics from various school subjects and to build links to regular curricular topics like fields and forces in physics, structure-property relations in chemistry, or electrophysiology in biology. With that in mind, the goal of the SOP school outreach program is to offer students insight into authentic interdisciplinary research, to teach about biomagnetic sensing through hands-on experiments, and to raise interest by showing the medical relevance of CRC research. The focus of the first funding period was the design of an in-school as well as out-of-school measure covering important concepts from the project areas **A** and **B**.

In our strategy, we used the *Model of Educational Reconstruction* in combination with a design-based research framework, stating that development and research take place through continuous cycles of design, enactment, analysis, and redesign [De03]. To identify important concepts in the CRC research, we analyzed CRC documents and used the first retreat meeting for goal clarifications. Existing teaching materials in the area and studies on learning outcomes were analyzed with regard to important concepts such as the interaction of matter and fields, magnetism, and forces. The first product was a content structure that was discussed with CRC researchers to ensure that it fits the research logic of the CRC. A group of teachers assessed the consistency and the educational value of the unit.

Following a cyclic, design-based research process, we designed (1) a teaching unit for in-school learning and (2) an out-of-school project day at the student lab *Kieler Forschungswerkstatt* (www.forschungs-werkstatt.de). The teaching unit is a four-week unit that teachers can implement in their classes. In the project day, the visiting school classes get a compact overview of the CRC research and experiment independently in small groups. Both designs have a similar content structure but make use of the special characteristics of the in-school and out-of-school setting, respectively. The structure is context-based, starting with a medical motivation, which is especially motivating for students of both genders [Ho07] [SOP-4]. Then, the students learn about the process of biomagnetic sensing with hands-on experiments. New experiments had been designed, allowing students to explore the functional principle of magnetoelectric sensors. A low-cost setup of a magnetostrictive cantilever

beam is used to quantitatively measure magnetostrictive characteristics of materials and to visualize the magnetostrictive effect via a laser beam on a screen (Fig. SOP-3). An experiment with piezo crystals demonstrates the properties of piezo materials and the piezoelectric effect. Both effects are linked when students create their own magnetoelectric sensors out of magnetostrictive and piezoelectric materials, test them, and optimize them. In both formats, authentic CRC media were implemented, including pictures, animations, graphs, and short researcher interview statements.

In order to support teachers with the teaching unit, a detailed teaching manual was created. It contains comments and suggestions on how to use the materials as well as detailed background information regarding CRC topics. To further increase teacher support, we provided teachers with a CRC kit that contains experimentation materials that might be not available in schools.

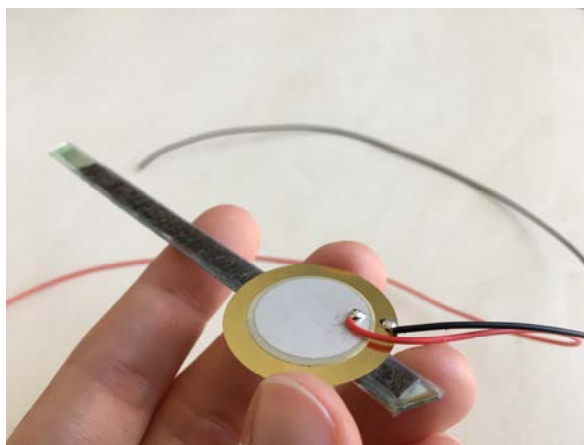


Fig. SOP-3: A simple and low-cost experiment for the qualitative and quantitative investigation of magnetostrictive characteristics, employing magnetostrictive laser deflection and optical amplification (left) and a magnetoelectric sensor built by a student as part of the out-of-school project day (right).

The SOP tested the measures with school classes. To date, three classes for the teaching unit and three classes for the out-of-school project day have participated. First evaluation results confirmed that students are especially interested in the medical applications of the CRC research. Students positively highlighted several structural aspects, such as the hands-on character, the opportunities to experiment freely, and building your own sensors. The evaluation made clear that there is still potential to improve the materials through providing different levels of difficulty, for example, for students with high prior knowledge, and to integrate authentic insight into signal processing.

The goal of testing the measures with 10 classes will be reached by the end of the current funding period, as there is a high demand for the teaching unit and a waiting list for the project day at the *Kieler Forschungswerkstatt*. In first presentations of the teaching unit at teacher workshops and conferences, the feedback was very positive and showed that there is a great demand for this type of interdisciplinary teaching concept and materials. More workshops for teachers are planned for 2020 to present the final teaching unit to an even broader range of science teachers. The developed experiments are in the process of being published in teacher journals [SOP-1]. Furthermore, the developed teaching manuals will be published on the new *Open Educational Resources Platform* at Kiel University, which will make the materials accessible to teachers all over Germany (<https://www.ipn.uni-kiel.de/de/forschung/projekte/oer-ipn>).

To address more interested and talented students, we have started a cooperation with the newly founded *Netzwerk Schülerforschungszentren Schleswig-Holstein* (<https://www.sfz-sh.de/standorte/kieler-forschungswerkstatt.html>) that provides opportunities to carry out scientific projects over a longer time span. We also integrated CRC outreach elements at the yearly Girls' Day (<https://www.girls-day.de/>) and at the physics project days in Kiel (<http://www.ppt2018.de/>).

Table SOP-2: School outreach program activities.

Date	Event	Target Group
09.-14.09.2019	Project days at Humboldt School, Kiel	Interested students
30.08.2019	Project day at <i>Kieler Forschungswerkstatt</i>	Secondary school class from Rudolf Steiner Schule Hamburg-Wandsbek

23.08.2019	Project day at <i>Kieler Forschungswerkstatt</i>	Secondary school class from Gemeinschaftsschule Friedrichsort, Kiel
24.-25.06.2019	Talk in a school and accompanying program at Faculty of Engineering	Secondary school class from Isarnwohld School Gettorf
24.06.2019	First implementation of the project day at <i>Kieler Forschungswerkstatt</i>	Secondary school class from Lernwerft, Kiel
28.03.2019	Girls' Day at CAU, Kiel	Female school students
26.03.2019	Presentation of the school outreach concept and materials at the DPG Spring Meeting, Aachen	Science teachers
24.03.2019	Presentation of the school outreach concept and materials at the national MNU teacher congress, Hannover	Science teachers
October-December 2018	Implementation of the teaching unit in three physics classes	Secondary school classes from Heinrich-Heine Gymnasium Heikendorf and Gymnasium Schloss Plön
04.09.2018	Teacher workshop presenting the developed experiments, Kiel	Science teachers
22.-25.08.2018	First implementation of experiments at Physics Project Days, Kiel	Female school students
02.-03.07.2018	Nano Summer School, Kiel	Science teachers
26.04.2018	Girls' Day at CAU, Kiel	Female school students
13.03.2018	Students course at the <i>Schülerforschungszentrum</i> , Kiel	Talented and interested students
27.04.2017	Girls' Day at CAU, Kiel	Female school students

Development of science communication training and support elements for doctoral researchers

Cooperation among scientists from different disciplines relies on interdisciplinary communication. Different challenges have been reported in the literature with regard to language, the use of special terms and representations, and the different levels of expertise (e.g. [Ko03]), leading to potential misunderstandings and barriers in communication, learning, and cooperation. The SOP aims to raise awareness for thoughtful communication to different audiences [Br10] and connects these interdisciplinary communication processes in the CRC with a specific focus on IRTG researchers, especially doctoral researchers.

The design of training and support elements was based on research on interdisciplinary science communication. It included three phases: (1) a presentation at the first retreat meeting combined with a workshop with the doctoral researchers to highlight challenges of interdisciplinary communication and cooperation. The goal was to sensitize doctoral researchers to their own modes of representation and explanations, like the use of terms, graphs or pictures, and those of the other disciplines, to lay the ground for a more explicit use of language during the internal CRC cooperation. (2) At the second retreat, the CRC members were asked to write down terms and representations that were hard to understand or used in another meaning during the talks from other project groups. The doctoral researchers then explained the collected terms and representations to each other in the student-only meetings, thus clarifying misunderstandings. (3) The third phase of designing training and support elements focused on external science communication. In a presentation at the retreat meeting, principles of external science communication were highlighted. This was accompanied by workshops for the IRTG group, e.g. practicing communicating about your own work to non-expert audiences by preparing and reflecting on "elevator pitches" (brief presentations that outline an idea or a project in the short time period of an elevator ride, usually 30-60 seconds). In another workshop, IRTG members reflected on how they can communicate about the CRC as an interdisciplinary research centre (Fig. SOP-4). A competition was initiated with the goal to design the best CRC giveaway for outreach events. The winning design – a stress ball in the shape of a brain with the CRC logo – was produced and disseminated at outreach events.



