Crystalline Solids and their Microstructure Division
Fachverband Kristalline Festkörper und deren Mikrostruktur (KFM)

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Overview of Invited Talks and Sessions

(Lecture halls H10, H47, PHY 5.0.20, and PHY 5.0.21; Poster C)

Invited Talks

KFM 4.1	Mon	9:30–10:00	H47	**Mixing microwave and light: up-conversion and frequency combs** — •Harald G. L. Schwefel
KFM 4.6	Mon	11:40–12:10	H47	**Nonlinear whispering gallery resonators for quantum optical technologies** — •Christoph Marquardt
KFM 5.1	Mon	15:00–15:30	PHY 5.0.21	**On-surface synthesis by atomic manipulation studied with AFM** — •Leo Gross
KFM 6.1	Mon	15:00–15:30	PHY 5.0.20	**Fifteen years of electron magnetic circular dichroism** — •Ján Rusz
KFM 6.6	Mon	17:10–17:40	PHY 5.0.20	**Advanced Imaging and Spectroscopy in an Ultrafast Transmission Electron Microscope** — •Armin Feist
KFM 8.5	Tue	11:10–11:40	PHY 5.0.20	**Development of Kinetic Inductance Detectors for polarimetric applications in plasma diagnostics** — •Francesco Mazzocchi, Eduard Driessen, Shibo Shu, Giovanni Grossetti, Dirk Strauss, Theo Scherer
KFM 9.1	Tue	9:30–10:00	PHY 5.0.21	**High Energy Density and Low Loss Dielectric Polymers for Electrical Applications** — •Lei Zhu
KFM 9.5	Tue	11:20–11:50	PHY 5.0.21	**Storing electrical energy using glasses and glass ceramics** — •Martin Letz

Invited talks of the joint Symposium SKM Dissertation-Prize 2019

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	**Synchronization and Waves in Confined Complex Active Media** — •Jan Frederik Totz
SYSD 1.2	Mon	9:50–10:10	H2	**Spin scattering of topologically protected electrons at defects** — •Philipp Rüßmann
SYSD 1.3	Mon	10:10–10:30	H2	**Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions** — •Chris W. Nicholson
SYSD 1.4	Mon	10:30–10:50	H2	**Thermodynamic bounds on current fluctuations** — •Patrick Pietzonka
SYSD 1.5	Mon	10:50–11:10	H2	**Lightwave-driven quasiparticle acceleration** — •Fabian Langer
SYSD 1.6	Mon	11:10–11:30	H2	**Ultrafast plasmon-driven point-projection electron microscopy** — •Jan Vogelsang
SYSD 1.7	Mon	11:30–11:50	H2	**Helimagnets, sand patterns and fingerprints linked by topology** — •Peggy Schönherr

Invited talks of the joint Symposium Mechanically Controlled Electrical Conductivity of Oxides

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	9:30–10:00	H1	**Dislocation Dynamics and Their Conductivities in Oxides** — •Yuichi Ikuhara

SYCO 1.2	Mon	10:00–10:30	H1	**Strain effects in ionic conductivity and electrode processes** — •Jürgen Janek
SYCO 1.3	Mon	10:30–11:00	H1	**Elastic dipoles of point defects in materials** — •Celine Varvenne
SYCO 1.4	Mon	11:30–12:00	H1	**Mapping strain/pressure with ZnO nanowire arrays by piezo-phototronic effect** — •Caofeng Pan
SYCO 1.5	Mon	12:00–12:30	H1	**Bulk and Flexo-photovoltaic effect** — •Marin Alexe

Invited talks of the joint Symposium Czech Republic as Guest of Honor

See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	**Crystal symmetries and transport phenomena in antiferromagnets** — •Tomas Jungwirth
SYCZ 1.2	Thu	10:00–10:30	H4	**Terahertz subcycle charge and spin control** — •Rupert Huber
SYCZ 1.3	Thu	10:30–11:00	H4	**1D molecular system on surfaces** — •Pavel Jelinek
SYCZ 1.4	Thu	11:15–11:45	H4	**Tunneling microscopy on insulators provides access to out-of-equilibrium charge states** — •Jascha Repp
SYCZ 1.5	Thu	11:45–12:15	H4	**Occam's razor and complex networks from brain to climate** — •Jaroslav Hlinka
SYCZ 1.6	Thu	12:15–12:45	H4	**Long range temporal correlations in complex systems** — •Holger Kantz

Invited talks of the joint Symposium Interactions and Spin in 2D Heterostructures

See SYIS for the full program of the symposium.

SYIS 1.1	Thu	15:00–15:30	H1	**Magic Angle Graphene: a New Platform for Strongly Correlated Physics** — •Pablo Jarillo-Herrero
SYIS 1.2	Thu	15:30–16:00	H1	**Bilayer Graphene Quantum Devices** — •Klaus Ensslin
SYIS 1.3	Thu	16:00–16:30	H1	**Light-Matter interaction in van der Waals heterostructures** — •Tobias Korn
SYIS 1.4	Thu	16:45–17:15	H1	**Spin transport in Van der Waals materials and heterostructures** — •Bart Van Wees
SYIS 1.5	Thu	17:15–17:45	H1	**Flipping the valley in graphene quantum dots** — •Markus Morgenstern

Sessions

KFM 1.1–1.3	Sun	16:00–18:15	H10	**Tutorial: Diamond-Growth, characterization, electronics and applications (joint session KFM/TUT)**
KFM 2.1–2.4	Mon	9:30–11:10	PHY 5.0.20	**Microstructure of Thin Films / Crystal Structure**
KFM 3.1–3.4	Mon	9:30–11:10	PHY 5.0.21	**Dielectric, Elastic and Electromechanical Properties**
KFM 4.1–4.10	Mon	9:30–13:30	H47	**Focus: Whispering-Gallery-Mode Resonators**
KFM 5.1–5.4	Mon	15:00–16:30	PHY 5.0.21	**Instrumentation for Micro-/Nano-Analysis and Lithography/Structuring (joint session KFM/DS/O)**
KFM 6.1–6.9	Mon	15:00–18:40	PHY 5.0.20	**Focus: Advanced TEM spectroscopy - low energy excitations and chemical composition at high resolution (joint session KFM/HL)**
KFM 7.1–7.9	Mon	15:00–18:30	H47	**Multiferroics**
KFM 8.1–8.6	Tue	9:30–12:00	PHY 5.0.20	**Diamond I (joint session KFM/HL)**
KFM 9.1–9.8	Tue	9:30–12:50	PHY 5.0.21	**Focus: Materials for Energy Storage**
KFM 10.1–10.11	Tue	9:30–12:50	H47	**Ferroics - Domains and Domain Walls**
KFM 11.1–11.6	Tue	14:00–15:45	H37	**Multiferroics and Magnetoelectric coupling I (joint session MA/KFM)**
KFM 12.1–12.5	Wed	9:30–11:30	PHY 5.0.20	**Diamond II (joint session KFM/HL)**
KFM 13.1–13.7	Wed	9:30–12:10	H47	**Microscopy, Tomography and Spectroscopy with X-ray Photons, Electrons, Ions and Positrons (joint session KFM/HL)**
KFM 14.1–14.36	Wed	16:00–18:30	Poster C	**Postersession KFM**
KFM 15	Wed	18:30–19:00	PHY 5.0.21	**Annual General Meeting of the KFM division**

KFM 16.1–16.9	Fri	9:30–11:45	H39	**Multiferroics and Magnetoelectric coupling II (joint session MA/KFM)**

Annual General Meeting of the Crystalline Solids and their Microstructure Division

Mittwoch 18:30–19:00 PHY 5.0.21

- Bericht
- Wahl
- Verschiedenes

KFM 1: Tutorial: Diamond-Growth, characterization, electronics and applications (joint session KFM/TUT)

This tutorial is dedicated to growth mechanisms of diamond (single and polycrystalline) and corresponding physical properties, used for electronic applications. Process technologies and production of diamond devices tailored for special technical applications will be discussed. Applications for diamond in high power and high frequency components will be presented.

Organized by Theo Scherer (KIT)

Time: Sunday 16:00–18:15 Location: H10

Tutorial KFM 1.1 Sun 16:00 H10
Diamond's bright future in electronics and quantum technology — •Matthias Schreck — Institut für Physik, Universität Augsburg

The present talk gives first a general introduction into diamond growth by chemical vapor deposition (CVD). Then, it describes the different approaches and the crucial steps for the realization of single crystal diamond on wafer scale. The focus will be on the heteroepitaxial multilayer system Dia/Ir/YSZ/Si which is currently the most advanced as demonstrated by the successful synthesis of a monocrystalline disc with a diameter of 92 mm and a mass of 155 ct.
The second part addresses current and potential future applications. Cutting tools for high precision machining, scalpels for eye surgery as well as visible/infrared optical elements based on CVD grown single crystals are already available on the market. Detectors for high energy ionizing radiation required at large particle physics research facilities like GSI or CERN are under development. In the field of high power electronics, diamond should outperform all other wide bandgap materials according to its intrinsic material parameters, but highly competitive devices that may be grown on the new wafers are still to be demonstrated. Finally, emerging quantum technologies based on color centers hosted in the diamond crystal lattice open a fascinating new field.

Tutorial KFM 1.2 Sun 16:45 H10
Microwave CVD of Diamond — •Volker Buck — Uni. Duisburg-Essen

The contribution starts with historic remarcs concerning microwave CVD of Diamond. Then basic physics of microwave plasmas are presented to explain the concepts of usual microwave reactors. After this, standard process parameters for deposition of microcrystalline diamond films are given. An overview of problems related with epitaxy leads to actual research and within this context also the state of the art of doping is discussed. Some general aspects of nanotechnology then leads to ultrananocrystalline diamond films (UNCD) and color centers. An outlook concludes the contribution.

Tutorial KFM 1.3 Sun 17:30 H10
High power and high frequency applications of diamond — •Dirk Strauss — KIT Karlsruhe, Deutschland

Content of this tutorial is the presentation of basic properties of polycrystalline as well as single crystalline CVD diamond in high frequency (GHz-THz) and high power (MW) applications with extreme low microwave losses. Starting with growth conditions of diamond, optimization of dielectric and thermal properties up to implementation in diamond window assembly structures for multi-frequency applications (step tunable and Brewster windows) the complete development process and the state of the art today will be presented. Main applications of this field are heating and diagnostic systems in nuclear fusion reactors, accelerator and laser devices, where such windows can be implemented with outstanding physical properties.

KFM 2: Microstructure of Thin Films / Crystal Structure

Chair: Enrico Langer (Technische Universität Dresden)

Time: Monday 9:30–11:10 Location: PHY 5.0.20

KFM 2.1 Mon 9:30 PHY 5.0.20
Structural modification of thin Bi(1 1 1) films by passivation and native oxide model — •Christian König[1], Stephen Fahy[1,2], and James C. Greer[3] — [1]Tyndall National Institute, University College Cork, Lee Maltings, Cork T12 R5CP, Ireland — [2]Department of Physics, University College Cork, College Road, Cork T12 K8AF, Ireland — [3]Nottingham Ningbo New Material Institute and Department of Electrical and Electronic Engineering, University of Nottingham Ningbo China, 199 Taikang East Road, Ningbo, 315100, China

Bismuth is a promising material for electronic devices on the nanometer scale. Although the bulk material is semimetallic, a band gap can be expected in a thin film or nanowire due to quantum confinement. We investigated the structure of thin Bi(1 1 1) films with a thickness of approximately 1 nm with density functional theory. In order to remove metallic surface states, a passivation of the devices is necessary. Our calculations show considerable interaction of the surface with passivants like hydrogen and hydroxyl. The orientation of the thin films is changed completely whereas thick films are only affected at the surface. As the electronic properties of the material depend on the crystal structure, this effect is detrimental for device performance. Furthermore, we present model structures for the native oxide which form a protective capping layer and interact only weakly with the film so that the crystal orientation remains unchanged.

KFM 2.2 Mon 9:50 PHY 5.0.20
Introducing Caesar: Ab Initio Modelling of the Properties of Materials over Large Temperature Ranges — •Mark Johnson and Richard Needs — Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, United Kingdom

Caesar is a new code which is capable of modelling crystalline materials across most of the temperature range at which they remain crystalline. Caesar aims to provide calculations at ab inito accuracies whilst being fast enough, and autonomous enough, to be used as part of high-throughput methods such as structure searching.

Caesar can be interfaced with any electronic structure code, which is used as an engine to map out the nuclear energy landscape under the Born-Oppenheimer approximation. Nuclear motion in this landscape is modelled under the formalism of coupled anharmonic phonons, using vibrational self-consistent field theory and related methods. This allows for behaviour over a range of temperatures to be calculated from a single mapping of the energy landscape, and for the simulation of materials which are dynamically unstable under the harmonic approximation.

This talk will highlight advances to vibrational methods made in the development of Caesar, focussing on the exploitation of symmetry to accelerate the calculation and improve its accuracy. The talk will also present an overview of the current and future applications of the code, including work employing CASTEP as the engine used to predict the phase diagrams of elemental systems from first principles.

Break 20 min

KFM 2.3 Mon 10:30 PHY 5.0.20
Time-resolved X-ray absorption spectroscopy on Al-Cu alloys – from solute copper to stable precipitates — Danny Petschke, Frank Lotter, Elischa Blaess, and •Torsten E.M. Staab — University Wuerzburg, Dep. of Chemistry, LCTM, Roentgenring 11, D-97070 Wuerzburg, Germany

Although binary aluminium alloys seem to be uninteresting and well known, some aspects of their precipitation sequence – especially the early stages immediately after quenching – are still not well understood. Since the Al-Cu system is the basis for many ternary and quaternary high-strength alloys with application in the aviation sector, it is important to understand this binary system in detail. This problem is here tackled by a unique combination of differential scanning calorimetry and X-ray absorption fine structure measurements, where relaxed atomic coordinates for simulation of the spectra have been obtained by ab initio calculations. Thereby, it is possible to attribute any exo- or endothermal peak to a certain type of precipitate, even though formation and dissolution regions have a large overlap in this system. This unique combination of experimental and numerical methods allows one to determine the local atomic environment around Cu atoms, thus following the formation and growth of Guinier-Preston zones, i.e. Cu platelets on {100} planes, during the precipitation process.

KFM 2.4 Mon 10:50 PHY 5.0.20

Distinctive bond breaking in crystalline phase-change materials and fingerprints for metavalent bonding — •Stefan Maier[1], Oana Cojocaru-Mirédin[1], Min Zhu[1], Antonio Mio[1], Jens Keutgen[1], Michael Küpers[2], Yuan Yu[1], Ju-Young Cho[1], Richard Dronskowski[2], and Matthias Wuttig[1,3] — [1]I. Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — [2]Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany — [3]JARA-FIT Institute Green-IT, RWTH Aachen University and Forschungszentrum Jülich, 52056 Aachen, Germany

The field evaporation of a number of crystalline and amorphous phase-change materials and other intermetallic compounds was studied by laser-assisted atom probe tomography. A high probability of multiple detector events (i.e. more than one ion detected per laser pulse was found for the crystalline materials. Amorphous phase-change materials and other materials showing classical metallic or covalent bonding, exhibit low probabilities. This unusual field evaporation is unlike any other known mechanism to result in high probabilities for multiple detector events. Hence, in the presented examples, laser-assisted field evaporation reveals striking differences in bond breaking. This is indicative for pronounced differences in the bonding mechanism (which we call metavalent bonding) and it implies the presence of chemical bonds, which differ significantly from classical covalent, ionic and metallic bonds. This is supported by other fingerprints, which are sensitive towards chemical bonding such as the optical dielectric constant.