Fig. SOP-4: Exhibition design meeting in April 2018 for preparing the event at Kieler Woche 2018 (left), SOP Workshop at the IRTG summer school in July 2018 in Eckernförde (middle), and IRTG members filming an outreach video in April 2017 (right).

Doctoral researchers were involved in the development of different outreach elements for the school outreach program as well as for the exhibitions (Fig. SOP-4). Evaluation results and observations showed that a lot of doctoral students were generally interested in participating in outreach activities but wished for more continuous exchange and feedback on the outreach activities conducted. We will adapt the program accordingly for the second funding period (see WP4 in the project plan).

During the funding period, the SOP and the IRTG board cooperated closely: Carolin Enzingmüller was a permanent participant during the IRTG meetings; this ensured a constant exchange on outreach and communication topics. The SOP conducted a formative and summative evaluation of the IRTG, monitoring different aspects of the communication in the IRTG and giving regular feedback to the IRTG board to support further planning. Part of the quality control was based on regular short questionnaires, evaluating the retreat and student-only meetings, and to monitor the perception of different elements of the IRTG (for details see chapter **IRTG**). The SOP was also active in advising the planning of summer schools and other support measures.

Evaluation and monitoring of the outreach activities

The *Model of Educational Reconstruction* as a design framework and the cyclic, design-based research approach already include various evaluation as well as monitoring elements in the design process. Feedback regarding relevance, accuracy, consistency, and practicability was collected from CRC researchers and the outreach target groups by using different evaluation methods like ratings, open and closed questionnaires, group discussions, and qualitative observations. The interactive touch screen has a built-in feedback section, where visitors can give their opinion on how to improve the interaction with the device. Differentiated analysis had been carried out with example target groups such as teachers and school classes for the school module and the microsite. A master's thesis project implemented and evaluated the design of the out-of-school project day. Interest, as one important prerequisite of out-of-school learning, was analyzed with regard to different CRC topics (How can different materials be combined to design a sensor? How can sensor signals be improved? What signals can be measured at the heart?). The evaluation and improvement of the outreach measures will continue and outcomes will be further studied.

In cooperation with the IRTG, the SOP conducted both a formative and a summative evaluation of the IRTG program. The IRTG measures were specially developed to increase the interdisciplinary communication and scientific activities between the different research areas. With the formative evaluation, it was possible to monitor and improve the quality of the measures in the process, e.g. by adapting the structure and content of retreat meetings, student-only meetings, or workshops for the IRTG group. The summative evaluation assessed the benefits of the IRTG program at the end of the funding period, facilitating evidence-based improvements of the program for the second funding period (for detailed concept and results see chapter **IRTG**).

Connecting outreach and press relations activities

The SOP connects outreach activities with press relations (PR) by collaborating closely with the University Office for Press, Communication and Marketing Services. Together, we supported researchers in the CRC by different means and advice. Press releases were written regularly and submitted in cooperation with the researchers and the SOP. The CAU social media channels (e.g. Facebook, Twitter, blogs, etc.) were used to communicate CRC milestones to different target groups (the public, students, sponsors, partners) and to enhance news and stories (research results, people, events, etc.) with photos, videos, charts, and graphics. The University Office for Press, Communication and Marketing Services also supported the CRC's presentation at

several outreach events, such as the *Kieler Uni live* or *Hannover Messe*. In addition, the outreach media developed in the SOP were collected in a media centre on the website, accompanied by additional information for different target groups, e.g. the interested public or teachers and students. A news section on the CRC website called “Outreach News” informs regularly about outreach events and the progress of outreach format design (Fig. SOP-5). We also developed a specific auxiliary website (“microsite”) that delivers focused, relevant content about CRC research in easy-to-understand language to a broader non-scientific audience (<http://info.sfb1261.de/de/>). Together with the University Office for Press, Communication and Marketing Services, an interview series with doctoral researchers was initiated. With the goal of giving exhibition visitors and school students authentic and personal insight into the work of young researchers, the participants were asked questions like “What subject did you study to become a scientist in the CRC?” and “How does a typical day at work look?”. This not only created interesting content but was also a great training opportunity for the doctoral researchers to practice talking to a media representative in a protected setting. The interviews are published on the CRC website (<http://www.sfb1261.de/index.php/en/mediacenter-en/nachwuchsforschende-wall>).

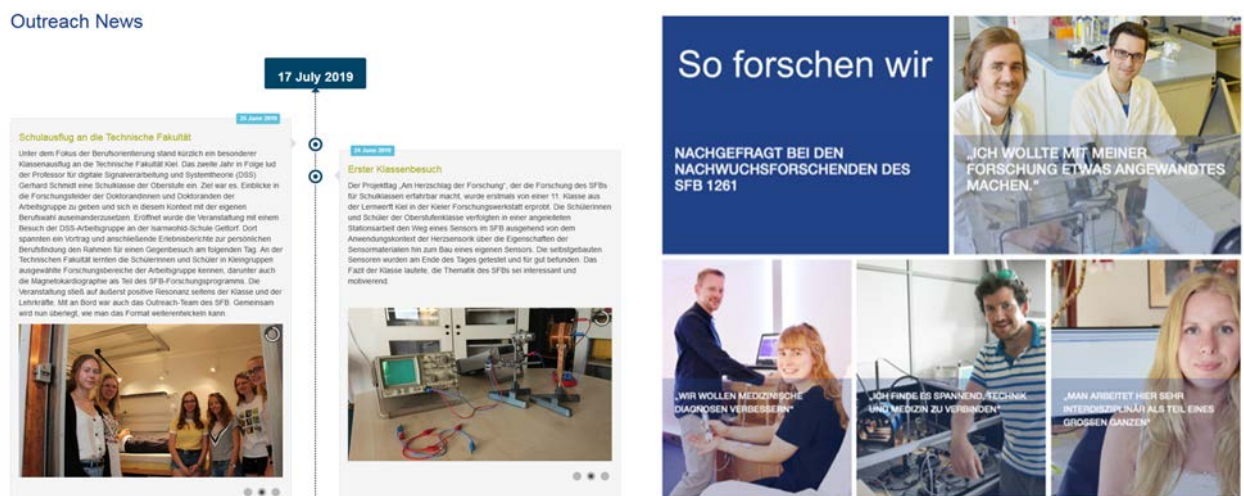


Fig. SOP-5: The outreach news that informs about the communication activities and events on the CRC website (left) and the interview series with IRTG researchers in cooperation with the University Office for Press, Communication and Marketing Services (right).