KFM 3: Dielectric, Elastic and Electromechanical Properties

Time: Monday 9:30–11:10 Location: PHY 5.0.21

KFM 3.1 Mon 9:30 PHY 5.0.21

Piezotronic material based on ZnO-ZnO interfaces — •Maximilian Gehringer — Technische Universität Darmstadt, Darmstadt, Deutschland

In recent years, the research field piezotronics gained a lot of attention. It has been shown to have huge potential for applications like nanogenerators, gated field effect transistors and sensors. Zinc oxide nanowires that allow extensive deformation were the focus of many investigations of metal-semiconductor Schottky-barriers. However, ZnO is also well known for polycrystalline ceramics with grain boundary potential barrier. In this case, the barriers at grain boundaries inhibit electrical transport until breakdown at high voltages. Therefore, ZnO is often used for surge protection or for voltage regulation.

In this work, the possibility of using bicrystals or polycrystalline materials with high grain boundary potential barrier for piezotronic applications will be discussed. Our investigations show a large impact of mechanical stress on the linear leakage current in polycrystalline ZnO samples and bicrystals. Extensive conductivity changes could be induced in this low voltage region via application of uniaxial pressure. Hence, very high possible gauge factors (figure of merit for the use in strain/stress sensors) around 1000 can be obtained. Commercial sensors can reach only a factor of 200 so far. A physical model will be introduced to explain the observed behavior and the results are compared with single crystal metal-ZnO Schottky barrier investigations. Evidence will be provided for varistor boundaries showing enhanced piezotronic properties compared to metal-ZnO Schottky barriers.

KFM 3.2 Mon 9:50 PHY 5.0.21

Characterization of extremely small nonlinearities of dielectric response in glasses and glass ceramics — •Florian Bergmann[1,2], Martin Letz[1,2], Gerhard Jakob[1], and Holger Maune[3] — [1]Johannes Gutenberg Universität Mainz — [2]Schott AG Mainz — [3]TU Darmstadt

The 5G mobile communication standard aims to provide massive data rates to an increasing number of devices. This requires the use of higher frequencies and the efficient use of the available frequencies. A major challenge in the efficient use of frequencies is cross talk between channels due to passive intermodulation (PIM). Due to the large differences in the intensity of receiving and transmitting channels, even tiniest intermodulation levels need to be controlled. One source of intermodulation is the nonlinear response of dielectrics to the electric field. However, it is hard to characterize the intrinsic material nonlinearity as the nonlinearity of the setup itself produces intermodulation. Following a resonator method exciting eigenresonances of three coupled cylindrical dielectric resonators enables to measure nonlinear behavior at high field strengths and allows isolating the resonators' material nonlinearities from other intermodulation sources. The setup enables to measure a third order nonlinear term being 10^{-10} times smaller than the linear response at electric field amplitudes of a few V/mm. We report on the characterization measurements of the nonlinearity of glasses and glass ceramics.

Break 20 min

KFM 3.3 Mon 10:30 PHY 5.0.21

Nonlocal Electrostatics: Lorentzian Kernels or Gradient Theories? — •Jakob Leck — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Nonlocal electrostatics is a continuum theory to be used on small length scales when effects of spatial dispersion become relevant. A common ansatz for the kernel in the nonlocal material law is the so-called Fourier-Lorentzian-model, a sum of a local term and the Green function of a Helmholtz-type operator. This leads to a fourth order differential equation for the potential. A different approach consists in a moment expansion of the material law, which leads to a gradient theory, implying similar equations for the potential. In this talk both approaches are compared and it is argued that the gradient theory is to be preferred because it does not require ad hoc assumptions about the kernel. The gradient theory is discussed up to second order and leads to a modified and non-singular near field behaviour in potentials and fields of point charges.

KFM 3.4 Mon 10:50 PHY 5.0.21

Aligning In-Plane Polarization Multiplies Piezoresponse In P(VDF-TrFE) Films On Graphite — •Robert Roth[1], Martin Koch[1], Jakob Schaab[2], Martin Lilienblum[2], Frank Syrowatka[3], Tino Band[1], Thomas Thurn-Albrecht[1], and Kathrin Dörr[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Department of Materials, ETH Zürich, Zürich, Switzerland — [3]Interdisciplinary Center of Materials Science, Martin Luther University Halle-Wittenberg, Halle, Germany

Ferroelectric polymers are attractive candidates for functional layers in electronic devices like non-volatile memories, piezo- and magnetoelectric sensors. However, thin films often reveal reduced di- and piezoelectric responses due to crystalline disorder and resulting non-aligned electrical dipoles leading to compensation effects. We will present results on controlled aligning of both in-plane and out-of-plane ferroelectric polarization in several 10 nm thick poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) films on graphite with a force microscope [1]. Micron-sized domains with well-defined shape can be written by a combined procedure of electrical poling and mechanical tip pressure scanning. The achieved uniform polarization orientation leads to strong enhancement in both, vertical and lateral piezoresponse. By variation of parameters, domain walls with defined angle can be formed within these areas and diverse special domain structures can be generated. This allows one to overcome compensation effects and get distinct domain patterns beneficial for various device applications.

[1] R. Roth et al., New J. Phys. 20 (2018), 103044.

KFM 4: Focus: Whispering-Gallery-Mode Resonators

Whispering Gallery Mode (WGM) resonators confine and enhance electro - magnetic fields almost entirely within a transparent dielectric. Strong light - matter interactions such as optical nonlinearities are the consequence. Therefore, these resonators are a link between the two continuously merging worlds of photonics and solid state physics. Research and applications using this type of resonators rely heavily on the availability of high quality linear and nonli near materials. Furthermore, advanced material processing for the fabrication of high quality resonators, in particular for on - chip integration is required. On the other hand, the strong light - matter interaction allows to study linear and nonlinear dielec tric material properties with high sensitivity over a huge wavelength regime from visible over infrared down to terahertz and microwave frequencies. WGM resonators can also serve as a widely tunable source of classical as well as quantum light which can be used for different types of high precision spectroscopy. The aim of this session is to cover the topics of this field and bring together the communities of photonics and solid state physics.

Chair: Florian Sedlmeir (Max Planck Institute for the Science of Light)

Time: Monday 9:30–13:30 Location: H47

Invited Talk KFM 4.1 Mon 9:30 H47

Mixing microwave and light: up-conversion and frequency combs — •Harald G. L. Schwefel — Dodd-Walls Centre for Photonic and Quantum Technology, New Zealand — Department of Physics, University of Otago, Dunedin, New Zealand

Dielectric whispering gallery mode resonators are a great tool to entrap electro-magnetic radiation throughout the dielectric's transparency range [1]. In small resonators this leads to high enough field amplification that nonlinear effects can readily be harnessed. I will discuss hybrid systems which are resonant for both microwave and optical fields and which are based on anisotropic crystalline dielectrics that allow for second order nonlinear effects, such as sum- and difference frequency generation.

In an efficient resonant system and for strong microwave and optical fields, sum- and difference frequency generation can cascade, leading to optical frequency combs [2]. Such combs are useful for telecommunication application such as wavelength division multiplexing and for sensing. For the limit of very weak microwaves and only sum frequency generation, coherent conversion of microwave signals allows the quantum state of individual microwave photons to be transferred into the optical domain [3]. This offers a way to coherently connect superconducting qubits to quantum networks, and allow the rapid scaling of quantum computers.

[1] D. V. Strekalov, *et al.*, J. Opt. **18**, 123002 (2016).
[2] A. Rueda, *et al.*, arXiv:1808.10608 [physics] (2018).
[3] A. Rueda, *et al.*, Optica, **3**, 597–604 (2016).

KFM 4.2 Mon 10:00 H47

Frequency comb up- and down-conversion in synchronously driven $\chi(2)$ optical microresonators — •Jan Szabados[1], Simon Johannes Herr[1], Victor Brasch[2], Ewelina Obrzud[2,3], Yuechen Jia[1], Steve Lecomte[2], Karsten Buse[1,4], Ingo Breunig[1,4], and Tobias Herr[2] — [1]Laboratory for Optical Systems, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 102, D-79110 Freiburg, Germany — [2]Swiss Center for Electronics and Microtechnology (CSEM), Time and Frequency, Rue de l'Observatoire 58, CH-2000 Neuchâtel, Switzerland — [3]Geneva Observatory, University of Geneva, Chemin des Maillettes 51, CH-1290 Versoix, Switzerland — [4]Fraunhofer Institute for Physical Measurement Techniques IPM, Heidenhofstraße 8, D-79110 Freiburg, Germany

We demonstrate the broadband conversion of a high-repetition rate frequency comb from the near-infrared (NIR) to the mid-infrared (MIR), visible (VIS) and ultraviolet (UV) wavelength domains. The employed lithium niobate WGRs are synchronously pumped by a frequency comb with a repetition rate in excess of 10 GHz and pico- to femtosecond pulse duration. Cascaded second-order nonlinear processes transfer significant parts of the fundamental frequency comb to harmonic and sub-harmonic optical frequencies. This way, the second and the third harmonics in the visible and the fourth harmonic in the ultra-violet spectral region are generated. Also, subharmonic generation of the fundamental comb lines into the mid-infrared spectral range via degenerate parametric oscillation is demonstrated. Non-degenerate processes enable wavelength-tunable signal- and idler-comb generation.

KFM 4.3 Mon 10:20 H47

Electro-optic tuning of whispering gallery resonators made of KTN crystals — •Ingo Breunig[1,2], Jan Szabados[1], and Karsten Buse[1,2] — [1]Laboratory for Optical Systems, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg, Germany — [2]4Fraunhofer Institute for Physical Measurement Techniques IPM, Heidenhofstraße 8, 79110 Freiburg, Germany

The electro-optic response of most centrosymmetric materials is neglected. Due to their symmetry, the Pockels coefficients are zero. The DC-Kerr coefficients are typically of the order of 10^{-22} m^2/V^2, i.e. very small. Consequently, refractive-index changes in centrosymmetric materials are induced by changing the temperature or by applying mechanical stress. However, potassium tantalate niobate crystals (KTN) operated at temperatures close to the paraelectric-ferroelectric phase transition provide DC-Kerr coefficients in the 10^{-15} m^2/V^2 range. Thus, although the material is centrosymmetric, it exhibits a strong electro-optic response. We have fabricated a millimeter-sized whispering gallery resonator made of KTN with a quality factor beyond 10^7 at 1 μm wavelength. By applying an electric field between its top and bottom surfaces, the eigenfrequencies of the cavity are shifted due to the DC-Kerr effect. For moderate field strengths of 250 V/mm, we achieve more than 100 GHz tuning. This exceeds the value reached with lithium niobate crystals by more than one order of magnitude. The results obtained here are of relevance for the realization of electro-optically tunable adiabatic frequency converters or Kerr frequency combs.

KFM 4.4 Mon 10:40 H47

Adiabatic frequency conversion in high-Q lithium niobate whispering gallery resonators — •Yannick Minet[1], Luís Reis[1], Ingo Breunig[1], and Karsten Buse[1,2] — [1]Laboratory for Optical Systems, Department of Microsystems Engineering, IMTEK, University of Freiburg, Georges- Köhler-Allee 102, D-79110 Freiburg, Germany — [2]Fraunhofer Institute for Physical Measurement Techniques IPM, Heidenhofstraße 8, D-79110 Freiburg, Germany

Optical frequency conversion in Whispering gallery resonators (WGRs) is mostly based on the nonlinear response of material polarization caused by intense laser light. For example in WGRs made of noncentrosymmetric materials tunable OPOs have been realized and in WGRs made of centrosymmetric materials frequency combs. Another way for frequency conversion is adiabatic tuning. Here, the optical length of the circumference of the resonator is changed during its ringdown time. This induces a frequency shift of the circulating light. Conventionally, this is achieved by changing the refractive index by generating free electrons or via the ac-Kerr effect. Both schemes require an additional pump laser. We present an alternative approach based on the linear electro-optic effect. Compared with the other schemes, the experimental setup is considerably simpler. Furthermore, it is applicable for all wavelengths in the transparency range of the resonator material used. Using this method, we can generate almost arbitrary waveforms and frequency shifts of several tens of GHz. We will also discuss a possible use of this technique for sensing and LIDAR applications.

KFM 4.5 Mon 11:00 H47

Dielectric tuning of millimeter-wave whispering-gallery modes for electro-optic phase matching — •Gabriel Santamaria Botello[1], Kerlos Atia Abdalmalak[1], Daniel Segovia Vargas[1], Luis Enrique Garcia Muñoz[1], and Zoya Popovic[2] — [1]Universidad Carlos III de Madrid — [2]University of Colorado Boulder

It has been shown that highly efficient electro-optic modulators can be designed in millimeter-sized high-Q whispering-gallery (WG) disk resonators made of nonlinear crystals, where a resonant optical field mixes with the modulating microwave field to produce a resonant sideband. This is potentially useful for high-sensitivity millimeter-wave detection, optical comb generation and up-conversion of quantum states. The interaction takes place only when the optical and microwave modes are phase matched, implying that the angular velocity is matched in the case of fundamental WG modes. Due to the high optical Q, the phase-matching condition is sensitive to fabrication tolerances of the resonator requiring an accuracy within less than 10um in all dimensions. In past demonstrations, a time-consuming iterative polishing process was performed to adjust the radius in small steps. In this work, we show that the phase-matching point can be found by perturbing the microwave mode with low-loss dielectric layer loadings on one or both sides. Thus, millimeter-sized lithium niobate resonators can be fabricated with tolerances up to 20um in height and 100um in radius. The conversion efficiency is not appreciably affected with this approach since no significant degradation of the microwave Q and field distribution is observed.

Break 20 min

Invited Talk KFM 4.6 Mon 11:40 H47

Nonlinear whispering gallery resonators for quantum optical technologies — •Christoph Marquardt — Max-Planck-Institut für die Physik des Lichts, Staudtstr. 2, 91058 Erlangen

In quantum information optical quantum states are an essential building block. Encoding quantum states in the optical field is important for travelling quantum states that can transfer quantum information, as well as in quantum sensing, imaging and photonic quantum computation. Nonlinear optical processes can be used to generate and process special quantum states. Nonlinear whispering gallery resonators provide an efficient platform towards these goals. I will review the current state of the field and discuss possible applications in quantum optical technology.

D. Strekalov et al., Journal of Optics 18(12) 123002 (2016)

KFM 4.7 Mon 12:10 H47

Non-classical light from a nonlinear crystalline whispering gallery mode resonator — •Alexander Otterpohl[1,2], Florian Sedlmeir[1,2], Thomas Dirmeier[1,2], Ulrich Vogl[1,2], Gerhard Schunk[1,2], Golnoush Shafiee[1,2], Dmitry Strekalov[1,2], Harald G. L. Schwefel[3], Tobias Gehring[4], Ulrik L. Andersen[4], Gerd Leuchs[1,2], and Christoph Marquardt[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany — [2]Institute of Optics, Information and Photonics, University Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [3]The Dodd-Walls Centre for Photonic and Quantum Technologies, Department of Physics, University of Otago, 730 Cumberland Street, 9016 Dunedin, New Zealand — [4]Department of Physics, Technical University of Denmark, Fysikvej, 2800 Kgs. Lyngby, Denmark

Macroscopic crystalline whispering gallery mode resonators (WGMR) made out of $LiNbO_3$ have turned out to be an efficient and compact source of non-classical light generated via optical parametric down-conversion [1,2]. We report on the generation of squeezed vacuum, which is a special subclass of non-classical light, and the associated experimental challenges such as temperature stabilization. Furthermore, we discuss possible future applications like CV quantum computing and optomechanics [3].