References

- [Br10] R. Bromme, D. Kienhues, T. Porsch, “Who knows what and who can we believe? Epistemological beliefs are beliefs about knowledge (mostly) attained from others” in *Personal Epistemology in the Classroom: Theory, Research, and Implications for Practice*, L. D. Bendixen, F. C. Feucht, Eds. (Cambridge University Press, Cambridge, 2010), pp. 163-193.
- [De03] The Design-Based Research Collective, Design-based research: An emerging paradigm for educational inquiry. *Educational Researcher* **32**(1), 5–8 (2003).
- [Du12] R. Duit, H. Gropengießer, U. Kattmann, M. Komorek, I. Parchmann, “The Model of Educational Reconstruction – a Framework for Improving Teaching and Learning Science” in *Science Education Research and Practice in Europe. Cultural Perspectives in Science Education*, D. Jorde, J. Dillon, Eds. (SensePublishers, Rotterdam, 2012), vol 5.
- [Ha14] E. R. Halverson, K. Sheridan, The maker movement in education. *Harvard educational review* **84**(4), 495-504 (2014).
- [Ho07] N. Holstermann, S. Bögeholz, Interesse von Jungen und Mädchen an naturwissenschaftlichen Themen am Ende der Sekundarstufe I, *ZfDN* **13**, 71-86 (2007).
- [Ka18] L. Kampschulte, “Lernorte mit Medien vernetzen!? Chancen und Herausforderungen der lernortübergreifenden Mediennutzung” in *Medieneinsatz im mathematisch-naturwissenschaftlichen Unterricht – Fachübergreifende Perspektiven auf zentrale Fragestellungen*, M. Ropohl, A. Lindmeier, H. Härtig, L. Kampschulte, A. Mühling, J. Schwanewedel, Eds. (Verlag der Joachim Herz Stiftung, 2018), pp. 138-174.
- [Ko03] R. Kozma, The material features of multiple representations and their cognitive and social affordances for science understanding, *Learning and Instruction* **13**, 205–226 (2003).
- [Ri18] J. Risien, M. Storksdieck, Unveiling Impact Identities: A Path for Connecting Science and Society. *Integrative and Comparative Biology* **58**, 58–66 (2018), <https://doi.org/10.1093/icb/icy011>

- [Su18] D. Sun, C.-K. Looi, Boundary interaction: Towards developing a mobile technology-enabled science curriculum to integrate learning in the informal spaces. *British Journal of Educational Technology* **49**, 505–515 (2018), <https://doi.org/10.1111/bjet.12555>
- [Ta10] P. Taskinen, „Naturwissenschaften als zukünftiges Berufsfeld für Schülerinnen und Schüler mit hoher naturwissenschaftlicher und mathematischer Kompetenz. Eine Untersuchung von Bedingungen für Berufserwartungen“, (Science as a future career field for pupils with high scientific and mathematical competence. An investigation of conditions for profession expectations), thesis, Kiel University (2010).

3.3.1 Project-related publications

- [SOP-1] D. Laumann, P. Hayes, C. Enzingmüller, E. Quandt, I. Parchmann, Magnetostriction Measurements with a Low-Cost Magnetostrictive Cantilever Beam, (2019), **Manuscript submitted for publication.**
- [SOP-2] C. Enzingmüller, L. Kampschulte, I. Parchmann, “Science Outreach in Sonderforschungsbereichen” in C. Maurer, Ed. (Universität Regensburg, 2019), *Naturwissenschaftliche Bildung als Grundlage für berufliche und gesellschaftliche Teilhabe: Gesellschaft für Didaktik der Chemie und Physik, Jahrestagung in Kiel*, pp. 548–551.
- [SOP-3] C. Enzingmüller, D. Laumann, L. Kampschulte, I. Parchmann, “Kommunikation interdisziplinärer Forschung im Bereich Biomagnetic Sensing” in C. Maurer, Ed. (Universität Regensburg, 2019), *Naturwissenschaftliche Bildung als Grundlage für berufliche und gesellschaftliche Teilhabe: Gesellschaft für Didaktik der Chemie und Physik, Jahrestagung in Kiel 2018*, pp. 564–567.
- [SOP-4] L. Kampschulte, C. Enzingmüller, W. Wentorf, E., Quandt, I. Parchmann, Medizinische Sensoren entwickeln: Zusammenarbeit verschiedener Disziplinen. *Naturwissenschaften im Unterricht – Chemie* **29**, 41–45 (2018).
- [SOP-5] H. Sevian, Y. J. Dori, I. Parchmann, How does STEM context-based learning work: what we know and what we still do not know, *International Journal of Science Education* **40**, 1095–1107 (2018).

3.4 Project plan

Objectives

Design-based research in the previous funding period has shown that the interdisciplinary CRC research can successfully be transformed into exhibition frameworks and learning environments. Evaluations showed that the context-orientation on medical applications and the integration of digital media, like VR tours, were effective in raising visitors’ and students’ interest in modern research on biomagnetic sensing. Furthermore, IRTG evaluations showed a high interest for science communication but also various challenges for doctoral researchers. We want to use this experience and these materials to gain deeper insights into how to engage audiences in modern research (interested public, stakeholders, school students). The aims of this funding period will be to (1) investigate how VR videos can best be designed and used to raise interest in outreach settings, for example through interactivity elements that increase the perception of authenticity, (2) derive a representative model of efficacy for interdisciplinary school outreach measures with a focus on differential and mid-term effects for different subgroups of students, and (3) derive success factors for integrating doctoral students in outreach activities via a science communication training that is formally implemented in the IRTG program. Based on such insights, outreach tools will be further developed and disseminated, and outreach events will be designed and supported in cooperation with the University Office for Press, Communication and Marketing Services. This way, the CRC research will be communicated to the public and stakeholders as well as to school students and their teachers through evidence-based and high quality outreach, while at the same time training doctoral researchers in science communication.

WP1: Content analysis

As a first step, new CRC research projects will be analyzed with regard to their outreach potential. The area of movement detection and analysis (**B9**) may provide a promising context as it combines the medical background of neurological diseases with movement detection techniques. The project on individualized deep brain stimulation (**T1**) has the potential to give insight into research-industry collaboration and can serve as a case study for medical technology development and translation into clinical practice. Another promising area would be to focus on research methods in addition to experiments, for example, the role of simulations in the CRC research, e.g. in predicting the prospect of success for sensor concepts by modelling material properties and simulating sensor setups (**A8**), and the real-time application signal processing tools like KiRAT developed by CRC researchers (<https://dss.tf.uni-kiel.de/index.php/research/realtime-framework>) (**B2**).

WP2: Co-planning and implementing exhibitions for engaging the public

We will present and extend exhibition elements from the first funding period that show the whole CRC research program at regular outreach events, like the *Kieler Uni live* at the *Kieler Woche* or the *European Researchers’*

Night to engage the public in modern research. CRC doctoral researchers will actively participate in the planning and conducting of public outreach activities, supported by training elements (see WP 4). As Kiel University is currently planning to enlarge its exhibition and meeting areas and programs towards a holistic concept of a *Science Dialog* at the Kiel Fjord area, the SOP will potentially be able to implement exhibits in the long run.

Since VR videos are a tool for authentic insight into laboratory and clinical workplaces, we will develop new videos on medical applications of the CRC sensors in virtual real-life environments. To make the VR experience even more engaging, we want to integrate interactive elements into the videos, like information boxes with further explanations or quotes from scientists. The new videos will be shown at public events and fairs but will also be integrated in the school outreach program, for example, in the out-of-school project day at the *Kieler Forschungswerkstatt*. The videos will be evaluated qualitatively with a think-aloud method carried out by a master student as part of his or her thesis.

This work package will also benefit from the close cooperation with the *Deutsches Museum* in Munich. The Deutsches Museum is Germany's most popular museum, with around 1.4 million visitors a year, and is one of the leading experts for communicating science and technology. The museum offers not only its expertise in the design of interactive exhibitions and large scale science outreach programs but also VR experience gained in the current research project Museum4.0 (<https://www.museum4punkt0.de/en/subproject/application-of-3d-visualization-in-museum-education/>). In 2021, the *Deutsches Museum* will open a new 1000m² exhibition "Health", thus establishing a perfect platform for CRC outreach. In this context, we will design together with the IRTG an additional exhibition element that links CRC research to the exhibition theme. This could be, for example, a special tour guide for the *Deutsches Museum App* that will present aspects of CRC research at different points of the exhibition or a more interactive format, like a science show that will be held for the visitors of Deutsches Museum. This cooperation with *Deutsches Museum* will boost the reach of the CRC outreach measures far beyond the Kiel area.

WP3: Designing measures for interest development and career orientation of school students

In the science education literature as well as in current political discussions, the integration of relevant contexts in the interface between science and society (so called socio-scientific issues) and a higher emphasis on creative activities ("from STEM to STEAM", meaning the integration of arts & design in STEM) is continuously pointed out. The research on sensor development in the CRC offers an outstanding content for both the connection to societal demands and the integration of creative design activities. The contextual framing of the CRC fundamental research in medical contexts permits addressing different STEM interest areas and school subjects. The outreach program will initiate early-on explorations for students to catch their interest, deepen their knowledge and experimentation skills as part of regular school teaching and out-of-school learning, and finally foster more interested and talented students through additional enrichment measures.