[1] J. U. Fürst *et al.*, Phys. Rev. Lett. **106**, 113901 (2011).
[2] M. Förtsch *et al.*, Nat. Commun. **4**, 1818 (2013).
[3] V. Peano *et al.*, Phys. Rev. Lett. **115**, 243603(2015).

KFM 4.8 Mon 12:30 H47

Single photon generation in a whispering gallery mode resonator — •Golnoush Shafiee[1,2], Florian Sedlmeir[1,2], Gerhard Schunk[1,2], Alexander Otterpohl[1,2], Ulrich Vogl[1,2], Dmitry Strekalov[1,2], Harald G. L. Schwefel[3,4], Gerd Leuchs[1,2], and Christoph Marquardt[1,2] — [1]MPL, Erlangen, Germany — [2]FAU, Erlangen, Germany — [3]University of Otago, Dunedin, New Zealand — [4]Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand

A whispering gallery resonator (WGR) is a versatile source of tunable, narrow-band and efficient single photons which can be used for quantum information processing [1,2,3]. Our WGR is made of nonlinear lithium niobate and its working principle is based on spontaneous parametric down-conversion where a pump photon decays into two cavity modes of different wavelengths named signal and idler. Here, we investigate parametric down-conversion in counter-propagating modes of one WGR. The interference of two photons from different propagation directions opens up the possibility of generating polarization-entangled states using only one resonator. A source of polarization-entangled states can greatly enhance the success rates of the proposed quantum repeaters. [1] M. Förtsch et al., Nat. Commun. 4, 1818 (2013). [2] J. U. Fürst et al., Phys. Rev. Lett. 106, 113901(2011). [3] G. Schunk et al., Optica 2, 773-778 (2015).

KFM 4.9 Mon 12:50 H47

The optical Möbius strip cavity: Tailoring geometric phases and far fields — •Jakob Kreismann and Martina Hentschel — Technische Universität Ilmenau, Ilmenau, Germany

The Möbius strip, a long sheet of paper whose ends are glued together after a 180° twist, has remarkable geometric and topological properties. Here, we consider di- electric Möbius strips of finite width and investigate the interplay between geometric properties and resonant light propagation. We show how the polarization dynamics of the electromagnetic wave depends on the topological properties, and demonstrate how the geometric phase can be manipulated between 0 and π through the system geom- etry. The loss of the Moöbius character in thick cavities and for small twist segment lengths allows one to manipulate the polarization dynamics and the far-field emission, and opens the venue for applications.

KFM 4.10 Mon 13:10 H47

Super-directional light emission from arrays of deformed microcavities — •Jakob Kreismann[1], Martina Hentschel[1], Arne Behrens[2], and Stefan Sinzinger[2] — [1]Institute for Physics, Theoretical Physics II/Computational Physics Group, Technische Universität Ilmenau, Germany — [2]Department of Mechanical Engineering, Optical Engineering Group, Technische Universität Ilmenau, Germany

Microcavity lasers made of deformed dielectric disk resonators such as the Limaçon-shaped cavity have attracted a lot of interest due to directional light emission from high quality factor modes. Here we investigate them in various array configurations of Limaçon-shaped microcavities and show that the directional emission is enhanced drastically. At the same time, emission into side peaks is reduced. Furthermore, we study the coupling mechanisms between Limaçon-resonators arranged in different array configurations. We show that far-field properties depend strongly on the coupling between the resonators in the array that is mostly determined by the inter-cavity distance as well as geometric imperfections.

KFM 5: Instrumentation for Micro-/Nano-Analysis and Lithography/Structuring (joint session KFM/DS/O)

Time: Monday 15:00–16:30 Location: PHY 5.0.21

Invited Talk KFM 5.1 Mon 15:00 PHY 5.0.21
On-surface synthesis by atomic manipulation studied with AFM — •Leo Gross — IBM Research - Zurich, Säumerstr. 4, 8003 Rüschlikon, Switzerland

Elusive molecules can be created using atomic manipulation with a combined atomic force/scanning tunneling microscope (AFM/STM). Molecules that are highly reactive and short-lived under ambient conditions can be stabilized at low temperature on inert surfaces. Employing high-resolution AFM with functionalized tips provides insights into the structure, geometry, aromaticity and bond orders of the molecules created and into the reactions performed [1].

We created radicals, diradicals [2], non-Kekulé molecules [3], antiaromatics [4], and polyynes [5] and studied their structural and electronic properties. We recently showed that the reorganization energy of a molecule on an insulator can be determined [6]. In addition, we expanded the toolbox for the synthesis of molecules by atomic manipulation, demonstrating reversible cyclisation reactions [2], skeletal rearrangements [5] and controlled reactions on insulating substrates by electron attachment/detachment [7].

References: [1] L. Gross et al. Angew. Chem Int. Ed 57, 3888 (2018). [2] B. Schuler et al. Nat. Chem. 8, 220 (2016). [3] N. Pavliček et al. Nat. Nano. 12, 308 (2017). [4] Z. Majzik et al. Nat. Commun. 9, 1198 (2018). [5] N. Pavliček et al. Nat. Chem. 10, 853 (2018). [6] S. Fatayer et al. Nat. Nano. 13, 376 (2018). [7] S. Fatayer et al. Phys. Rev. Lett. 121, 226101 (2018).

KFM 5.2 Mon 15:30 PHY 5.0.21
Additive laser fabrication of silver and silver-composite 3D micro-structures — •Erik H. Waller[1] and Georg von Freymann[1,2] — [1]Physics department and State Research Center OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern — [2]Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern

We present direct laser writing (DLW) of silver and silver-composite microstructures via photoreduction in liquid resists. Several photoresist compositions are compared based on visual inspection of 2D and 3D test structures complemented by EDS and spectral resonance measurements.

Compared to common approaches for additive manufacturing of 3D metallic structures, e.g., selective laser melting or sintering, DLW is a very precise fabrication technology allowing sub-micrometer feature sizes. However, structures fabricated by DLW are usually made of polymers. Renewed interest in DLW of metallic microstructures has emerged due to their potential, e.g., in plasmonics. The underlying principle of metal DLW is photo-induced reduction of a precursor to neutral metal within the laser focus. The metal particles subsequently agglomerate to form the building block of a structure. Adverse effects are mainly heating of and scattering by the evolving structure as well as low quantum yield and slow speed of the reaction. Thus, we here test different photoresist compositions with respect to the above mentioned criteria and identify key parameters to best control these photoreactions.

KFM 5.3 Mon 15:50 PHY 5.0.21
Hard X-ray Photoelectron Diffraction in Graphite — •Olena Fedchenko[1], Sergey Chernov[1], Katerina Medjanik[1], Sergey Babenkov[1], Dmitry Vasilyev[1], Aimo Winkelmann[2], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]JGU, Institut für Physik, Mainz — [2]Laser Zentrum, Hannover

A new high-energy momentum microscope (kinetic energies up to >7 keV) allows full-field imaging of the (k_x-k_y) photoelectron distribution with a large field of view (up to 20 $Å^{-1}$ dia.) in momentum space and ToF energy recording. Avoiding symmetry-varying rotation of sample and/or analyser, "full-field k-imaging" provides an ideal means for X-ray photoelectron diffraction (XPD) studies. High-resolution ($< 0.1°$) diffractograms can be recorded within minutes thanks to the high brilliance of beamline P22 at PETRA III [1]. We present an XPD study for electrons from the C 1s core level in graphite in a wide energy range from 2840 to 7283 eV. Fine details in the diffractograms reflect the large number of scatterers (10^5-10^6) due to the large inelastic mean free path. A calculation based on the Bloch wave approach to electron diffraction by lattice planes [2] shows excellent agreement. The short photoelectron wavelength (10% of the interatomic distance) "amplifies" phase differences and turns hard X-ray XPD into a very sensitive structural tool. The results are important for valence band XPD [3].

[1] C. Schlueter et al., Synchr. Radiation News 31, 29 (2018); [2] A. Winkelmann et al., New J. of Phys. 10, 113002 (2008); [3] G. Schönhense et al., arXiv 1806.05871 (2018).

KFM 5.4 Mon 16:10 PHY 5.0.21
High-Resolution High-Sensitivity Characterization using SIMS based Correlative Microscopy — •Santhana Eswara, Alisa Pshenova, Jean-Nicolas Audinot, and Tom Wirtz — Advanced Instrumentation for Ion Nano-Analytics, MRT, Luxembourg Institute of Science and Technology, L-4422 Belvaux, Luxembourg

Technological materials are being increasingly engineered by optimizing the structure at the nanometer-level and the chemical composition at the dopant-level. Therefore, analytical techniques capable of both high-resolution and high-sensitivity are indispensable. Transmission Electron Microscopy (TEM) offers excellent lateral resolution down to atomic scale, but the analytical techniques typically available in a TEM such as EDX or EELS do not have the sensitivity to analyze trace elements (e.g. dopants). In comparison, Secondary Ion Mass Spectrometry (SIMS) is well-known for high-sensitivity analysis of materials down to the ppm level. However, the lateral resolution of SIMS is fundamentally limited by the ion-solid interaction volume to ~ 10 nm. Recently we developed SIMS in a Helium Ion Microscope (HIM) and demonstrated a SIMS lateral resolution of ~ 15 nm[1]. While this is a remarkable breakthrough, it is still 2 to 3 orders-of-magnitude poorer in comparison to high-resolution techniques such as TEM imaging. To overcome this limitation, we developed correlative microscopy methods combining SIMS imaging with high-resolution techniques such as TEM and HIM (SE mode). We will discuss the HIM-SIMS and in-situ TEM-SIMS correlative techniques[2]. [1] D. Dowsett et al, Anal. Chem., 89, 8957-8965, 2017 [2] L. Yedra et al, Sci. Rep. 6, 28705, 2016

KFM 6: Focus: Advanced TEM spectroscopy - low energy excitations and chemical composition at high resolution (joint session KFM/HL)

The recent progress in transmission electron microscope (TEM) based spectroscopies in terms of spatial, temporal and spectral resolution allows to address new regimes of electronic and vibrational excitations and therefore widened our understanding of condensed matter. This session focuses on recent developments and applications of spectroscopy techniques in the TEM, in particular electron energy loss spectroscopy in the low-loss regime for optical properties and core-loss regime for chemical analysis, at both atomic and medium resolution. Moreover, contributions on ultrafast techniques as well as energy dispersive X-ray spectroscopy, hardware and technique developments, theory and simulation and data processing will be discussed.

Organizer and Chair: Axel Lubk (IFW Dresden)

Time: Monday 15:00–18:40 Location: PHY 5.0.20

Invited Talk KFM 6.1 Mon 15:00 PHY 5.0.20

Fifteen years of electron magnetic circular dichroism — •Ján Rusz — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Electron magnetic circular dichroism (EMCD; [1]) has been proposed in 2003 and for the first time experimentally realized in 2006. Since then the method went through a rapid development at both fronts - experimental and theoretical. Dynamical diffraction effects severely complicate EMCD detection and often reduce the its strength. To circumvent this, numerous ways of acquiring EMCD have been proposed and many of them were experimentally tested. Recently, EMCD was detected using astigmatic electron beams on antiferromagnets, or with convergent probes, resolving magnetic signals from areas smaller than a square nanometer. In high-resolution TEM setting, EMCD signal from individual atomic planes was detected using the PICO instrument, where a crucial role was played by chromatic aberration corrector. Theory predicts that electron vortex beams should be efficient probes of EMCD at atomic resolution. Successful realization of this experiment could be extended further to probe the third dimension by means of magnetic depth sectioning. We will review the recent history of EMCD, its present state-of-art and discuss some of its challenges for the near future.

[1] P. Schattschneider et al., Nature **441**, 486 (2006).

KFM 6.2 Mon 15:30 PHY 5.0.20

Spectral Field Mapping of Surface Plasmon Resonances using High Energy Electrons — •Jonas Krehl[1], Giulio Guzzinati[2], Johannes Schultz[1], Pavel Potapov[1], Jerome Martin[3], Jo Verbeeck[2], Bernd Büchner[1], and Axel Lubk[1] — [1]IFW Dresden, Dresden, Deutschland — [2]EMAT, Antwerpen, Belgien — [3]Institute Charles Delaunay, Troyes, Frankreich

Surface plasmons resonances (SPR) are discrete modes in the response of the electron gas near the surface of a metallic nanoparticle. They contain very strong and localized electric and magnetic fields which enables interesting nanophotonic applications. Conventional electron energy-loss spectroscopy (EELS) is readily used for mapping the loss probablity of these modes with high energy and high spatial resolution.

The energy-loss signal only entails the longitudinal inelastic momentum transfer (IMT), so for a more comprehensive study of the fields of plasmon modes the lateral IMT components are crucial. The associated beam deflection is only a few μrad so we needed to develop a especially low-angle TEM setup for energy-filtered diffraction. With the energy slit set to a particular mode, the full IMT corresponds to a spectral component of the projected (along the beam trajectory) fields.

We demonstrated this technique in mapping the electric field at the dipole mode of an aluminium nanorod and compared the results with boundary-element-method simulations where we reached reasonable quantitative agreement. We are developing several extensions to this technique which e.g. tackle methodic problems or enable the mapping of magnetic fields.

KFM 6.3 Mon 15:50 PHY 5.0.20

Automatic Truncation of Principal Components in the PCA Analysis of EELS and EDX Spectrum-Images — •Pavel Potapov[1], Paolo Longo[2], and Axel Lubk[1] — [1]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany — [2]Gatan Inc, Pleasanton, CA, USA

The Principal Component Analysis (PCA) allows to denoise drastically STEM EELS and EDX spectrum-images by extracting the meaningful fraction of data while cutting off the irrelevant noise. The number of meaningful PCA components is usually estimated through the evaluation of a scree plot - a dependence of the log eigenvalues (variances) on the component index. This strategy however introduces some subjectivity in the treatment. A novel promising method for the truncation of principal components is the analysis of bivariate scatter plots. This method can be easily implemented in automatic algorithms promoting a smooth, unsupervised data treatment flow.

KFM 6.4 Mon 16:10 PHY 5.0.20

Synthesis and high-resolution structural and chemical analysis of iron-manganese-oxide core-shell nanoparticles — •Aladin Ullrich, Mohammad Mostafizar Rahman, and Siegfried Horn — Universität Augsburg, Universitätsstr. 1, 86159 Augsburg

Nanoparticles were synthesized by thermal decomposition of a mixture of iron oleate and manganese oleate precursors in high-boiling solvents in the presence of Na-oleate and oleic acid as surfactants. The structural and chemical composition of the nanoparticles was investigated by high-resolution analytical transmission electron microscopy (TEM). The particles appear core-shell like in bright field TEM images. High-resolution TEM (HRTEM) analysis reveals a FeO/MnO like structure in the core and a spinel like structure in the shell. With high-resolution analytical methods like energy dispersive x-ray spectroscopy and electron energy loss spectroscopy, the distribution of the metals Mn and Fe, respectively, was investigated. Furthermore, differences in the oxidation state of these metals were found between the core and the shell region. The presence of sodium from the used surfactant (Na-oleate) on the surface of the particles has been proved.

KFM 6.5 Mon 16:30 PHY 5.0.20

How sharp are atomically sharp interfaces in complex functional oxide heterostructures? — •Peter A. van Aken — Max Planck Institute for Solid State Research, Stuttgart Center for Electron Microscopy, Stuttgart, Germany

Complex functional oxide heterostructures have been serving as a multi-directional platform for engineering novel interface functionalities. Recent technical improvements of the epitaxial growth techniques enable fabricating high-quality thin films and heterostructures. The phenomena occurring at their interfaces can be tailored depending on the choice of the constituents. The key factor dominating the interface functionalities is the control of interface sharpness. Therefore, examining the interfacial structure and chemistry is vital for correlating with the underlying physical properties.