Design-based research has shown that the interdisciplinary structure of the teaching unit and the out-of-school project day is successful with regard to relevance, accuracy, consistency, and practicability. Now, we will systematically evaluate differential effects with representative sample sizes, investigating efficacy of the measures for different subgroups of students, for example, regarding gender or school type. We will include follow-up surveys to check the stability of effects. Based on these findings, we will design a follow-up format at the *Schülerforschungszentrum Kiel*, tailored to the needs of interested and talented students, like a medical sensor design academy. Creativity elements will be a focus in the process of designing your own sensors, as emphasized in the internationally growing „maker“ scene [Ha14]. Interested IRTG doctoral researchers will actively engage in these school outreach activities, supported by the SOP (see WP 4). By involving both experts and novices in design thinking projects, as being realized for example in the Fraunhofer citizen science project *CitizenSensor* (<https://www.imw.fraunhofer.de/en/research/innovation-acceptance/projects/Citizen-Sensor.html>), new insights about future-oriented participatory communication models between research and society are gained.

In addition to accompanying evaluation studies, e.g., on interest, an empirical research study will be carried out. The goal of the research of the doctoral researcher in the SOP will be to design and evaluate this new measure for interested and talented students and to connect it to the existing school outreach measures by developing and testing so-called *boundary objects*, which connect different learning spaces [Su18]. A boundary object can be an explanation concept, like the on-going understanding of the sensor concept in science classes and out-of-school activities, or a physical object created in the classroom and brought to an informal learning space, like a model sensor designed and further developed by groups of students. More recently, mobile technologies allow for creating a wide range of digital artifacts that can be used as boundary objects, like concept maps, drawings, photos, and videos [Ka18]. Following a design-based research paradigm, the doctoral researcher will develop potential boundary objects and empirically test their effects on the continuation

of interest and motivation with a specific focus on study and career perspectives and their support of deepening understanding. This will lead to new insights about how to better connect regular school teaching, school enrichment, and out-of-school programs in STEM.

WP4: Implementation and evaluation of science communication training for IRTG members

Doctoral researchers have to learn to communicate in many different contexts as part of their research activities. The formats and norms of communication differ in audience and relation (PhD student - supervisor, peer-to-peer, teaching and learning, public outreach) as well as in the goals and conditions of the communication activity. The SOP provides reflection and training tools for communication in general, in close cooperation with the Graduate Centre, and for public and educational outreach in particular. In the first funding phase, a lot of doctoral researchers showed high interest in direct involvement in science communication but also expressed various challenges in selecting, planning, practicing, and reflecting outreach activities. In this work package, we will formally implement and evaluate a module-based program that is oriented towards the needs of doctoral researchers in the CRC but also applicable to other research centers (Fig. SOP-6). This work package requires continuous communication and feedback with the **IRTG**.

The first module will provide tools and formats that reflect interdisciplinary science communication, a topic that is especially important during the starting phase of a new interdisciplinary project. The IRTG members will gain insight into goals, tools, language, and representations in general, which the IRTG members apply to their own fields of research and can use to reflect on differences and similarities between the disciplines.

The second module focuses on outreach at CAU, with the goal of explaining your own research and knowledge background to novices. The participants get to know different CAU outreach formats and their specific benefits and challenges. Based on this overview, the participants choose an outreach focus in public outreach or school outreach. Depending on their focus, they will prepare an authentic CRC outreach event in teams, for example for the *European Researchers' Night* (public outreach) or as part of the CRC school program (school outreach). The material from the first module will be adapted for this outreach context, enriched by a specific approach, like a societal contextualization of personal research or inquiry learning.

The third module combines these learning experiences and expands them beyond the location of CAU to the setting of a research museum, here the *Deutsches Museum*, where public and educational outreach meet and get connected to current overarching societal questions. The whole IRTG group designs a participation tool or program within a joint project between the CRC and the *Deutsches Museum*. Via the *Kerschensteiner Kolleg*, a renowned training institution for science communication at the *Deutsches Museum*, it will be possible to offer IRTG members a complete training element in an authentic museum setting.

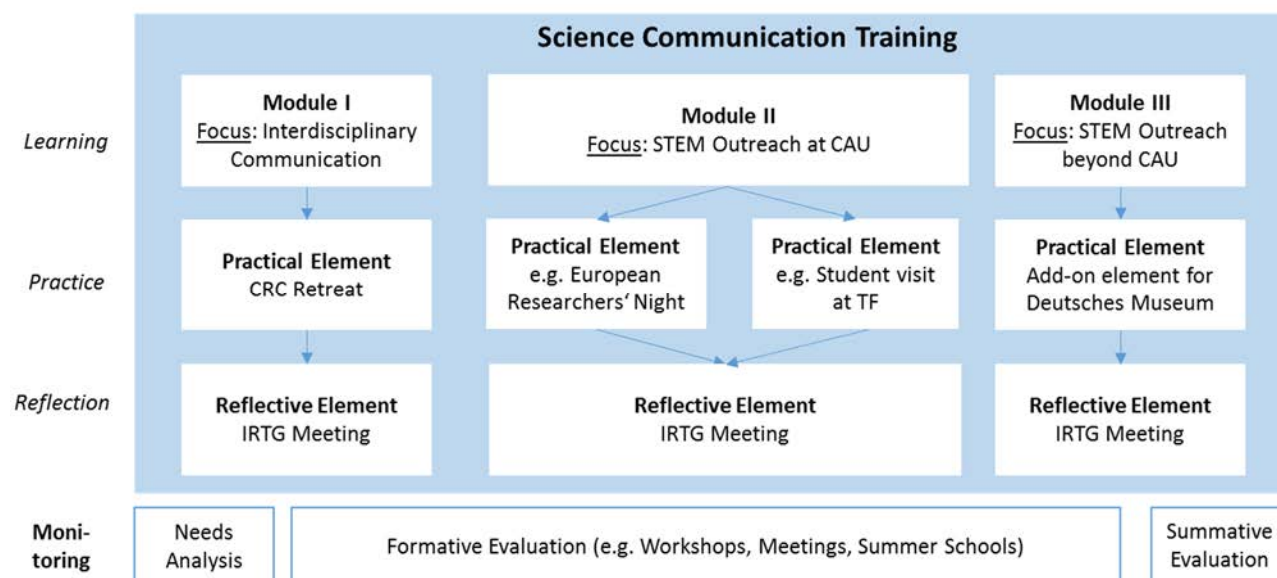


Fig. SOP-6: Science outreach training program consisting of systematic and cumulative learning opportunities in science communication, application of knowledge in authentic outreach event settings, and reflection on experiences in the IRTG group.

The outreach training elements in the IRTG will be based on research on effective science communication training, like the concept of impact identity, that incorporates a scientist's discipline and scholarship, personal preferences, capacities, skills, institutional context, and the various communities or social settings in which she/he participates [Ri18]. They will consist of workshop elements, practice units in authentic communication settings, and reflection phases. This allows for reflecting on differences and similarities between audiences and learning how to adapt to these communication scenarios. In accordance with literature on scientists' outreach motivation, evaluation carried out during the first funding period showed that acknowledgment and appreciation are important factors for the participation of doctoral researchers in outreach activities. The SOP outreach activities will be formally implemented in the IRTG credit point scheme (see **IRTG**) as regular part of the work of IRTG members. With that step, the CRC commits to the important role of active science communication for research institutions.

WP5: Monitoring and evaluation of the outreach activities

The outreach measures are accompanied by continuous evaluation and monitoring of the SOP's activities and the IRTG program. Interviews, questionnaires, and other test instruments will be used to analyze differential and mid-term effects of the school outreach measures with regard to interest as well as study and career orientation and involvement in enrichment programs (following the catch-and-hold framework). Outcomes will be investigated in a pre-post-follow-up design. The personal data collected will be pseudonymized. Before each study, there will be an approval obtained by the IPN ethics committee.

To evaluate the SOP elements of the IRTG training, we will conduct group interviews and use questionnaires. Furthermore, the SOP will evaluate the IRTG program as a whole by using short questionnaires at regular intervals (e.g. summer schools, retreat meetings) to monitor the perception of the different elements of the IRTG, e.g. with regard to the estimated relevance, the perceived learning outcomes, and additional demands of qualification. Results from the accompanying research, especially WPs 3-5, as well as the products of the design in the WPs 2-4, will be presented at conferences for teachers and science education researchers and published in journals for both groups by the SOP PIs and the doctoral researcher.