High-resolution analytical STEM investigations on various complex functional oxide heterostructures exhibiting different interface sharpness and different functionalities will be presented yielding that i) the growth technique has a direct impact on the structural and chemical sharpness of the interfaces, ii) two-dimensional doping of La2CuO4-based multilayers results in different dopant distribution at both sides of the interfaces which induces different superconducting mechanisms, iii) the choice of the dopant directly affects the interface sharpness. The effect of dopant distribution at interfaces on physical properties will be discussed.

Break 20 min

Invited Talk KFM 6.6 Mon 17:10 PHY 5.0.20

Advanced Imaging and Spectroscopy in an Ultrafast Transmission Electron Microscope — •Armin Feist — IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany

Electron microscopy is tremendously successful in studying complex nanostructured systems, with a temporal resolution governed by typical detector response times. Overcoming these time-domain limitations, ultrafast transmission electron microscopy (UTEM) combines the versatile imaging, diffraction and spectroscopy capabilities of state-of-the-art TEM with femtosecond temporal resolution achieved by a laser pump/electron probe scheme [1,2].

Here, I will briefly introduce the UTEM methodology and show recent results of the Göttingen UTEM instrument, which features high coherence electron pulses generated from nanoscale field emitter tips [2]. The novel applications of UTEM include the study of coherent inelastic electron-light scattering (IELS) at laser-excited nanostructures [3,4]. Besides nanometer mapping of optical near-fields and plasmonic modes, IELS enables the transverse and longitudinal phase control of the free-electron wavefunction [4,5], as evident from characteristic multiphoton gain and loss spectra. In particular, this new concept now allows us to generate attosecond electron pulse trains with applications for optically phase-resolved electron microscopy [5].

[1] A. H. Zewail, Science **328**, 187 (2010). [2] A. Feist *et al.*, Ultramicroscopy **176**, 63 (2017). [3] Barwick *et al.*, Nature **462**, 902 (2009). [4] A. Feist *et al.*, Nature **521**, 200 (2015). [5] K. E. Priebe *et al.*, Nat. Photonics **11**, 793 (2017).

KFM 6.7 Mon 17:40 PHY 5.0.20

Spectroscopic coincidence experiments in Transmission Electron Microscopy — •Daen Jannis[1], Knut Müller-Caspary[1], Armand Béché[1], Andreas Oelsner[2], and Jo Verbeeck[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]Surface Concept GmbH, Am Sägewerk 23a, 55124 Mainz, Germany

Modern transmission electron microscopes are often equipped with EELS and EDX spectrometers. Both measurement techniques share the fact that excitations of atomic states are involved. Indeed, there is for every emitted X-ray photon at least one electron that transfers a part of its energy to excite the atom in the first place, and therefore one could imagine that they convey very similar information. Since the two signals originate from the same process, the temporal correlation between these signals can be measured. Our current setup consists of a novel delay line detector setup for EELS and a Super-X EDX detector. These allow to detect the energy and arrival time (time resolution 270 ns) of every incoming electron and X-ray. This setup keeps all detected events and allows for extensive post processing. By the measurement of every event, it is possible to disentangle the background from the coincidence signal opening up the possibility of background free EELS and EDX with EELS resolution.

[1] D. Jannis, K. Müller-Caspary, A. Béché A. Oelsner and J. Verbeeck. Unpublished Paper, 2018.

[2] D.J., A.B. and J.V. acknowledge funding from the Flemish Research Fund FWO under projectno. G093417N

KFM 6.8 Mon 18:00 PHY 5.0.20

High-resolution EFTEM at very low accelerating voltages — •Martin Linck[1], Michael Mohn[2], Johannes Biskupek[2], Heiko Müller[1], Stephan Uhlemann[1], and Max Haider[1] — [1]CEOS GmbH, Englerstr. 28, D-69126 Heidelberg, Germany — [2]Central facility of electron microscopy, Ulm University, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

Simultaneous correction of both, spherical and chromatic aberration in a dedicated low-voltage transmission electron microscope (TEM) has enabled atomic resolution TEM observations on beam sensitive materials at beam energies from 20 to 80 keV (SALVE project). The reduction of focus spread due to chromatic aberration correction, however, not only allows for highest resolution atomic phase contrast (elastic zero-loss imaging) but also enables high-resolution imaging capabilities over significant energy windows in energy-filtered (EF)TEM. In order to provide a significant field of view on the energy filter's camera device, it is essential that the corrector is free of chromatic distortions, i.e. image distortions which change with electron energy. It has been shown that the SALVE corrector is well-suited for such ambitious investigations. First experimental results, in fact, show that high-resolution EFTEM is feasible in the SALVE microscope. The subsequent interpretation of such data, however, is very challenging due to the multiple scattering, i.e. mixture of elastic and inelastic scattering.

KFM 6.9 Mon 18:20 PHY 5.0.20

Plasmonics in topological insulators — •Johannes Schultz[1], Axel Lubk[1], Flavio Nogueira[2], Darius Pohl[3], and Bernd Büchner[1] — [1]IFF, IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]ITF, IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [3]Dresden Center for Nanoanalysis, TU Dresden, 01062 Dresden

Surface plasmons are self-sustaining resonances occuring at interfaces between media whose permittivities have a different sign. They are associated with strongly enhanced, localized electrical fields, which may be coupled to external optical excitations. Surface plasmons can be used for the sub-wavelength control of electromagnetic fields. Based on this, novel electronic devices can be realized, for instance on-chip light spectrometers and linear accelerators, plasmonic rectennas for the harvesting of light or LEDs and photovoltaics with a higher efficiency. We study the properties of these surface plasmons when they are localized on a surface of a topological insulator like Bismuth selenide.

Surfaces of topological insulators contain conducting states which leads to negative permittivity on the surface and positive permittivity in the bulk. Consequently topological insulators can in principle sustain surface plasmons if they are embedded in a dielectric environment with positive permittivity. To characterize this localized surface plasmon-modes on the surfaces of topological insulators we use low loss spectroscopy techniques in the TEM.

KFM 7: Multiferroics

Time: Monday 15:00–18:30 Location: H47

KFM 7.1 Mon 15:00 H47

Insights into the coupled domains in conical spin-driven multiferroics — •Jonas K. H. Fischer, Kenta Kimura, Ryusuke Misawa, and Tsuyoshi Kimura — Department of Advanced Materials Science, University of Tokyo, Japan

Multiferroics offer opportunities for new and previously unattainable applications [1]. Especially sought-after is the mutual control of magnetization and electric polarization by electric and magnetic fields, the so-called magnetoelectric effect. The "conical spin structure" is a rather complicated spiral magnetic order that breaks both time-reversal and space-inversion symmetries and leads to a ferromagnetic-ferroelectric, i.e., multiferroic ground state. So far only a few conical spin-driven multiferroics have been reported, among them spinel-type $CoCr_2O_4$ [2] and olivine-type Mn_2GeO_4 [3]. Recently, an intriguing domain coupling, that is, magnetoelectric inversion of domain patterns, has been reported in Mn_2GeO_4 [4,5].
However, the coupling mechanism among the various domains of the conical spin-driven multiferroics has not yet been fully understood. In addition to electric and magnetic fields, uniaxial pressure is expected to affect their domain coupling. In this study, the effect of uniaxial stress on the magnetoelectric properties is examined.
[1] M. Fiebig *et al.*, Nat. Rev. Mater. **1**, 16046 (2016).
[2] Y. Yamasaki *et al.* Phys. Rev. Lett. **96**, 207204 (2006).
[3] J. S. White *et al.* Phys. Rev. Lett. **108**, 077204 (2012).
[4] T. Honda *et al.* Nat. Commun. **8**, 15457 (2017).
[5] N. Leo *et al.*, Nature **560**, 466 (2018).

KFM 7.2 Mon 15:20 H47

Domain dynamics in $LiCuVO_4$: Evidence for polarized nanoregions — •Christoph P. Grams[1], Severin Kopatz[1], Daniel Brüning[1], Sebastian Biesenkamp[1], Petra Becker[2], Ladislav Bohatý[2], Thomas Lorenz[1], and Joachim Hemberger[1] — [1]University of Cologne, Institute of Physics II, Zülpicher Str. 77, 50937 Cologne, Germany — [2]University of Cologne, Institute of Geology and Mineralogy, Section Crystallography, Zülpicher Str. 49b, 50674 Cologne, Germany

$LiCuVO_4$ is a model system of a 1D spin-1/2 chain that enters a multiferroic planar spin-spiral ground state below its Néel temperature of

2.4 K with electric polarization along the a axis. With external magnetic fields in c direction T_N can be suppressed down to 0 K at 7.4 T.

Here we report dynamical measurements of the polarization from $P(E)$-hysteresis loops, magnetic field dependent pyro-current and non-linear dielectric spectroscopy as well as thermal expansion and magnetostriction measurements at very low temperatures. Our measurements find a sizable magnetoelastic coupling in $LiCuVO_4$ that strongly influences all observed quantities. Most striking is the observation of a growth dimension $d \approx 0.25$, i.e. strong pinning of the domain walls, from the non-linear polarization dynamics. Further analysis finds the domain sizes to be in the nm range.

This work was supported by the Deutsche Forschungsgemeinschaft through CRC 1238 and HE-3219/2-1.

KFM 7.3 Mon 15:40 H47

Low frequency phonons in rare-earth langasites — •Lorenz Bergen[1], Lukas Weymann[1], Andrei Pimenov[1], Artem Kuzmenko[2], Alexander A. Mukhin[2], and Evan Constable[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia

Rare-earth langasites are characterized by geometric magnetic frustration exhibiting magneto-electric effects, high piezoelectric properties, and may even support a spin-liquid ground state. To better understand the interplay between the structural and magnetic degrees of freedom it is important to study the phonon and crystal electric field spectra that can be observed in the far infrared (FIR) range. The langasite structure crystallizes in the P321 space group with a general formula $A_3BC_3D_2O_{14}$. Our study presents spectra of the rare-earth langasite $N_3Ga_5SiO_{14}$ using far-infrared reflection spectroscopy. Experiments have been performed with polarized radiation along different crystallographic axes and under different sample temperatures. Phonon excitations at unusually low frequencies are observed that brings the crystal structure of langasites close to a lattice instability. The results of neodymium and holmium-substituted langasites will be compared with the pure $La_3Ga_5SiO_{14}$ langasite compound that does not show effects like magnetic frustration.

KFM 7.4 Mon 16:00 H47

Magnetic Structure and Magnetoelectricity in Holmium-Doped Langasite — •Lukas Weymann[1], Lorenz Bergen[1], Thomas Kain[1], Anna Pimenov[1], Alexey Shuvaev[1], Evan Constable[1], David Szaller[1], Artem M. Kuzmenko[2], Alexander A. Mukhin[2], Vsevolod Yu. Ivanov[2], Nadezhda V. Kostyuchenko[1,3], Maxim Mostovoy[4], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]A. M. Prokhorov General Physics Institute of Russian Academy of Sciences, 119991 Moscow, Russia — [3]Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Moscow region, Russia — [4]Theory of Condensed Matter, Zernike Institute for Advanced Materials, 9747 AG Groningen, The Netherlands

The family of the rare-earth langasites $R_3Ga_5SiO_{14}$ attracted significant attention due to their intriguing magnetic and magnetoelectric properties. However, in the langasites with only one magnetic sublattice of the rare-earth ions no magnetoelectric effect was observed till now.

In this work we present the results on a magnetoelectric effect, i.e. electric polarization induced by an external magnetic field, in the diluted rare-earth langasite $(Ho_{0.03}La_{0.97})_3Ga_5SiO_{14}$, with an unusual six-fold symmetry. Its rather complex magnetic structure can be resolved via magnetization, torque and dynamic experiments. Magnetic and magnetoelectric properties can be understood by taking into account the interplay between crystal symmetry and the local symmetry of the Holmium ions.

KFM 7.5 Mon 16:20 H47

Orbital-Order Driven Ferroelectricity and Dipolar Relaxation Dynamics in Multiferroic $GaMo_4S_8$ — •Korbinian Geirhos[1], Peter Lunkenheimer[1], Hiroyuki Nakamura[2], Takeshi Waki[2], Yoshikazu Tabata[2], and Istvan Kezsmarki[1] — [1]Experimental Physics V, EKM, University of Augsburg — [2]Department of Materials Science and Engineering, Kyoto University, Japan

$GaMo_4S_8$, a compound of the lacunar spinel family, was recently shown to exhibit non-canonical, orbitally-driven ferroelectricity [1]. Our dielectric spectroscopy measurements on this multiferroic material reveal complex relaxation dynamics, above as well as below its Jahn-Teller transition at T_{JT} = 47 K [2]. Above the Jahn-Teller transition, two types of coupled dipolar-orbital dynamics were found: On the one hand, relaxations within cluster-like regions with short-range polar order, as known from relaxor ferroelectrics. On the other hand, critical fluctuations of only weakly interacting dipoles, resembling the typical dynamics of order-disorder type ferroelectrics. Below T_{JT}, the system is driven into long range ferrolectric order by the onset of orbital order and dipolar dynamics within the ferroelectric domains is observed: The found marked differences to the skyrmion host GaV_4S_8, seem to be related to the different structural distortions in these systems.

[1] E. Neuber,*et al.*, J. Phys.: Condens. Matter **30**, 445402 (2018) [2] K. Geirhos, *et al.*, arXiv:1810.07145

Break

KFM 7.6 Mon 17:10 H47

Interplay of structural distortions and magnetism in lacunar spinels — •Sergey Artyukhin[1], Giulia Biffi[1], and István Kézsmárki[2] — [1]Italian Institute of Technology, Genova, Italy — [2]University of Augsburg, Germany

Lacunar spinels contain tetrahedral clusters of transition metal compounds whose molecular orbitals host electrons, delocalized over the cluster. Partial occupations of degenerate molecular orbitals are thought to lead to Jahn-Teller distortions that influence magnetic exchange interactions between clusters, giving rise to a multitude of distortion patterns and magnetic ground states, including non-collinear states and skyrmion lattices. Here we use effective Hamiltonians with parameters derived from ab-initio calculations to address the complex phase diagram of these compounds.

KFM 7.7 Mon 17:30 H47

Imaging of ferroelectric domains in $Ca_3Mn_{1.9}Ti_{0.1}O_7$ by second harmonic generation — •Yannik Zemp[1], Mads C. Weber[1], Thomas Lottermoser[1], Bin Gao[2], Sang-Wook Cheong[2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Rutgers University, New Jersey

One of the most important challenges towards the application of multiferroics – materials with coexisting magnetic and ferroelectric order, is to find a material with a robust coupling between ferroelectricity and magnetism and a sufficiently large polarisation at high temperatures. Magnetic hybrid-improper ferroelectrics, in particular $Ca_3Mn_2O_7$, where magnetism and ferroelectricity are induced through the same lattice instability, were theoretically proposed as a possible solution. Experimentally, however, ferroelectric switching at room temperature has still not been achieved. Already an important hallmark for ferroelectricity would be the observation of polar domains. Here, we investigate Ti-stabilised $Ca_3Mn_2O_7$ by optical second harmonic generation imaging – a method that is highly sensitive to a breaking of inversion symmetry and hence the ideal non-destructive tool to probe for ferroelectricity. We show the existence of polar domains, oriented 90° towards each other, at room temperature and additional 180° domains within them. This domain structure can be directly linked to the complex structural distortion mechanism and gives rise to a rich domain wall structure. These findings are an important milestone towards the detection of multiferroicity and magnetoelectric coupling in $Ca_3Mn_2O_7$.

KFM 7.8 Mon 17:50 H47

The ultrathin limit of improper ferroelectricity — •Johanna Nordlander[1], Marco Campanini[2], Marta D. Rossell[2], Rolf Erni[2], Quintin N. Meier[1], Andres Cano[1,3], Nicola A. Spaldin[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials – ETH, Zurich, Switzerland — [2]Electron Microscopy Center – EMPA, Dübendorf, Switzerland — [3]Institut Néel – CNRS, Grenoble, France

The secondary nature of spontaneous polarization in improper ferroelectrics is known to promote functional properties beyond those of conventional ferroelectrics. In technologically relevant ultrathin films, however, the improper ferroelectric behavior remains largely unexplored. Using state-of-the-art in-situ second harmonic generation and transmission electron microscopy, we probe the coupled improper polarization and primary order parameter in $YMnO_3$ thin films. The polarization displays a pronounced thickness dependence, which we show to originate from the strong modification of the primary order at epitaxial interfaces. Finite-size effects reduce the temperature of the phase transition, allowing us to reveal its order-disorder character with atomic resolution. Our results lay the foundation for understanding the emergence of improper ferroelectricity within the confinement of ultrathin films – essential for the successful implementation of these exotic materials in nanoscale devices.

KFM 7.9 Mon 18:10 H47

Magnetic monopoles in $LuFeO_3$: modelling inelastic neutron scattering and magnetoelectric effect — Francesco Foggetti[1,2], Sang-Wook Cheong[3], and •Sergey Artyukhin[1] — [1]Italian Institute of Technology — [2]University of Genova, Italy — [3]Rutgers University, USA

Multiferroic hexagonal manganites are an interesting realization of frustrated triangular lattice, where magnetic order is coupled to ferroelectricity and trimerization. They support 120 degrees antiferromagnetism with spin canting due to Dzyaloshinskii-Moriya interaction leading to magnetoelectricity. Here we study the possible spin orders and their neutron scattering signatures, as well as their connection to magnetoelectric effect. The calculations are performed using spin wave approximation, within the microscopic model that involves spin and structural degrees of freedom.

KFM 8: Diamond I (joint session KFM/HL)

This session represents the physics, the production and applications of diamond and diamond related materials in the fields of dielectrics, electronics, high frequency techniques, GHz * THz * applications, mechanics and optics and biological applications as well. Defects in diamond have a large influence to the physical properties (e. g. NV-centers). Applications of diamond (single, poly-crystalline, UNCD, etc.) or related materials in technical systems are part of this session (Nuclear fusion applications, high frequency heating systems and material processing).

Chair: Dirk Strauss (KIT)

Time: Tuesday 9:30–12:00 Location: PHY 5.0.20

KFM 8.1 Tue 9:30 PHY 5.0.20

The ITER Diamond Window - Qualification Program Development of a Safety Important Component — •Sabine Schreck, Gaetano Aiello, Andreas Meier, Theo Scherer, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, Hermann-von-Helmholtz-Platz 1,

An important component of the ITER ECRH Upper Launcher system is the torus diamond window, which serves as primary vacuum and tritium boundary of the ITER vacuum vessel and allows the transmission of high power mm-waves coming from the gyrotrons into the plasma. The window consists of an ultra-low loss CVD diamond disk mounted in a system of metallic parts and is integrated into the transmission line system. Because of its confinement function the window is classified as Protection Important Component (PIC) and high requirements for quality and safety apply. An ad-hoc qualification program is required for this specific component because it cannot be entirely covered by codes and standards.

Diamond disks with a diameter of about 70 mm and a thickness of 1.11 mm (resonance thickness for 170 GHz) will be used and need to be qualified with respect to their mm-wave transmission capability and mechanical stability. Qualification procedures are also to be established for the joining of the disk to the metallic structure, which is performed by brazing and finally for the qualification of the complete housing made of metallic parts, that are welded together.

The status of the window qualification program will be given together with results of already performed prototype tests.

KFM 8.2 Tue 9:50 PHY 5.0.20

Development of Diamond Windows Diagnostics for fusion applications — •Theo Scherer, Aurelian Tesniere, Gaetano Aiello, Francesco Mazzocchi, Andreas Meier, Sabine Schreck, and Dirk Strauss — Karlsruhe Institut für Technologie KIT, IAM-AWP, D-76344 Eggenstein-Leopoldshafen, Hermann-von-Helmholtz-Platz 1, Germany

The future nuclear fusion power plants will require Electron Cyclotron Heating and Current Drive (ECH&CD) systems to heat up and stabilize the plasma inside the vacuum vessel. One of the key components of such systems is the Chemical Vapor Deposition (CVD) diamond window. The purpose of this device is to act as vacuum and tritium boundary while providing a high microwave transparency with minimal reflectivity. Although suited for high power microwave operation, the windows shall be internally monitored in order to properly ensure the ECH system efficiency and safety. In this paper, the latest assessment study on a set of diagnostics to be part of the window assembly is shown. The required diagnostics include arc and tritium detection, microwave stray radiation (perpendicular to the main beam and generated by cracks in the windows), pressure and disk temperature measurements. To accommodate the diagnostics previously mentioned, a new design for the window housing was developed.

KFM 8.3 Tue 10:10 PHY 5.0.20

Brewster-angle diamond window for microwave application — •Gaetano Aiello[1], Theo Scherer[1], Thomas Franke[2], John Jelonnek[1], Andreas Meier[1], Dirk Strauss[1], Quang Tran[3], Christoph Wild[4], and Eckhard Woerner[4] — [1]KIT, Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, Germany, 76344 — [2]EUROfusion Consortium, Boltzmannstrasse 2, Garching, Germany, 85748 — [3]Swiss Plasma Center (SPC), EPFL, Lausanne, Switzerland, 1015 — [4]Diamond Materials GmbH, Hans-Bunte-Strasse 19, Freiburg, Germany, 79108

The Brewster-angle diamond window is a broadband window solution for the frequency step-tunable gyrotrons in the context of the DEMO EC H&CD system. It consists of an elliptical CVD diamond disk brazed to two copper WGs at the Brewster angle of 67.2° for diamond. This window concept is being investigated for long pulse gyrotron operation at 2 MW power. Main challenges along this path are the production of very large area optical grade diamond disks suited for a 63.5 mm WG aperture, the proper joining of the disks to the WGs and the design of an effective cooling layout. A 63.5 mm WG requires a minimum disk diameter of 180 mm and 2 mm thickness. Available state of the art microwave plasma reactors are not able of growing diamond disks of such size. In collaboration with Diamond Materials GmbH, tests aiming to obtain large disks were thus investigated by different methods and experiments are still ongoing. In this work, the results of these experiments shall be reported, also together with the results of the FEM analyses aiming to investigate different window cooling layouts.

Break 20 min

KFM 8.4 Tue 10:50 PHY 5.0.20

ECRH system development for nuclear fusion reactors: Antenna design and diamond window implementation — •Dirk Strauss, Theo Scherer, Sabine Schreck, Peter Spaeh, Gaetano Aiello, Andreas Meier, and Francesco Mazzocchi — KIT Karlsruhe, Deutschland

The ITER ECRH system consists of 24 gyrotrons with up to 24 MW millimeter wave heating power at 170 GHz, power supplies, control system, transmission lines, one Equatorial and the four Upper Launchers. With its high frequency and small beam focus the ECRH has the unique capability of driving locally current. While the Equatorial Launcher mainly acts for central heating and current profile shaping, the Upper Launchers aim on suppressing MHD instabilities, especially neoclassical tearing modes triggering plasma disruptions. The Upper Launchers inject millimeter waves through a quasi-optical section. The eight overlapping beams have focal points optimized for suppression of NTMs. Changes in the design include new ex-vessel waveguide components with a reduced aperture and redesigned ultra low-loss CVD diamond windows.

Invited Talk KFM 8.5 Tue 11:10 PHY 5.0.20

Development of Kinetic Inductance Detectors for polarimetric applications in plasma diagnostics — •Francesco Mazzocchi[1], Eduard Driessen[2], Shibo Shu[2], Giovanni Grossetti[1], Dirk Strauss[1], and Theo Scherer[1] — [1]Karlsruhe Institute of Technology, Eggenstein Loepoldshafen, Germany — [2]Institute de RadioAstronomie Millimetrique, Grenoble, France

Polarimetry is a technique that measures the Faraday rotation in a magnetized medium, such as a fusion plasma. It allows to determine various fundamental plasma parameters, such as current density when used independently from other diagnostics and like poloidal field and electron density when coupled to specific systems (i.e. interferometry). To mitigate these issues of current systems, we have considered to use in our device a Quantum Cascade Laser (QCL). The lack of power of such source requires the use of extremely sensitive detectors, hence the development of custom superconducting Kinetic Inductance Detector (KID) presented in this work. The whole system will be composed of a cryostat containing the source and the detector (both of which require cryogenic temperatures to operate optimally) and a beam delivery system, consisting of suitable waveguides and a diamond window on the reactor side, to have a very strong pressure barrier between the tritium rich atmosphere of the fusion reactor and the vacuum of the polarimeter side waveguides. The dielectric and mechanical properties of the synthetic diamond allow us to have such barrier without compromising the beam transmission factor.

KFM 8.6 Tue 11:40 PHY 5.0.20

Diamant und die Knickpyramide in Ägypten: Eine überraschende Gemeinsamkeit — •Peter-Michael Wilde — 15711 Königs Wusterhausen, Deutschland

Der Habitus und die Zusammensetzung von kristallinen Mikroobjekten auf Silicium (111)- Substraten wurden mit SEM und EDX aufgeklärt. Mittels des LPE Verfahrens waren Felder von Mikropyramiden erzeugt worden, deren Böschungswinkel typisch sind für die kubische Struktur von Diamant. Mikroanalysen ergaben die Zusammensetzung C - Si - Ge, wobei die Verhältnisse dieser drei Elemente bei konstantem Böschungswinkel gezielt variiert werden können. Die aus Kalkstein errichtete Kickpyramide von Dahschur mit über 105 m Höhe weist fast bis zur Hälfte den gleichen Böschungswinkel von 54,5 Grad auf, wie er für die Diamantstruktur typisch ist. Über die geometrische Tangens-Funktion ergibt sich ein Zahlenwert von 1,41 in sehr guter Übereinstimmung mit dem Wert Quadratwurzel aus 2. Auch bei der Realisierung des oberen Teils der Knickpyramide kommt eine Wurzelfunktion von 2 zum Tragen. Das sind überraschende Befunde, da die Mathematik der alten Ägypter die Operation des Radizierens nicht kannte. Es wird eine Erklärung hierzu vorgestellt.

KFM 9: Focus: Materials for Energy Storage

On the one hand efficient energy storage is a necessary prerequisite for a continuous electrical power supply on the basis of fluctuating energy sources like wind and solar energy. On the other hand the replacement of combustion engines in cars by electric motors requires energy storage systems with optimized properties like high power density, high energy density, low discharge and high reliability. The aim of the focus-session will be the discussion of different energy storage concepts with a main focus on capacitors, supercaps and other methods of direct electric energy storage, but not limited to these methods.

Chair: Martin Diestelhorst (Martin-Luther-University Halle-Wittenberg)

Time: Tuesday 9:30–12:50 Location: PHY 5.0.21

Invited Talk KFM 9.1 Tue 9:30 PHY 5.0.21

High Energy Density and Low Loss Dielectric Polymers for Electrical Applications — •Lei Zhu — Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106-7202, United States

High dielectric constant polymers find numerous advanced electrical and power applications such as pulsed power, power conditioning, gate dielectrics for field-effect transistors, electrocaloric cooling, and electromechanical actuation. Unfortunately, it is generally observed that polymers do not have high dielectric constants (only 2-5) and high polarization tends to cause a significantly dielectric loss. Therefore, it is highly desirable that the fundamental science of all types of polarization and loss mechanisms be thoroughly understood for dielectric polymers. In this presentation, we intend to explore advantages and disadvantages for different types of polarization. Among a number of approaches, orientational polarization is promising for high dielectric constant and low loss polymer dielectrics, if the dipolar relaxation peak can be pushed to towards the gigahertz range. In particular, dipolar glass, paraelectric, and relaxor ferroelectric polymers will be discussed for the orientational polarization approach.

KFM 9.2 Tue 10:00 PHY 5.0.21

Self-discharge behaviour of poly(vinylidene fluoride-hexafluoropropylene) for dielectric energy storage — •Tino Band[1], Till Mälzer[2,3], Sandra Wickert[4], Hartmut S. Leipner[2], Stefan G. Ebbinghaus[4], Kathrin Dörr[1], and Martin Diestelhorst[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06099 Halle, Germany — [2]Interdisciplinary Center of Materials Science, Martin Luther University Halle-Wittenberg, Heinrich-Damerow-Straße 3, 06099 Halle, Germany — [3]enspring GmbH, Weinbergweg 23, 06120 Halle, Germany — [4]Institute of Chemistry, Martin Luther University Halle-Wittenberg, Kurt-Mothes-Straße 2, 06099 Halle, Germany

We present results about dielectric energy storage mechanisms in doctor blade coated P(VDF-HFP). One approach is using cyclic unipolar *D-E* characteristics to study conduction mechanisms. We define an effective conductivity for each cycle observing a Curie-von Schweidler law with steady-state conductivity. Therefore, an effective relaxation time can be obtained which is connected to self-discharge rate of the polymer. A second approach is made inversely. The self-discharge is directly investigated by means of charging-lift-discharging measurements, where the contact between measurement tip and electrode is interrupted for a specific time between charging and discharging process. Based on the self-discharge behaviour, we can conclude on conduction mechanisms. So we are able to separate the influence of polarization, depolarization and conduction mechanisms on the energy storage properties of dielectric materials in detail.

KFM 9.3 Tue 10:20 PHY 5.0.21

Influence of the morphology on the electrical conductivity of ceramic-polymer composite dielectrics — •Till Mälzer[1,3], Tino Band[2], Marius Falkenstein[2], Robert Schlegel[3], Martin Diestelhorst[2], Stefan Ebbinghaus[4], and Hartmut S. Leipner[1] — [1]Center of Materials Science, Martin-Luther-University Halle-Wittenberg (MLU), D06120 Halle (Saale) — [2]Department of Physics, MLU — [3]enspring GmbH, D06120 Halle (Saale) — [4]Department of Chemistry, MLU

Ceramic-polymer composites have been evaluated as a candidate for dielectric materials for a new type of capacitors, due to the possibility to tailor materials properties by proper design for specific applications. By rising the content of high-k ceramic filler, the energy density of composite materials can be increased. However, it causes also an increase in the electrical conductivity, a fact which has been disregarded in many studies.

We report on the influence of morphological aspects like particle size, particle distribution, agglomerate structure and percolating agglomerates on the electrical conductivity of the composite. The investigated material system consists of P(VDF-HFP) as polymer matrix and $BaTiO_3$ or TiO_2 as filler. Composite films with a variation of the particle size and the concentration of the filler, as well as different film thicknesses have been fabricated via a solution cast doctor blade method.

We have applied charge-voltage measurements for electrical investigations and for morphological studies scanning electron microscopy and 3D X-ray microscopy.