WP6: Dissemination and cooperation with the University Office for Press, Communication and Marketing Services

The focus of our dissemination activities will be on making the CRC research and outreach activities visible and accessible to audiences beyond our direct outreach events. We will be closely collaborating with the University Office for Press, Communication and Marketing Services to support researchers in the CRC by writing press releases as well as in posting news on CAU social media channels (Twitter, Instagram, etc.). The CRC website is an important tool for dissemination and will be updated regularly by interacting closely with CRC scientists. The outreach section of the CRC website will be restructured and will be connected to a new platform called *ScienceSurfers*, developed by the *Kiel Science Outreach Campus*, that will guide students through outreach topics and activities. Through the close cooperation with partners like *Deutsches Museum* as well as science education networks, e.g. the German wide network of student laboratories and student research centers (LernortLabor), or the international cooperation partners of the *Kiel Science Outreach Campus*, the designed outreach programs will be transferred beyond the location of Kiel. School outreach material will be made available for teachers, students, and out-of-school labs by the *Open Educational Resources Platform* currently developed at IPN and Kiel University.

Table SOP-3. Work schedule

	Work Package	2020		2021				2022				2023				2024	
		III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II
WP 1	Development of a core concept for content to be disseminated (updates after each retreat)																
WP 2	Update of exhibition elements																
	Presentation of exhibition elements at outreach events																
	Development, production, and editing of new videos																
WP 3	Updating out-of-school project day at Kieler Forschungswerkstatt																
	Offering out-of-school project day at Kieler Forschungswerkstatt																
	Literature research																

	Development of follow-up format for interested students, designing boundary objects																		
	Pre-studies, pilot test, and revision of instruments for empirical studies																		
	first test cycle																		
	Improvement																		
	second test cycle																		
	Dissemination at teacher meetings and conferences																		
W	Refinement of core concept for IRTG communication training																		
P	Implementation of training program																		
4	Evaluation and further development of the program																		
	Dissemination of success factors and best-practice examples																		
W	Monitoring of exhibitions																		
P	Evaluation of out-of-school project day																		
5	Evaluation of communication training and support in IRTG group																		
	Monitoring IRTG activities																		
W	Communication (e.g. press releases, website maintenance)																		
P	Maintenance, updating and improvement of CRC website																		
6																			

Prospects

In cooperation with IPN, outreach and enrichment have become substantial research and development subjects at Kiel University that will be continued and expanded in the near future, strengthened through the *Kiel Science Outreach Campus*. The SOP activities will be embedded in these outreach concepts at Kiel University. We expect that the work of the SOP will not only contribute to communicating and disseminating CRC research to different important target groups (public, stakeholders, educational institutions) but also gain new insights into interdisciplinary public and educational outreach design and training. The designs developed and investigated in the first and second funding period of the CRC will be an excellent base for the further investigation on successful designs in that area. We will further expand the focus of the school outreach design and research towards long-term effects, investigating processes like identity building and fostering a sense of belonging to STEM areas. The long-term goals will be to develop integrated programs to foster identity building and a sense of belonging, especially for underrepresented STEM students. The training program for doctoral researchers will be designed and documented in a way that makes it transferable to other interdisciplinary research groups. Successful elements will be integrated permanently into the training structures at Kiel University.

3.5 Project funding

3.5.1 Previous funding

The project is currently funded from 1.7.2016 – 30.6.2020.

3.5.2 Existing funds for the new funding period

	2020/2	2021	2022	2023	2023/1
Sum of existing funds from IPN/ Kieler Forschungswerk-	1500	3000	3000	3000	1500
Sum of requested funds	7.500	15.000	13.000	13.000	5.500

(All figures in euros)

3.5.3 Requested funding for the new funding period

	2020/2		2021		2022		2023		2023/1	
Staff	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum	Quantity	Sum
Doctoral researcher, 65% E13	1	21.550	1	43.100	1	43.100	1	43.100	1	21.550
Graphic designer, 15% E9	1	3.000	1	6.000	1	6.000	1	6.000	1	3.000
Total		24.550		49.100		49.100		49.100		24.550
Global funds	Sum		Sum		Sum		Sum		Sum	
Public relations	7.500		15.000		13.000		13.000		5.500	
Grand total	32.050		64.100		62.100		62.100		30.050	

(All figures in euros)

3.5.4 Requested funding for staff

Existing staff	Se-quential no.	Name, academic degree, position	Field of research	Department of university or non-university institution	Project commitment in hours per week	Funding source
Research staff	1.	Parchmann, Ilka, Prof. Dr.	Chemistry Education	IPN	4	Core Support
	2.	Enzingmüller, Carolin, Dr.	Science Outreach	IPN	5	Core Support
	3.	Eckhard Quandt, Prof. Dr.-Ing.	Functional Materials	IMS	1	Core Support
	4.	Gerhard Schmidt, Prof. Dr.-Ing.	System Theory	DSS	1	Core Support
Non-research staff	5.	Henrike Bratz		Kieler Forschungswerkstatt	1	IPN
	6.	Julia Siekmann		Priority research area KINSIS, public relations	2	Core Support
	7.	Martin Laß		IPN	2	IPN
Requested						
Research staff	8.	Cara Broß		IPN	E13	
	9.	N.N.		IPN	E9	

Job descriptions of staff for the proposed funding period (existing staff):

1. Prof. Dr. Ilka Parchmann is responsible for the coordination and the scientific management of the SOP. She will be actively involved in the development of the overall evaluation framework and will supervise the PhD student and the scientific publications. She will coordinate the institutional integration of outreach measures into CAU institutions.
2. Dr. Carolin Enzingmüller will supervise the school outreach design and will support the doctoral researcher in designing the materials. She will design and evaluate the outreach training for the IRTG doctoral researchers, will coordinate these efforts with the IRTG manager and representatives from the *Kiel Science Outreach Campus*, and will generate transferable best-practice examples for an integrated outreach training.

3. Prof. Dr.-Ing. Eckhard Quandt in his role as spokesman of the CRC will advise the SOP on strategic communication in order to strengthen the overall message of all outreach and communication activities. Furthermore, he will support the SOP with his scientific knowledge to ensure the quality of the content.
4. Prof. Dr.-Ing. Gerhard Schmidt will support the doctoral researcher in designing effective school outreach measures for the CRC with a focus on career orientation.
5. Henrike Bratz will support the doctoral researcher in all issues regarding the organization of projects at the student lab *Kieler Forschungswerkstatt*.
6. Julia Siekmann will support the SOP in general PR work such as press releases, social media activities, as well as support in presenting the exhibitions, e.g. at the science festival *Kieler Woche*.
7. Martin Laß will support the SOP by constructing and building models and experimental setups for exhibitions and teaching modules.

Job descriptions of staff for the proposed funding period (requested staff):

8. Cara Broß is currently working as a master's student in the SOP and will continue as a doctoral researcher (E13, 65%). The work will comprise the responsible coordination and administration, educational attendance, evaluation and re-design of all measures in school and out-of-school settings within the project.
9. N.N., a communication & graphic designer from the IPN graphic department (E9, 15%) will support the SOP with the (re-)design of the website, the digital exhibition, the teacher and student materials as well as the IRTG guide.