KFM 9.4 Tue 10:40 PHY 5.0.21

The effect of filler distribution in the enhancement of the energy storage in nanocomposites — •Elshad Allahyarrov — Theoretical Chemistry, Essen, UDE — Physics Department, CWRU, Cleveland OH, USA — Theoretical Department, RAS Moscow, Russia

Mixing dielectric polymers with high permittivity nano-sized inclusions affects their electrical properties. These nanocomposites are extensively used in actuation applications via employing electrostriction properties of the matrix, and in electrostatic energy storage applications employing high polarization fields of the fillers. In both cases existing theoretical studies mostly utilize mixing rule approaches that consider a homogeneous filler distribution in the matrix. Consequently, the effective permittivity of the composite never exceeds the the permittivity of the filler. We show that much higher effective permittivities can be achieved by manipulating the morphology of the inclusion distribution in the matrix. Simulation results for the field distribution reveal an enhancement of the field localization and dipole-dipole correlation effects in some proposed morphologies. By considering several possible clustering scenarios we found that a cylindrical clustering along the applied field has a potential to achieve an order of magnitude increase in the effective permittivity. The issue of chained filler configurations which lower the breakdown field threshold for the material is also addressed.

Break 20 min

Invited Talk KFM 9.5 Tue 11:20 PHY 5.0.21

Storing electrical energy using glasses and glass ceramics — •Martin Letz — SCHOTT AG, Hattenbergstr. 10, 55122 Mainz, Germany

Power electronics is a strongly growing field since highly fluctuating demand and supply of electrical energy needs efficient electronics for switching or for transformation between different voltage levels. In this situation the classes of materials, glasses (i) and glass ceramics (ii), which are nearly ever used as dielectrics for capacitors can enable innovations. Recent technical development makes it possible to produce ultrathin glasses (i) with extremly large dielectric breakdown strength up to 600 kV/mm which enable high storage densities at elevated temperatures. Glass ceramics (ii) allow to reach higher polarizabilities and are produced in a two step process. In a first step a transparent glass with a solely amorphous structure is molten. In a second and independent step crystallites are grown in such glasses by applying a well defined time–temperature profile. By growing nanosized crystallites with ferro- or para-electric phases, pore free dielectric materials with very high homogeneity and high dielectric strength can be obtained. We present two types of such material. Besides capacitors there are further fields of applications for glasses and glass ceramics in improving saftey and storage density of batteries.

KFM 9.6 Tue 11:50 PHY 5.0.21

Properties of composite films for Li-ion batteries — •Lena Kuske[1], Frank Apsel[2], Robert Schlegel[2], Till Mälzer[1,2], Richard Schalinski[3], Stefan Ebbinghaus[4], Ralf Wehrspohn[3], and Hartmut Leipner[1] — [1]Center of Materials Science, Martin-Luther-University Halle-Wittenberg (MLU), 06120 Halle (Saale) — [2]enspring GmbH, 06120 Halle (Saale) — [3]Department of Physics, MLU — [4]Department of Chemistry, MLU

The development of new, safer and good performing materials for long life batteries to provide storage possibilities that fulfil the distinct requests of different portable devices is highly demanded.

A promising material class for lithium ion batteries are polymer composite materials. We combine the distinct properties of P(VdF-HFP) as a flexible and mechanical stable polymer matrix with the electric properties of nanosized ceramic $Li_7La_3Zr_2O_{12}$ as a highly Li-ion conducting material and different Lithium salts to develop electrolyte materials with the desired properties of high ionic and low electron conductivity, good mechanical stability and homogeneity.

Thin layers of the composite materials were fabricated via a solution cast doctor blade process. Their ion and electron conductivity was analysed in view of their use as electrolyte material in lithium ion batteries. Besides electrochemical investigations, the morphology of the composite layers were studied with X-ray diffraction and electron microscopy.

KFM 9.7 Tue 12:10 PHY 5.0.21

Tungsten sulfide: An intercalation-type anode material for potassium-ion battery — •Yuhan Wu, Yang Xu, Chenglin Zhang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

The intercalation-type materials have rarely been discovered as anodes for potassium-ion batteries (PIBs) except graphite and conventional transition metal oxides. Here we reported the first two-dimensional transition metal dichalcogenide (2D TMD), WS2, as an intercalation-type anode material for PIBs. It is found for the first time that the WS2 undergoes an unexpected intercalation dominated K storage at deep-discharge condition (0.01 V vs. K+/K), attributing to the facilitation of K+ transport derived from the intercalation reaction that is confirmed by a kinetic study. Electrochemical characterizations reveal that WS2 exhibited a reversible capacity of 103 mAh/g at 0.1 A/g after 100 cycles. It also delivered a high rate capability (62 mAh/g at 0.8 A/g) and long-term stability at high rate (90% retention at 0.5 A/g after 400 cycles). Furthermore, a full-cell with intercalation-type WS2 as anode and Prussian blue as cathode exhibited a charge plateau around 3.3 V and a discharge slope between 1.5 and 3.2 V, delivering a reversible capacity of 60 mAh/g at 0.1 A/g after 50 cycles. This work highlights the unusual electrochemical properties when replacing Li+ and Na+ with K+ for the battery application, and may induce more future work in this regard.

KFM 9.8 Tue 12:30 PHY 5.0.21

Water splitting by pyroelectric single crystals — •Wolfram Münchgesang, Thomas Köhler, Erik Mehner, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany

The generation of hydrogen through water electrolysis has been understood for a long time and will be used for large-scale conversion of electrical energy into chemical energy in the future. The direct conversion of residual heat into hydrogen is completely new to our knowledge, but feasible when making use of pyroelectric materials. In pyroelectrolysis, a cyclic temperature excitation generates an electric field between the crystal surfaces due to an imbalance between polarization and compensation charges. This field can be used for water splitting, theoretical.

For the verification of the water splitting with pyroelectric single crystals an electrochemical measuring cell with optical heating was developed. With this setup, the proof of water splitting has been achieved. Furthermore, the reaction rates could be determined from the amount of transferred charges and compared with the theory.

KFM 10: Ferroics - Domains and Domain Walls

Time: Tuesday 9:30–12:50 Location: H47

KFM 10.1 Tue 9:30 H47

Ferroic transition in single-crystal $BaTiO_3$ — Asaf Hershkovitz[1], •Florian Johann[2], Maya Barzilay[1], Alon Avidor[1], and Yachin Ivry[1] — [1]Department of Materials Science and Engineering, Technion, Israel Institute of Technology, Haifa, Israel — [2]Asylum Research, an Oxford Instruments company, Wiesbaden, German

Variable-temperature piezoresponse force microscopy was used to image real-time dynamics of ferroelastic domains during the orthorhombic-tetragonal ferroic phase transition in single-crystal BaTiO3. We demonstrate multiscale stress releasing mechanism at the time space. This mechanism comprises domain wrinkling at the pre-transition state, followed by domain wedging during the transition and ending with domain zipping after the transition, in which striped ferroelastic domains are broadened.

KFM 10.2 Tue 9:45 H47

External-field induced domain wall dynamics in $LiNbO_3$ and $BaTiO_3$ single crystals imaged by in-situ 3D Cherenkov second harmonic generation microscopy — •Benjamin Kirbus, Christian Godau, Lukas Wehmeier, Elke Beyreuther, Alexander Haussmann, and Lukas Eng — Institut für Angewandte Physik, TU Dresden, Nöthnitzer Str. 61, 01187 Dresden

Cherenkov second harmonic generation (CSHG) microscopy poses a powerful new tool [1,2] for the 3D imaging of ferroelectric domain walls (DWs). Investigating $LiNbO_3$ crystals, 10-nm-thick Cr electrodes were deposited onto the samples. The z^+ side was grounded and a ramped potential applied to the z^- side. When increasing the field up to +4.0 kV/mm, laser-poled hexagonal domains were observed in real-time and *in-situ* to collapse into inclined, coned structures, forming highly conductive head-to-head DWs [3]. Consequently, the domain-wall current (DWC) increased by over 4 orders of magnitude, reaching values of >1 μA. A reversed poling field down to -3.6 kV/mm led to reversible and irreversible domain-shape recovery. Expansion of spike domains increased the DWC up to >1 mA.
The crystal symmetry of $BaTiO_3$ allows much more complex domain patterns [4], such as 90° domain walls. Their kinetics upon phase transition will also be discussed using 3D CSHG imagery.

[1] L. Wehmeier et al. *Phys. Status Solidi RRL* **11**, 1700267 (2017).
[2] T. Kämpfe et al. *Phys. Rev. B* **8**, 035314 (2014).
[3] C. Godau et al. *ACS Nano* **11**, 4816 (2017).
[4] J. Döring et al. *J. Appl. Phys.* **120**, 084103 (2016).

KFM 10.3 Tue 10:00 H47

Tuning ferroelectric phase transition temperatures in epitaxial $K_xNa_{1-x}NbO_3$ thin films — •Leonard von Helden[1], Laura Bogula[1], Pierre-Eymeric Janolin[2], Michael Hanke[3], Martin Schmidbauer[1], and Jutta Schwarzkopf[1] — [1]Leibniz Institute for Crystal Growth, Berlin, Germany — [2]Laboratoire SPMS, CNRS-École Centrale Paris, France — [3]Paul-Drude-Institute for Solid State Electronics, Berlin, Germany

$K_xNa_{1-x}NbO_3$ is a promising material for, e.g., surface acoustic wave (SAW) sensors based on ferroelectric thin films. For these systems a strong enhancement of SAW transmission coefficients in the vicinity of phase transition temperatures has been reported, recently.[1] Hence, it is desirable to deliberately tune those phase transitions.

Here, we present a first systematic study in which ferroelectric phase transition temperatures in epitaxial $K_xNa_{1-x}NbO_3$ films could be altered by choice of different (110) oriented rare earth scandate substrates and variation of the K-to-Na ratio in the film. Sample preparation was conducted by liquid delivery metal organic vapor phase epitaxy (MOVPE). Our results reveal the possibility to continuously shift the ferroelectric-ferroelectric transition between monoclinic M_C and c-phase by about 400 K via application of compressive strain. The phase transition was investigated in detail by temperature dependent piezoresponse force microscopy (PFM), X-ray diffraction (XRD) and laser interferometry.

[1] S. Liang et al., Appl. Phys. Lett. 113, 052901 (2018)

KFM 10.4 Tue 10:15 H47

Transient depolarizing field effects leading to domain formation in the ultrathin regime — •Nives Strkalj[1], Gabriele De Luca[1], Marco Campanini[2], Shovon Pal[1], Jakob Schaab[1], Chiara Gattinoni[1], Nicola A. Spaldin[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]EMPA, Switzerland

A major challenge for the ferroelectric-based device miniaturization is to stabilize a robust polarization. In the ultrathin regime, however, the interface-related effects can drastically alter the polarization behavior and in extreme case lead to annihilation of the ferroelectric state. Because the ferroelectric layers are usually grown below their Curie temperature, their polarization state is set during the heterostructure growth. We thus track the evolution of polarization state using in situ optical second harmonic generation [1]. Taking $SrRuO_3$-$BaTiO_3$-$SrRuO_3$ capacitor heterostructure as a model system, we observe an abrupt domain formation leading to a net polarization quench during the top electrode deposition. We show a reduced conductivity in the ultrathin regime of the top electrode, leading to an inferior charge screening efficiency and therefore transient depolarizing field enhancement [2]. We demonstrate a healing route to the single domain state by post-growth thermal annealing above the strain-engineered Curie temperature. Our in-situ approach addresses transient electrostatic effects during the deposition and sheds light on the emergence of complex domain architectures in ferroelectric superlattices. [1] G. De Luca et al. Nat. Commun. 8, 1419 (2017) [2] N. Strkalj et al. (submitted)

KFM 10.5 Tue 10:30 H47

Deconvoluting conductance contributions at charged ferroelectric domain walls — •Theodor Secanell Holstad[1], Donald Malcolm Evans[1], Didrik René Småbråten[1], Joshua Agar[2], Stephan Krohns[3], Zewu Yan[4], Edith Bourret[4], Sverre Magnus Selbach[1], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology, Norway. — [2]Department of Materials Science and Engineering, University of Lehigh, USA. — [3]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany. — [4]Materials Sciences Division, Lawrence Berkeley National Laboratory, USA.

Ferroelectric domain walls are spatially mobile interfaces that naturally occur in materials that develop a spontaneous electric polarization. Because of their unique electronic properties, such walls hold great promise as functional 2D systems, but the characterization of their intrinsic transport properties remains a challenging task. Here, we combine scanning probe microscopy (SPM) with machine learning to gain new insight into the local electronic domain wall properties and to enhance the informational value of local conductance measurements. As a model case, we study the transport at ferroelectric domain walls in $(Er_{0.99}, Zr_{0.01})MnO_3$: At low voltages, head-to-head domain walls appear to be conducting. At higher voltages, however, the same domain walls are insulating. Using machine learning, we disentangle different conduction contributions and explain these seemingly contradictory results, highlighting how machine detection enhances the SPM output.

KFM 10.6 Tue 10:45 H47

Interplay of domain structure and phase transitions and its impact on functional responses — •Anna Grünebohm[1] and Madhura Marathe[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institut de Ciència de Materials de Barcelona, Spain

It is well established that the domain structure of ferroelectrics depends on crystal structure as well as the elastic and electric boundary conditions. However, the knowledge on the interplay of domain structure and structural phase transitions is incomplete. In this *ab initio* based study we focus on the domain structure at the tetragonal to orthorhombic phase transition in $BaTiO_3$ which has been less studied than the high temperature paraelectric to ferroelectric transition [1]. In particular, we show how domain engineering may allow to reduce the thermal hysteresis of the transition and how this allows to optimize functional responses such as the electrocaloric effect.

[1] T. Limboek and E. Soergel, Appl. Phys. Lett. **105**, 152901, 2014

Break

KFM 10.7 Tue 11:35 H47

Electric-field poling of an improper ferroelectric — Alexander Ruff[1], Jakob Schaab[2], Manfred Fiebig[2], Dennis Meier[3], and •Stephan Krohns[1] — [1]Experimental Physics V, Center for Electronic Correlation and Magnetism, University of Augsburg, Augsburg 86159, Germany — [2]Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [3]Department of Materials Science and Engineering, Norwegian University of Science and Technology

Manipulation of domains within ferroelectric semiconductors has attracted attention in recent years for potentially allowing domains and domain walls to be used as functional elements in nanoelectronics. Hexagonal manganites have shown particular potential because of their unusual, improper ferroelectric properties. Here, we provide an electric-field poling study of h-$ErMnO_3$. From a detailed dielectric analysis [1], we deduce the temperature- and frequency-dependent range for which single-crystalline h-$ErMnO_3$ exhibits purely intrinsic dielectric behavior [2]. In this temperature range, the ferroelectric switching kinetics, which is mainly driven by domain-wall motion, is investigated without superimposing extrinsic contributions. Controlling the domain walls via electric fields will bring us an important step closer to their utilization in domain-wall-based electronics [3].

[1] E. Ruff et al., Phys. Rev. Lett. 118, 036803 (2017).
[2] A. Ruff et al., Appl. Phys. Lett. 112, 182908 (2018).
[3] J. Schaab et al., Nature Nanotechnology, 13, 1028 (2018).

KFM 10.8 Tue 11:50 H47

Local manipulation of improper ferroelectric domains in $YMnO_3$ using scanning probe microscopy at low temperatures — •L. Kuerten[1], P. Schoenherr[1], S. Krohns[2], D. Meier[3], E. Pomjakushina[4], K. Conder[4], Th. Lottermoser[1], and M. Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Experimental Physics V, University of Augsburg — [3]Department of Materials Science and Engineering, NTNU, Trondheim — [4]Laboratory for Scientific Developments and Novel Materials, PSI, Villigen

In hexagonal manganites, the conductivity can differ by orders of magnitude between ferroelectric domains and domain walls. In order to utilize this technological potential, control over the domain wall position and orientation is necessary. In $YMnO_3$, switching of the bulk polarization has been achieved at low temperatures using co-planar electrodes. However, the microscopic mechanism of domain switching and the role played by domain wall motion and domain nucleation are still unknown. In particular, the multi-domain state of the surface appears unaffected when observed at room temperature before and after switching. Here, we investigate the microscopic mechanism of domain manipulation in situ at low temperature using piezoresponse force microscopy (PFM). By applying DC voltages to the PFM tip, we reveal signatures of polarization reversal at the sample surface indicating local domain switching. However, charge injection via the tip also plays a crucial role, which is demonstrated for regions on the nanometer scale. These charged regions remain stable for days at low temperatures, but vanish for increased temperatures.