3.5.5 Global funds

	2020/2	2021	2022	2023	2024/1
Chemicals, materials, and digital tools for school outreach events and project days at the <i>Kieler Forschungswerkstatt</i> , workshop and teaching materials for teachers, workshop and training materials for the IRTG program	3.000	6.000	5.000	5.000	4.000
Travel costs for network meetings (e.g. with the Deutsches Museum, Munich)	500	1.000	1.000	1.000	500
Simulation software for the sensor simulations in the school outreach program, new VR glasses	2.000	-	-	-	-
Video conception and production	-	6.000	6.000	6.000	-
Update of the digital exhibits, structural improvements and expansion of the website	2.000	2.000	1.000	1.000	1.000

(All figures in euros)

3.1 General Information about the administrative project Z3

3.1.1 Title: Central tasks of the Collaborative Research Centre

3.1.2 Principal investigator(s)

Quandt, Eckhard, Prof. Dr.-Ing.
05.04.1960

Inorganic Functional Materials
Institute for Materials Science
Christian-Albrechts-Universität zu Kiel
Kaiserstr. 2, D-24143 Kiel

Phone: +49 (0) 431 880 6200
Fax: +49 (0) 431 880 6203
E-Mail: eq@tf.uni-kiel.de

Do the above mentioned persons hold fixed-term positions? no

3.2 Documentation of the central activities of the Collaborative Research Centre

3.3 Project funding

3.3.1 Existing funds for the new funding period

Existing Staff	Sequential no.	Name, academic degree, position	Field of research	Department of university or non-university institution	Project commitment in hours per week	Funding source
Research staff	1	Quandt, Eckhard, Prof. Dr.-Ing., CRC Coordinator	Functional Materials	IMS	6	Core support
	2	Deuschl, Günther, Prof. Dr. med.	Neurology	UKSH neuro	1	Core support
	3	Gerken, Martina, Prof. Dr.	Theoretical Electrical Engineering	EEIT	1	Core support

Job description of staff (supported through available funds)

1. Prof. Dr.-Ing. Eckhard Quandt, coordinator, spokesperson: The coordinator is in charge of the administrative project of the CRC 1261. He is responsible for the general scientific programme, is coordinating the steering committee meetings as well as the general assembly and is responsible for planning funds and resources. The coordinator is representing the CRC outside and inside of the university and is the contact partner for DFG representatives.
2. Prof. Dr. med. Günther Deuschl: The deputy coordinator is supporting the coordinator in all duties described before. Furthermore, he builds the contact between the Faculty of Engineering and the Faculty of Medicine and coordinates the projects with medical content.
3. Prof. Dr. Martina Gerken: The deputy coordinator is supporting the coordinator in all duties described before, especially concerning all contents of the IRTG.

	2020/1	2021	2022	2023	2024/1
existing funds from Kiel University	1.50	3.00	3.00	3.00	1.50
Sum of existing funds	1.50	3.00	3.00	3.00	1.50
Sum of requested funds	172.60	345.00	345.00	345.00	172.60

3.3.2 Requested funding for the new funding period

Funding for	2020/2		2021		2022		2023		2024/1	
Staff	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum	Qty	Sum
Secretary 100%	1	25.50	1	51.00	1	51.00	1	51.00	1	25.50
Student research assistants	28	32.80	28	65.50	28	65.50	28	65.50	28	32.80
Total		57.60		115.00		115.00		115.00		57.60
Direct costs	Sum		Sum		Sum		Sum		Sum	
Travel costs	35.00		70.00		70.00		70.00		35.00	
Visiting Researchers	6.00		12.00		12.00		12.00		6.00	
Total	41.00		82.00		82.00		82.00		41.00	
Global Funds	Sum		Sum		Sum		Sum		Sum	
Workshops / Colloquia	9.00		18.00		18.00		18.00		9.00	
Gender Equality	15.00		30.00		30.00		30.00		15.00	
Lump Sum	50.00		100.00		100.00		100.00		50.00	
Total	74.00		148.00		148.00		148.00		74.00	
Total	172.60		345.00		345.00		345.00		172.60	

3.3.3 Requested funding for staff

	2020/2	2021	2022	2023	2024/1
Coordination					
Secretary (100%): The secretary will be the administrative coordinator of the CRC and will take care of: - budget planning and financial administration; - staff affairs (contracts, visa etc.); - travel planning; - general correspondence; - organization of meetings, workshops and conferences.	24.80	49.50	49.50	49.50	24.80
Student Research Assistants					
For every requested researcher (E13, E14) a student assistant position with 30 h / month is requested. A standard local fee is 390 € / month, each student assistant position amounts 4680 € / year. This gives 131.000 € per year, from which half of the costs (65.500 € per year) are covered by the Kiel University. The table is showing the funds requested from DFG for 28 student assistants. For job descriptions of each student assistant see below.	32.80	65.50	65.50	65.50	32.80

(All figures in k€)

Job description of the student research assistants

- A1 (McCord):** The student assistant supports the doctoral researcher in carrying out the research project. The assistant will be introduced to magneto-optical microscopy in order to perform standard magneto-optical experiments. Moreover, the assistant will contribute to the magnetic characterization by BH-looper and ME measurements and will be engaged in the data analysis.
- A1 (Meyners):** After being introduced to standard optical lithography the student assistant will perform UV light exposure of resist coated magnetostrictive multilayer systems. The assistant will conduct pattern transfer to the functional magnetostrictive layers using established etching procedures. And the assistant will contribute to the magnetic and ME characterization of ME composites by means of Vibrating Sample Magnetometry, magnetostriction and ME coefficient measurements.
- A2 (Adelung):** The student assistant will be employed to help the doctoral researcher in the fabrication of magnetoactive material by weighing precursor material, mixing particles in prepolymers, and molding or printing the magnetoactive material. The assistant will also help in postprocessing the magnetoactive material but cutting or field annealing.
- A2 (Faupel):** The student assistant helps the doctoral researcher in terms of electret synthesis and the measurement of resulting electret properties. Furthermore the student assistant will perform routine tasks in the iCVD synthesis like cleaning and mounting the samples, as well as preparing sets of samples with already specified deposition parameters.
- A4 (Faupel):** The student assistant will be introduced to the impedance analyser and carry out routine tasks in sensor characterization in WP1. This will include preparation of the MEMS layout for measurement as well as testing the electromechanical key parameters of the different MEMS structures.
- A4 (Rieger):** The student assistant will aid in chip layout and verification for the CMOS and MEMS designs. The assistant will also help the doctoral researcher with the fabrication and installation of measurement setups for chip evaluation. In addition, the assistant will contribute to common lab routine tasks.
- A5 (Adelung):** After an introduction to the measurement system the student assistant will perform routine characterization measurements of the piezotronics sensors. Furthermore, the assistant will help in sensor preparation, e.g. sputtering, soldering contact wires and mechanical mounting of the sensors.
- A6 (Murphy):** The student assistant will carry out both X-ray at our Kiel Lab X-ray source and electrical measurements for thin film samples and nano-rod samples. The data will be evaluated and will contribute to the project. The student will also help prepare for the synchrotron experiments.
- A6 (Kienle):** The project includes time-consuming and sophisticated TEM sample preparation which can be done by a talented student assistant in order to support the doctoral researcher working on the project. The lab job offers the possibility for the student to be involvement on a qualified level into the project work.
- A7 (Quandt):** The student assistant will support the doctoral researcher in the fabrication and characterization of the inverse ME sensors. In particular, the student assistant will work on the coil fabrication, the mounting of the sensors and the functional characterization, especially of the ME properties.

- A8 (Gerken):** In the area of sensor simulation both student assistants will be trained in the area of finite-element method (FEM) simulations. The first stand assistant shall carry out parameter studies of different sensor geometries and material combinations. The second student assistant will perform simulations on the the behavior of specific types of sensors under inhomogeneous field excitation. This includes the analysis of the results regarding the establishment of a transfer function.
- A9 (Quandt):** The student assistant will support the doctoral researcher in the clean room fabrication of the SAW sensors at Kiel University. This includes lithography, etching and thin film deposition.
- A9 (Lofink):** The student assistant will conduct his work at Fraunhofer ISIT. He/she will assist the doctoral researcher in the electrical/piezoelectric characterization and optical inspection of thin-film SAW sensors on waferlevel to select promising devices for further investigations. Another second will be to perform and protocol a functional characterization of devices.
- A10 (McCord):** The student assistant supports the doctoral researcher in carrying out time-resolved magneto-optical microscopy experiments. The assistant will also conduct modeling experiments, especially varying the physical parameter space for systematic studies. Moreover, the assistant will contribute to the general magnetic characterization by BH-looper and ME measurements and will be engaged in the data analysis.
- A10 (Wulfinghoff):** The student assistant will be introduced into the finite element method and theory of micromagnetism. She or he will support the doctoral candidate in terms of mesh generation, parameter studies and different implementation tasks.
- B1 (Höft):** The first student assistant is required for support in the construction of discrete sensor electronics, e.g. manufacturing of printed circuit boards and microcontroller programming, as well as for support in the construction of permeameters. In addition, the student assistant will support measurements for sensor system evaluations and characterizations.
- B1 (Bahr)** The second student assistant is required for support in the characterization of the application specific integrated circuits. He will also carry out the assembly of the various analogue front-end designs and will be involved in its verification as well as in system design and assembly for small sensor arrays for biomedical applications.
- B2 (Schmidt):** The student assistant is required for helping with the assembly of hardware for the sensor interfaces and for programming parts of the graphical user interface. Furthermore, she or he should help when measurement series are required.
- B7 (Faupel):** The student assistant will help with routine tasks in the magnetic particle mapping such as systematic variations of single parameters. Furthermore the student assistant will assist the doctoral researcher in the characterization of the magnetic properties of samples with different concentrations and distributions of magnetic nanoparticles.
- B7 (Selhuber-Unkel):** The student assistant will support the doctoral researcher in fabricating and biofunctionalizing scaffold materials. Furthermore, the student assistant will take over tasks in cell cultivation and will support the doctoral researcher in MSPM experiments.

- B9 (Schmidt / Maetzler)** The student assistant will support the medical team in patient management. More specifically, the person will help with recruitment and assessment issues. Moreover, she or he will be involved in measurement procedures and prepare data from the measurements for statistical analysis.
- B10 (Frey, Schmidt):** The student assistant will support the medical team in patient management. More specifically, the person will help with recruitment and assessment issues. Moreover, she or he will be involved in measurement procedures and prepare data from the measurements for the corresponding analyses.
- T1 (Deuschl, Höft, Helmers):** The student assistant is needed to assist in performing magnetic field measurements on the phantom and testing the sensors through the test pipeline. He or she will also be involved in data processing and mainly in system integration in the second phase of the period. Besides, he or she will consistently participate in programming of modeling approaches in Lead-DBS and Matlab.
- Z1 (Meyners):** The student assistant will conduct his work in the faculty's cleanroom facility Kieler Nanolabor. He will assist the postdoctoral researcher in processing bulk-micromachined ME sensors by conducting established process steps. These processing tasks comprise thin film deposition, lithography and patterning by wet or dry etching.
- Z1 (Niekiel):** The student assistant will support the postdoctoral researcher in the ISIT cleanroom with respect to the fabrication of ME sensors. He/she will conduct fabrication relevant measurements to establish process control. He/she will learn the relevant measurement techniques and get insights into the microsystem fabrication processes.
- Z2 (Höft, Schmidt):** The student assistant is required for supporting the construction and improvement of measurement hardware and software for the functional characterization of the ME sensors. She or he will also support the construction of the required multitude of analogue and digital circuits for biomagnetic measurements consisting of different single sensors, 3D sensors, and small arrays of 1D or 3D sensors, respectively.
- SOP (Parchmann, Enzingmüller):** The student assistant will support the doctoral researcher in developing and presenting outreach materials as well as gathering and handling of research data. Furthermore, the student will support the carrying out of the project days at the student lab Kieler Forschungswerkstatt and assist schools in carrying out the teaching module.

3.3.4 Requested funding for direct costs

	2020/2	2021	2022	2023	2024/1
Travel Costs					
For each project and principal investigator (in total 35) 2000 € / year are planned for attending national and international conferences	35.00	70.00	70.00	70.00	35.00
National / International Guests					
It is of vital interest for the research program of the CRC to establish close scientific collaborations with international experts. In average 12 visits / year are planned with 1000 € / visit.	6.00	12.00	12.00	12.00	6.00

(All figures in k€)

3.3.5 Requested global funds

	2020/2	2021	2022	2023	2024/1
Workshops / Colloquia					
Two half annual two-day symposia of the CRC for scientific discussion of all projects will take place for intensive exchange of information and for internal evaluation of achieved research results.	9.00	18.00	18.00	18.00	9.00
Gender equality and family measures					
An aim of the CRC is the support of female researchers in their career planning and development. Therefore, several measures are planned, which are: - Support of the "Girls Day", where interested girls can spend a day at the Faculty of Engineering - Invitation of interested female Master students to the retreats and summer schools of the CRC - Program for female Master students including a student assistant position, conference visit and mentoring by a female principle investigator	15.00	30.00	30.00	30.00	15.00
Lump sum					
The lump sum will be used to support highly qualified young academics, who have their scientific background in a CRC related research area and who want to work on their own research project within the CRC. The support may also lead to own research proposals of the young academics. Furthermore the lump sum should be used for the acquisition of innovative laboratory equipment, for which the need of acquisition was not foreseeable at the time of the application of the CRC.	50.00	100.00	100.00	100.00	50.00

(All figures in k€)

4 Bylaws of the Collaborative Research Centre

§1 Kennzeichnung und Aufgaben

1. Der Sonderforschungsbereich (SFB) 1261 ist eine Einrichtung der Christian-Albrechts-Universität zu Kiel gemäß den Richtlinien des Wissenschaftsrates und der Deutschen Forschungsgemeinschaft.
2. In dem Sonderforschungsbereich werden miteinander zusammenhängende Forschungsvorhaben aus den Gebieten Materialwissenschaft, Physik, Elektrotechnik und Medizin bearbeitet. Er gliedert sich in Projektbereiche und Teilprojekte.
3. Des Weiteren setzt sich der Forschungsverbund zur Aufgabe, die Interaktion mit anderen Forschungseinrichtungen, den wissenschaftlichen Nachwuchs und die internationale Zusammenarbeit zu fördern.
4. Die Mittelverwaltung erfolgt durch die Universität Kiel.

§2 Organisatorischer Aufbau

1. Der SFB hat folgende Organe:
 - Sprecherin / Sprecher und zwei stellvertretende Sprecherinnen / Sprecher
 - Vorstand
 - Versammlung der Teilprojektleiter/innen und
 - Versammlung der Mitglieder
2. Der SFB gliedert sich in z. Zt. 15 wissenschaftliche Teilprojekte, die in zwei Projektbereiche zusammengefasst sind, sowie zwei Serviceprojekte, ein Verwaltungsprojekt, das Integrierte Graduiertenkolleg und das Projekt Öffentlichkeitsarbeit.

§3 Mitgliedschaft

1. Alle Teilprojektleiter*innen der von der DFG genehmigten Teilprojekte im SFB 1261 (namentlich in Kapitel 1.1.2 des Antrages aufgeführt) sind Mitglieder, falls ihre Mitgliedschaft nicht beendet wurde.
2. Alle Mitarbeiter*innen, die über den SFB finanziert werden sind Mitglieder.
3. Alle promovierten Wissenschaftler*innen, die im Themenbereich des SFB tätig sind, können die Mitgliedschaft beantragen. Anträge auf Mitgliedschaft nimmt die Sprecherin / der Sprecher entgegen. Über die Aufnahme neuer Mitglieder entscheidet die Versammlung der Teilprojektleiterinnen und Teilprojektleiter mit einfacher Mehrheit in geheimer Abstimmung.
4. Mitglieder können durch Beschluss mit 2/3 Mehrheit aller Mitglieder ausgeschlossen werden. Wenn das ausgeschlossene Mitglied ein*e Teilprojektleiter*in ist, informiert die Sprecherin oder der Sprecher die Deutsche Forschungsgemeinschaft und entscheidet dann in Abstimmung mit dieser über die wissenschaftliche Weiterführung des betroffenen Teilprojekts und über die zugewiesenen Mittel.
5. Die Mitgliedschaft im SFB beginnt mit dem Förderungsbeginn durch die DFG bzw. mit dem Moment des Beschlusses durch die Versammlung der Teilprojektleiter*innen. Die Mitgliedschaft endet mit der Beendigung der Förderung des von der Teilprojektleiterin / vom Teilprojektleiter geleiteten Teilprojektes durch die DFG, durch den Ausschluss durch die Versammlung der Teilprojektleiter*innen mit dem Moment dieser Entscheidung oder falls ein Mitglied seinen Austritt gegenüber der Sprecherin / dem Sprecher erklärt.