KFM 10.9 Tue 12:05 H47

Charge-carrier localization at ferroelectric domain walls in $BiFeO_3$ — •Sabine Körbel and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

$BiFeO_3$ is a prototype material for investigating the photovoltaic effect in ferroelectrics, and it has been suggested that ferroelectric domain walls in $BiFeO_3$ and other ferroelectrics are beneficial for separating charge carriers.

In order to elucidate the role of the domain walls in the separation of photogenerated charge carriers, we studied electron and hole localization at ferroelectric domain walls in $BiFeO_3$, using density-functional theory.

In this talk we will discuss the localization behavior of separate electrons and holes and that of electron-hole pairs.

KFM 10.10 Tue 12:20 H47

Hall effect probed within highly- conducting ferroelectric domain walls in single-crystalline Lithium Niobate — •Henrik Beccard, Benjamin Kirbus, Alexander Haussmann, Elke Beyreuther, and Lukas M. Eng — Institute of Applied Physics, TU Dresden, Nöthnitzer-Str. 61, 01187 Dresden, Germany

Conducting domain walls (CDWs) in single-crystalline lithium niobate (LNO) are promising candidates for generating a manifold of possible nanoscale devices, especially based on electronic and optical properties [1]. Much works focused on improving imaging methods [2] and developing new devices utilizing CDWs. Moreover, novel protocols have been proposed that allow to tuned the domain wall current up to the mA regime [3]. Nevertheless, some of the most fundamental properties of charge carrier transport within these CDWs could not be measured accurately. We thus thoroughly inspected a single CDW in LNO using macroscopic Hall transport measurements. As a result, the mobility and charge carrier density of CDWs in LNO could be determined. Additionally, the influence of UV illumination on charge the charge carrier density within the wall was investigated. Utilizing Cherenkov second-harmonic generation, we were also able to record 3D images of these domain walls hence correlating [4] the Hall transport current to the local inclination of the domain within the LNO single crystal.

[1] G. Catalan et al. Rev. Mod. Phys. 84, 119 (2012).
[2] T. Kämpfe et al. Phys. Rev. B 8, 035314 (2014).
[3] C. Godau et al. ACS Nano 11, 4816 (2017).
[4] B. Wolba et al. Adv. Electron. Mater. 4, 1700242 (2017).

KFM 10.11 Tue 12:35 H47

Nonlinear optical crystals in tightly focused laser beams: A spatially resolved second-harmonic analysis in the focal plane — •Kai Spychala, Peter Mackwitz, Alex Widhalm, Gerhard Berth, and Artur Zrenner — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

In this work the nonlinear light-matter interaction in tightly focused optical systems is characterized. The study comprises the development of a theoretical model and a detailed experimental verification of the behaviour of second-harmonic (SH) generation in nonlinear optical crystals by focused light beams. We apply a direct imaging technique which records the spatial distribution of the second-harmonic signal in the back focal plane. Besides a profound understanding of the interaction which takes place in the focal region, the objective of this work is to develop the necessary numerical tool kit for in-depth data analysis. Our rigorous simulation, which is based on a vectorial description of the propagating light-fields, models the generated nonlinear signal in the case of (high NA) SH-microscopy and is verified via focal plane mapping in lithium niobate and potassium titanyl phosphate in a surface near regime. The calculations predict the symmetry and shape of the corresponding signals very well. In combination with experimental results it is now possible to extract information about the crystal symmetry. In this respect, our experiments verify the vectorial interaction processes, which lead to a specific and well-understood response in the SH signal.

KFM 11: Multiferroics and Magnetoelectric coupling I (joint session MA/KFM)

Time: Tuesday 14:00–15:45 Location: H37

Invited Talk KFM 11.1 Tue 14:00 H37

Magnetoelectric Inversion of Domain Patterns — •Naëmi Leo[1,2,3], Vera Carolus[4], Jonathan White[3], Michel Kenzelmann[3], Matthias Hudl[5], Pierre Toledano[6], Takashi Honda[7], Tsuyoshi Kimura[8], Sergey Ivanov[9], Matthias Weil[10], Thomas Lottermoser[2], Dennis Meier[11], and Manfred Fiebig[2] — [1]CIC nanoGUNE, Spain — [2]ETH Zürich, Switzerland — [3]Paul Scherrer Institute, Switzerland — [4]Bonn University, Germany — [5]Stockholm University, Sweden — [6]Université de Picardie, France — [7]High Energy Accelerator Research Organization (KEK), Japan — [8]University of Tokyo, Japan — [9]Karpov Insitute of Physical Chemistry, Russia — [10]TU Wien, Austria — [11]Norwegian University of Science and Technology, Norway

The global inversion of an inhomogeneous distribution of ferromagnetic or ferroelectric domains within a material is surprisingly difficult: Field poling creates a single-domain state, and piece-by-piece inversion using a scanning tip is impractical. Here we report inversion of entire domain patterns in the magnetoelectric material Co_3TeO_6 and the multiferroic material Mn_2GeO_4. In these materials, an applied magnetic field reverses the magnetization or polarization, respectively, of each domain, but leaves the overall domain pattern intact. This effect originates from a trilinear coupling term containing a "hidden" order parameter which retains the relative orientation of the field-driven and the observed order parameters. Such behaviour might also occur in other complex materials where coexisting order parameters are available for combination.

KFM 11.2 Tue 14:30 H37

Dielectric response of a vector-chiral magnetic ordering — •David Rivas Gongora[1], Martina Dragičević[1], Željko Rapljenović[1], Mirta Herak[1], Tomislav Ivek[1], Matej Pregelj[2], Andrej Zorko[2], Helmuth Berger[3], and Denis Arčon[2] — [1]Institute of Physics, Bijenička cesta 46, HR-10000 Zagreb, Croatia — [2]Jožef Stefan Institute, Jamova c. 39, 1000 Ljubljana, Slovenia — [3]Ecole polytechnique federale de Lausanne, CH-1015 Lausanne, Switzerland

β-TeVO4 is a zig-zag spin-1/2 quasi-one-dimensional system with a rich low-temperature phase diagram. Its vanadium spins interact through a nearest ferromagnetic (V-O-V) and next-nearest antiferromagnetic (V-O-Te-O-V) superexchange. The resulting frustration assisted by quantum fluctuations gives rise to three magnetic phase transitions [1]: paramagnetic to incommensurate spin density wave at TN1=4.65 K, followed by the so-called stripe phase under TN2=3.28 K, and lastly at TN3=2.28 K the system enters the vector-chiral ground state [2]. Interestingly, the complex magnetic landscape makes β-TeVO4 an ideal candidate for non-conventional magnetoelectric phases due to a symmetry which does not forbid the formation of electric dipoles [2,3]. We present the dynamic dielectric response of β-TeVO4 single crystal samples in the presence of a magnetic field and discuss it in the context of low-temperature magnetic ordering as a potentially multiferroic phase.

[1] Y. Savina et al. Phys. Rev. B 84, 104447 (2011). [2] M. Pregelj et al. Nature Communications 6 (2015), 10.1038/ncomms8255. [3] K. F. Wang et at. Adv. Phys 58, 321-448 (2009).

KFM 11.3 Tue 14:45 H37

Magnetoelectric Red-Ox switching of magnetism in iron oxide/iron nanostructures — •Jonas Zehner[1,2], Ivan Soldatov[1], Rudolf Schäfer[1], Sebastian Fähler[1], Kornelius Nielsch[1,2], and Karin Leistner[1,2] — [1]IFW Dresden — [2]TU Dresden - Institute of Material Science

Low power voltage-control of magnetism in metals can be achieved by electrical gating of magnetic nanostructures. Recent approaches focus on ion displacement and electrochemical reactions in oxide/metal films[1,2]. All solid state architectures suffer from a low ion mobility at room temperature (RT) and focus on ultrathin films so far[3]. Utilizing liquid electrolytes allows us to overcome these limitations and achieve large voltage induced changes of magnetization and anisotropy within several nanometer thick oxide/metal heterostructures[4]. In this case, typical alkaline battery electrolytes are used and merely 1V is applied to induce electrochemical RedOx processes in nanostructured FeOx/Fe films[4,5]. For FeOx/Fe nanoislands, ON/OFF switching of magnetization has been probed by two independent integral methods: in situ AHE and in situ FMR. A novel in situ Kerr set up has been developed, which allows us to observe also local changes of the magnetic microstructure during the RedOx operations. We find, for the first time, significant voltage-induced changes of the domain size in continuous FeOx/Fe thin films upon RedOx reactions. [1]Song et al., Prog. Mater Sci. 87, 33,2017, [2]Leistner et al., PRB 87, 224411,2013, [3]Bauer et al., Nat. Mater. 14, 174,2015, [4]Duschek et al. APL Mater.4, 32301,2016 [5]Duschek et al., J. Mater. Chem. C 6, 8411,2018

KFM 11.4 Tue 15:00 H37

Switchable one-way transparency via coupled magnetic and electric resonances — •David Szaller[1], Artem Kuz'menko[2], Alexander A. Mukhin[2], Alexey Shuvaev[1], Urmas Nagel[3], Toomas Rõõm[3], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

The strong anisotropy in the absorption of counter-propagating light beams approaching the limit of one-way transparency[1] became an intensively studied topic of simultaneously magnetic and polar (i.e. multiferroic) crystals, motivated by both the fundamentals of nonreciprocity and the possible information-technology applications. However, due to the limited understanding of the phenomenon the design of one-way transparent devices with specified optical spectrum is still an open task. On the basis of symmetry analysis and statistical physical considerations[2], it is possible to construct a minimal model of one-way transparency consisting of a pair of coupled magnetic and electric resonances. This model can be realized in certain multiferroic crystals and also in metamaterial structures, opening the path to custom-designed, electrically[3] or magnetically[1] switchable optical response.

[1] I. Kézsmárki, D. Szaller et al., Nat. Commun. 5, 3203 (2014)
[2] D. Szaller et al., PRB 87, 014421 (2013) and PRB 89, 184419 (2014)
[3] A. M. Kuz'menko, D. Szaller et al., PRL 120, 027203 (2018)

KFM 11.5 Tue 15:15 H37

Multiferroic domain inversion in $NaFeGe_2O_6$ — •Sebastian Biesenkamp[1], Dmitry Gorkov[1], Tobias Fröhlich[1], Jonas Stein[1], Karin Schmalzl[2], Wolfgang Schmidt[2], Yvan Sidis[3], and Markus Braden[1] — [1]Institute of Physics II, University of Cologne — [2]JCNS at ILL, Grenoble — [3]Laboratoire Léon Brillouin, CEA-CNRS, CEA/Saclay

Multiferroic materials attracted a considerable interest during the last decade, as the electric control of chiral magnetism implies a promising potential of applicability in the field of data storage devices or sensors. Fundamentally for all kind of applications is the knowledge of the relaxation times of multiferroic domain inversion, when switching applied external electric fields. Here we report time-resolved neutron scattering studies of the relaxations times in the multiferroic pyroxene $NaFeGe_2O_6$. They can be followed over a broad timescale, ranging from microseconds to several minutes and we found that the temperature and electric field dependence of the rise-times can be well described by a simple activation and Merz's law respectively.

KFM 11.6 Tue 15:30 H37

Temperature- and pressure-dependent optical measurements on the photo-response in multiferroic $BiFeO_3$ — •Fabian Meggle[1], Jihaan Ebad-Allah[1,2], Michel Viret[3], Jens Kreisel[4,5], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, Tanta University, 31527 Tanta, Egypt — [3]Service de Physique de l'État Condenseé, SPEC, CEA Saclay, CNRS, Université Paris-Saclay, 91191 Gif sur Yvette, France — [4]Physics and Materials Science Research Unit, University of Luxembourg, 4422 Belvaux, Luxembourg — [5]Department Materials Research and Technology, Luxembourg Institute of Science and Technology, 41 Rue du Brill, 4422 Belvaux, Luxembourg

$BiFeO_3$ exhibits three absorption features in the optical transmission spectrum between 1.0 and 2.2 eV during laser illumination.[1] These features were ascribed to excitons, which are proposed to be relevant for the ultrafast photostriction effect in $BiFeO_3$.[2] We studied the impact of low temperature and high pressure on the photo-induced features by using optical spectroscopy. Our temperature-dependent findings suppose a possible coupling between absorption features and lattice vibrations, whereas the spin degree of freedom might be also involved. The pressure-dependent measurements show a vanishing of the absorption features above 3.5 GPa, where $BiFeO_3$ is reported to undergo a phase transition from polar to a non-ferroelectric phase.[3] [1]Burkert et al., Appl. Phys. Lett. **109**, 182903 (2016); [2]Schick et al., Phys. Rev. Lett. **112**, 97602 (2014); [3]Belik et al., Chem. Mater. **21**, 3400 (2009)

KFM 12: Diamond II (joint session KFM/HL)

This session represents the physics, the production and applications of diamond and diamond related materials in the fields of dielectrics, electronics, high frequency techniques, GHz * THz * applications, mechanics and optics and biological applications as well. Defects in diamond have a large influence to the physical properties (e. g. NV-centers). Applications of diamond (single, poly-crystalline, UNCD, etc.) or related materials in technical systems are part of this session (Nuclear fusion applications, high frequency heating systems and material processing).

Chair: Theo Scherer (KIT)

Time: Wednesday 9:30–11:30 Location: PHY 5.0.20

KFM 12.1 Wed 9:30 PHY 5.0.20

Antibacterial propensities of UNCD with embedded silver nanodroplets — •Daniel Merker[1], Blagovesta Popova[2], Tobias Weingärtner[3], Thomas Bergfeldt[3], Gerhard Braus[2], Johann Peter Reithmaier[1], and Cyril Popov[1] — [1]Institute of Nanostructure Technologies and Analytics, Universität Kassel, Kassel, Germany — [2]Institute for Microbiology and Genetics, Universität Göttingen, Göttingen, Germany — [3]Institute of Applied Materials - Applied Materials Physics, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen, Germany

Thin diamond films are considered a promising material for coating of implants due to the mechanical and chemical durability in combination with biological compatibility. These properties are utilized to increase the lifetime and support the tissue integration of the implant. In this work we address another issue for implantation surgery, namely the danger of a bacterial infection. We prepared ultrananocrystalline diamond (UNCD) films with embedded silver nanodroplets to utilize the well-known antibacterial effect of silver ions. The changes in the morphology of the Ag nanodroplets depending on the conditions for their preparation was investigated by SEM and AFM and afterwards the composition of the resulting UNCD/Ag/UNCD layers was revealed by AES. The thickness of the capping UNCD layer can provide a control mechanism for the silver release. Therefore, we prepared samples with different capping layer thicknesses and investigated the amount of the released Ag into water with ICP-MS. Finally, we tested the layers against two bacteria: E. coli and B. subtilis.