§4 Rechte und Pflichten der Teilprojektleiter und Mitglieder

1. Teilprojektleiter*innen sind durch die Förderung zur regelmäßigen Berichtsabgabe verpflichtet. Sie liefern rechtzeitig der Sprecherin / dem Sprecher Arbeits- und Ergebnisberichte über ihre Forschungsarbeiten, und sie sind verpflichtet, an der Berichterstattung gegenüber der Deutschen Forschungsgemeinschaft aktiv mitzuarbeiten und bei Beendigung der Mitgliedschaft vor Ablauf der Förderperiode einen Abschlussbericht anzufertigen.
2. Teilprojektleiter*innen sind für die ordnungsgemäße Verwendung der für ihr Teilprojekt zugewiesenen Mittel der DFG verantwortlich. Sie tragen die Verantwortung für die Pflege und Funktionsfähigkeit der ihnen zugewiesenen Geräte und treffen die Entscheidungen über die Einstellung von wissenschaftlichem und technischem Personal auf die Ihnen genehmigten Stellen. Sie verpflichten sich, die angegebenen Anteile ihrer Grundausstattung für die von ihnen bearbeiteten Teilprojekte des SFBs zur Verfügung zu stellen.
3. Mitglieder sind zur Teilnahme an den Veranstaltungen des SFBs (Symposien etc.) berechtigt.
4. Mitglieder sind zur Nutzung der dem SFB gemeinschaftlich zur Verfügung stehenden Ressourcen berechtigt.
5. Mitglieder des SFBs sind verpflichtet, bei Publikationen, die aus SFB-Arbeiten hervorgehen, die Förderung durch den SFB anzugeben.
6. Von den Mitgliedern des SFBs wird eine aktive Mitarbeit am Integrierten Graduiertenkolleg erwartet.

§5 Mitgliederversammlung

Die Mitgliederversammlung findet mindestens einmal jährlich statt. Sie informiert die Mitglieder über den Stand im SFB, insbesondere über wissenschaftliche Ergebnisse, Finanzen und geplante neue Projekte. Die

Mitgliederversammlung wird von der Sprecherin / vom Sprecher einberufen, wobei zwischen Einladung und Termin mindestens 14 Tage liegen müssen. Auf Verlangen der Hälfte der Mitglieder hat der Sprecher die Versammlung binnen 4 Wochen einzuladen.

§6 Versammlung der Teilprojektleiter

Stimmberechtigte Mitglieder dieser Versammlung sind die Teilprojektleiter*innen. Mitglieder des SFBs, die nicht Teilprojektleiter*in sind, können beratend an der Versammlung teilnehmen.

Die Versammlung der Teilprojektleiter*innen hat folgende Aufgaben:

1. Wiederwahl/Neuwahl der Sprecherin / des Sprechers, der stellvertretenden Sprecherinnen / Sprecher, sowie der übrigen Mitglieder des Vorstandes jeweils Ende des dritten Jahres des laufenden Antragszeitraums für einen Zeitraum von 4 Jahren.
2. Abwahl der Sprecherin / des Sprechers, der stellvertretenden Sprecherinnen / Sprecher, sowie der übrigen Mitglieder des Vorstandes.
3. Beratung und Beschluss über Mitgliedschaft im SFB.
4. Entscheidung über Beschlussvorlagen des Vorstandes zu Fragen der Terminplanung des SFB sowie zur Mittelverteilung, soweit sie nicht durch die Bewilligung festgelegt sind; in konkreten Fällen können die Sprecherin / der Sprecher oder der Vorstand zu Entscheidungen ermächtigt werden.
5. Beratung und Verabschiedung von Anträgen und Berichten.
6. Beratung und Beschluss über Programmänderungen und Mittelumdispositionen.
7. Entscheidung über die Verteilungsrichtlinien der gemeinsamen Mittel für Publikationen, Symposien, Gäste und Reisen aus dem Projektteil Z2.
8. Entscheidung über die Einsatzrichtlinien der pauschalen Mittel des SFBs.
9. Änderung der Ordnung des SFBs 1261.

Bei den Ziffern 1-3 und 9 entscheidet die Versammlung der Teilprojektleiter*innen mit einfacher Mehrheit der Stimmberechtigten, in den anderen Punkten mit einfacher Mehrheit der Anwesenden.

Die Versammlung der Teilprojektleiter*innen wird von der Sprecherin / vom Sprecher einberufen, wobei zwischen Einladung und Termin mindestens 5 Werktage liegen müssen. Auf Verlangen der Hälfte der Teilprojektleiter*innen hat die Sprecherin / der Sprecher die Versammlung binnen 3 Wochen einzuladen. Die Versammlung der Teilprojektleiter*innen ist beschlussfähig, wenn mindestens die Hälfte der Mitglieder anwesend ist.

§7 Vorstand und Sprecher

Der Vorstand besteht aus der Sprecherin / dem Sprecher, je einer Vertreterin / einem Vertreter der drei Fachbereiche (Materialwissenschaft, Elektrotechnik, Medizin), von denen einer Mitglied im Vorstand des integrierten Graduiertenkollegs ist, sowie einem studentischen Mitglied. Zwei Mitglieder des Vorstandes fungieren als stellvertretende Sprecher*innen. Sie werden von der Versammlung der Teilprojektleiter*innen gewählt und müssen selbst Leiter*in eines Teilprojekts sein.

Der Vorstand führt die laufenden Geschäfte und trägt die Verantwortung für die Erarbeitung von Neuansträgen und Berichten sowie die ordnungsgemäße Verwendung der zentralen Mittel des SFB für Publikationen, Symposien, Gäste, Reisen und der pauschalen Mittel. In dringenden Fällen kann der Vorstand Eilentscheidungen treffen.

Die Sprecherin / der Sprecher vertritt den SFB nach außen, insbesondere gegenüber der DFG und den Organen der Universität. Sie oder er ist Vorsitzende*r des Vorstandes und der Versammlung der Teilprojektleiter*innen und beruft diese ein. Sie oder er unterrichtet die Teilprojektleiter*innen über die wissenschaftliche, personelle und finanzielle Situation des SFB und bereitet diesbezüglich Beschlüsse der Versammlung der Teilprojektleiter*innen vor.

Die Wahl der Sprecherin / des Sprechers und der anderen vier Vorstandsmitglieder erfolgt durch die Versammlung der Teilprojektleiter*innen mit einfacher Mehrheit der Stimmberechtigten. Mindestens ein Jahr vor der Antragstellung auf Weiterförderung erfolgt eine Neuwahl des gesamten Vorstands. Eine Wiederwahl von Vorstandsmitgliedern ist möglich. Die Versammlung der Teilprojektleiter*innen kann Vorstandsmitglieder und die Sprecherin / den Sprecher während ihrer Amtszeit mit einfacher Mehrheit der Stimmberechtigten abwählen. Voraussetzung dafür ist, dass in einem unmittelbar folgenden Wahlgang eine Ersatzwahl erfolgt.

§8 Hinweis

Im Übrigen finden die Richtlinien der Deutschen Forschungsgemeinschaft für Sonderforschungsbereiche in der jeweils gültigen Fassung und die einschlägigen Erlasse des Ministeriums für Wissenschaft, Wirtschaft und Verkehr des Landes Schleswig-Holstein Anwendung.

5 Declaration on working space for the Collaborative Research Centre

Is the existing office and/or lab space sufficient to accommodate the Collaborative Research Centre at the time of submitting the proposal? yes

Will there be sufficient office and/or lab space to accommodate the Collaborative Research Centre including possible extensions in the financial years...

2020/2	yes
2021	yes
2022	yes
2023	yes
2024/1	yes

If working groups participating in the Collaborative Research Centre are planned to be moved into newly built or rebuilt rooms, please state the time of the relocation:

none

Kiel, 08.01.2020

Place and Date

Claudia Ricarda Meyer
(Chancellor of the Christian-Albrechts-Universität zu Kiel)

6 Declaration on lists of publications

We hereby declare that the lists of publications included in this proposal and in the attached research profiles of the principal investigators were compiled in accordance with DFG rules on publication lists.

Kiel, 08.01.2020

Place and Date

Prof. Dr.-Ing. Eckhard Quandt
(Spokesperson of the CRC 1261)

Kiel, 08.01.2020

Place and Date

Prof. Dr. Lutz Kipp
(President of the Christian-Albrechts-Universität zu Kiel)