KFM 12.2 Wed 9:50 PHY 5.0.20

Fabrication of Photonic Crystals Based on Planarized Nanocrystalline Diamond Films — •Julia Heupel, Johann Peter Reithmaier, and Cyril Popov — Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Utilizing nanocrystalline diamond (NCD) membranes deposited on silicon dioxide/silicon substrates, two-dimensional photonic crystal slabs were fabricated. For adjusting the NCD film thickness as well as for smoothening the intrinsically rough surface, a planarization process was developed and investigated regarding the NCD surface roughness and overall thickness reduction. This procedure comprises the application and polymerization of spin-on glass (SOG), forming an even surface layer on NCD, followed by an inductively coupled plasma reactive ion etching (ICP RIE) step. The photonic crystal structures were prepared in NCD samples with a planarized surface by means of electron beam lithography (EBL) and ICP RIE. By underetching of the sacrificial silicon dioxide layer with a hydrofluoric acid solution, the photonic crystals were made suspended in air. The effect of the variation of the exposure dose factors on the air hole diameter and shape in the photonic hexagonal lattice was examined. Different established recipes for dry etching of the silicon dioxide hard mask were studied and analyzed.

KFM 12.3 Wed 10:10 PHY 5.0.20

Improving magnetic nanoimaging using diamond-AFM-tips containing NV centers — •Arne Götze, Christoph Schreyvogel, Christian Giese, Claudia Widmann, Christoph Nebel, and Oliver Ambacher — Fraunhofer Institut für angewandte Festkörperphysik, Tullastraße 72, 79108 Freiburg, Germany

The fabrication of microelectronic components is approaching its physical limits. The gate length of modern transistors is now below 10 nm. Further miniaturization could lead to a reduction in costs and energy consumption, but as the devices become smaller the failure rate during production increases. Diamond-AFM-tips containing single NV centers that enable the imaging of the magnetic field strength with high sensitivity and spatial resolution even at room temperature will help uncover the reasons for this.

The focus of our work is to improve the performance of the NV-tips by producing diamond with high crystal quality and single NV centers. One goal is to create single NV centers close to the surface of the tip during CVD diamond growth by coating microstructured diamond tips with a thin layer of N-doped diamond. This will lead to longer spin coherence times and improved sensitivity compared to N-implantation. In order to better understand the N-doping and NV-formation processes we study the tips by using a confocal microscope and measuring 3D photoluminescence distributions. With this knowledge we are able to tailor the CVD processes and improve the measurement capabilities of magnetic imaging using diamond-AFM-tips.

Break 20 min

KFM 12.4 Wed 10:50 PHY 5.0.20

High nitrogen doping of CVD-diamond — •Julia Langer[1], Volker Cimalla[1], Verena Zürbig[1], Jan Jeske[1], Tim Eichhorn[2], Brett Johnson[3], Lutz Kirste[1], Christoph Schreyvogel[1], Arne Götze[1], and Oliver Ambacher[1] — [1]Fraunhofer Institute for Applied Solid State Physics, Tullastraße 72, 79108 Freiburg — [2]NVision Imaging Technologies GmbH, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [3]The University of Melbourne, Victoria 3010, Australia

Nitrogen-vacancy centers in diamond are studied extensively over the past decades. Their properties as quantum system feature a wide range of applicability. A new approach is the growth of high nitrogen doped CVD-diamond to create ensembles of nitrogen-vacancy centers for the purpose of measuring sensitive magnetic fields by laser threshold magnetometry. The challenge arises from keeping detrimental material effects low such as absorption and the incorporation of other magnetic moments. Within this study we investigate the nitrogen incorporation in CVD-diamond depending on nitrogen flow and growth rates. A comparison of growth series with different crystallographic oriented substrates shows new insight in the varying dependencies.

KFM 12.5 Wed 11:10 PHY 5.0.20

Thermoelectric generator made of tailored carbon allotropes — •Rudolf Borchardt, Timo Fromm, and Stefan Rosiwal — Chair of Materials Science and Engineering for Metals, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

A thermoelectric generator (TEG) can be used to recover energy by the conversion of waste heat into electricity. Therefore such generators use thermoelectric materials that directly generate electrical power from a temperature difference, without any moving parts. However common thermoelectric materials suffer from rarity, are toxic or are not temperature stable for a long time. Our aim is to develop new thermoelectric materials with good availability base on carbon allotropes. Here we show a TEG made out of three different kinds of carbon allotropes: micro crystalline diamond for fast thermal transport, as well as p-type nano crystalline diamond and n-type graphene nanowalls as the active materials for the energy conversion. The materials were produced as freestanding foils by chemical vapor deposition (CVD), and laser cut pieces of the foils were brazed with an active silver-titanium solder to fabricate the TEG. This TEG was tested up to a temperature difference of 200 K, resulting in an open circuit voltage of over 120 mV and an output power of 118 μW.

KFM 13: Microscopy, Tomography and Spectroscopy with X-ray Photons, Electrons, Ions and Positrons (joint session KFM/HL)

Chair: Enrico Langer (Technische Universität Dresden)

Time: Wednesday 9:30–12:10 Location: H47

KFM 13.1 Wed 9:30 H47

Phase Retrieval in X-Ray Near-Field Holography on Strong Objects — •Johannes Hagemann — DESY, Notkestraße 85, 22607 Hamburg

Lensless imaging techniques in the hard x-ray regime have become popular over the last two decades since no image forming optic is needed. Instead, the image is formed a posteriori numerically by reconstruction algorithms, which solve the ill-posed phase problem inherent to the measured data. Lensless techniques are demanding in terms of the radiation's properties used for illumination i.e. coherence, monochromaticity and fluence. The image reconstruction is often carried out under idealized assumptions of the probing illumination. The effects of failing these assumptions on the result of the reconstruction have been studied earlier in greater detail [1, 2]. For this work we study the effects of the object under reconstruction in the setting of x-ray near-field holography in greater detail. By numerical modelling and experiment we investigate the aspects of (i) the contrast of a hologram as a function of Fresnel number and phase shift, and (ii) the influence of strong objects on the image reconstruction process by phase retrieval. Our results indicate a maximum of contrast at Fresnel number $10^{-5} - 10^{-4}$.

[1] J. Hagemann and T. Salditt, "The fluence-resolution relationship in holographic and coherent diffractive imaging", J. Appl. Crystallogr., 50 (2017)

[2] J. Hagemann and T. Salditt, "The Coherence-resolution relationship in holographic and coherent diffractive imaging", Opt. Express, 26 (2017)

KFM 13.2 Wed 9:50 H47

X-ray phase-contrast micro-CT of biological tissues at a rotating anode source — •Jasper Frohn and Tim Salditt — Institut für Röntgenphysik, Göttingen

X-ray phase-contrast offers the possibility of enhancing the image contrast for low absorbing materials such as biological soft tissues. Applied in a tomographic setup, the phase-contrast can be utilized to investigate the structure of such samples in 3d in a non-invasive way. One method to realize phase contrast images is "propagation-based imaging (PBI)", which is based on the free space propagation from the sample to the detector. To perform PBI tomography inhouse, x-ray sources are required with a certain degree of coherence. We were able to establish a high resolving propagation-based phase-contrast tomographic setup at a microfocus x-ray source with a rotating copper anode in our laboratory. The 3d resolution is in the range of few micrometers, achieved with a high resolving detector in inverse geometry. Results will be presented and compared with the synchrotron tomography endstation "GINIX" (P10 at PETRA III/DESY).

KFM 13.3 Wed 10:10 H47

Atomic Resolution Differential Phase Contrast STEM investigations of electric fields in ZnO nanostructures — •Julius Bürger, Julia Weiss, Dennis Meinderink, Katja Engelkemeier, Wolfgang Bremser, Guido Grundmeier, Mirko Schaper, and Jörg K. N. Lindner — Paderborn University, Paderborn, Germany

Differential phase contrast (DPC) is one of the most promising techniques for future research with scanning transmission electron microscopy (STEM) giving rise to a new range of measurable material properties. By detecting phase gradients, i.e. by quantifying the electron beam deflection on a specimen site with a segmented detector, electric and magnetic field components can be detected. With an installed C_s-corrector the projected charge carrier distribution and electric fields can be estimated with a resolution much smaller than typical atomic distances. Zinc oxide (ZnO) is a piezoelectric material with excellent optical and semiconductor properties. Hence ZnO is promising for green energy harvesting converting mechanical stress into electric energy. For optimization of ZnO-based piezoelectric devices the operating principles and charge carrier displacements resulting from mechanical stress have to be understood down to the sub-nanoscale. In this presentation, the electric fields and charge carrier distributions of bent ZnO nanobelts, ZnO nanorods, nanowall network hollow body microspheres and ZnO-functionalized carbon fibers are revealed for the first time by DPC-STEM both at a macroscopic scale and with atomic resolution.

KFM 13.4 Wed 10:30 H47

Investigation of superlattice defects in magnetite mesocrystals via (S)TEM tomography — •Sebastian Sturm[1], Daniel Wolf[1], Julian Brunner[2], Elena Sturm[2], Axel Lubk[1], and Bernd Büchner[1] — [1]IFW Dresden, Deutschland — [2]FB Chemie, Universität Konstanz, Deutschland

Mesocrystals are a special sub class of colloidal crystals fulfilling the definition of a crystal on two different hierarchical levels, exhibiting single crystal like diffraction pattern in small angles as well as single or texture like pattern in wide angles. They are thus formed by assembly of single crystalline building blocks in a long range ordered superlattice with reoccurring specific crystallographic orientation of the crystalline building blocks. In order to characterize the growth mechanism and investigate the defect structure of 3D iron oxide self-assembled mesocrystaline materials, we employed electron tomography on specifically picked areas. This allows to resolve structural defects generated within the superlattice during the self-assembly process inside the crystal in three dimensions. In case of a mesocrystal with fcc superlattice, grown by dislocation driven crystal growth mechanism, the disintegration of a (111) plane intersecting screw dislocation defect structure, in two Shockley-partials has been resolved, very similar to traditional fcc crystals. The aim is to study the structure of these partials and relate it to the elastic properties of the mesocrystal.

KFM 13.5 Wed 10:50 H47

Thickness Determination on Molecular Thick Carbon Nanomembranes by HIM, XPS and EFTEM — •Daniel Emmrich[1], Annalena Wolff[2], Nikolaus Meyerbröker[3], Jörg K. N. Lindner[4], André Beyer[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Germany — [2]Queensland University of Technology, Australia — [3]CNM Technologies GmbH, 33607 Bielefeld, Germany — [4]Paderborn University, Germany

The Helium Ion Microscope (HIM) offers a lateral imaging resolution of 0.3 nm and is known for its excellent sub 10 nm milling capabilities [1]. While imaging with secondary electrons (SE) is well established for this microscope, the ion transmission signal attracts growing attention. Imaging in transmission offers additional information on membranes [2] and core shell nanoparticles [3]. Monolayer thin membranes have not been studied so far. Our systems are molecular thick Carbon Nanomembranes which are made of self-assembled monolayers that are cross-linked by low energy electrons [4]. We are able to measure dark field transmission of the same sample area at different acceptance angles using a SE conversion holder. The image contrast at different acceptance angles is compared to simulations and the membrane thickness is determined. We demonstrate our concept for different energies and thicknesses. We compare our results to standard techniques, e.g., XPS and EFTEM. [1] G. Hlawacek, A. Gölzhäuser (Eds.), Springer

Intl., Switzerland 2016. [2] A. R. Hall, Microsc Microanal 2013, 19, 740. [3] T. J. Woehl et al., Microsc Anal, 2016, 22, 544. [4] A. Turchanin, A. Gölzhäuser, Adv. Mater 2016, 28, 6075.

Break 20 min

KFM 13.6 Wed 11:30 H47

Positron Annihilation Studies using a Superconducting Electron LINAC — •Maik Butterling[1], Andreas Wagner[1], Maciej Oskar Liedke[1], Eric Hirschmann[1,2], Ahmed G. Attallah Elsherif[1], Reinhard Krause-Rehberg[2], and Kay Potzger[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany

The Helmholtz-Center at Dresden-Rossendorf operates several user beamlines for materials research using different techniques for positron annihilation spectroscopy. Two of them are being operated at a superconducting electron linear accelerator producing positrons via pair production from electron-bremsstrahlung. While one of the sources uses bremsstrahlung to directly generate positrons inside the sample of interest, in the second source (MePS), monoenergetic positrons with energies ranging from 500 eV to 25 keV are used for thin-film studies of porosity and defect distributions. The MePS beam line is currently complemented by a new in-situ end station (AIDA-2), where defect studies can be performed in a wide temperature range during thin film growth and ion irradiation. Developments as well as examples of recent experimental results at all facilities will be presented. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). The AIDA facility was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox) and through the Helmholtz Energy Materials Characterization Platform.

KFM 13.7 Wed 11:50 H47

The influence of trace element additions to Al-1.7 at.% Cu alloys: preservation of quenched-in vacancies and atomistic mechanisms supporting θ'-formation — •Torsten E.M. Staab[1], Frank Lotter[1], Uwe Mühle[2], Mohamed Elsayed[3], Danny Petschke[1], Thomas Schubert[4], Reinhard Krause-Rehberg[3], and Bernd Kieback[2,4] — [1]University Wuerzburg, Dep. of Chemistry, LCTM, Roentgenring 11, D-97070 Wuerzburg — [2]TU Dresden, Institute of Materials Science; Helmholtzstr. 7, D-01069 Dresden — [3]Martin-Luther-University Halle-Wittenberg; Faculty of Natural Science II; von-Danckelmann-Platz 3; D-06120 Halle — [4]Fraunhofer IFAM, Winterbergstrasse 28, D-01277 Dresden

Aluminium-copper alloys of the 2xxx type receive their strength during hardening at room or elevated temperature by the formation of copper-rich precipitates. They are responsible for the final mechanical properties of these alloys. Alloying small amounts of Cd, In or Sn influences the precipitation behavior as well as the final strength of Al-Cu alloys. Obviously, quenched-in vacancies are bound to trace element atoms in the aluminium matrix. Thus, the diffusion behavior of the copper atoms is influenced and the main type of the formed precipitates changes. For high-purity ternary alloys we investigate the interaction of copper atoms and trace elements (In, Sn, and Pb) with quenched-in vacancies. By employing Differential Scanning Calorimetry (DSC), Small Angle X-Ray Scattering (SAXS), Positron Annihilation Lifetime Spectroscopy (PALS) as well as Transmission Electron Microscopy (TEM) we obtain a comprehensive picture.

KFM 14: Postersession KFM

Time: Wednesday 16:00–18:30 Location: Poster C

KFM 14.1 Wed 16:00 Poster C

Fabrication of polymeric Whispering-Gallery-Mode resonators on tunable liquid crystal elastomer substrates using Deep-UV — •Lukas Mall, Simon Woska, Jannis Hessenauer, Carolin Klusmann, Tobias Siegle, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Whispering-Gallery-Mode (WGM) micro resonators offer huge potential for future applications in photonic devices. For many applications, a cheap and upscalable production is indispensable, which requires the development of reproducible and fast production processes. Polymers as resonator material open up the possibility to structure WGM resonators using Deep-UV lithography. This method allows parallel production of a large number of resonators at low costs.

Polymers also allow implementation of flexible photonic components like photonic molecules with a tunable inter-cavity gap. Such elements are achieved by structuring WGM resonators on flexible substrates. Especially promising substrates are made from liquid crystal elastomers (LCEs) which show thermally induced geometrical modifications.

In this contribution, we detail the production process of DUV-structured high-Q WGM resonators made from poly (methyl methacrylate) (PMMA) on LCE substrates. To overcome problems regarding stability, adhesion, process reliability etc., we employ stacked layers of several different polymers utilizing their very own characteristics.

KFM 14.2 Wed 16:00 Poster C

Tunable Whispering-Gallery-Mode Resonators made from Liquid Crystal Elastomers — •Jannis Hessenauer, Carolin Klusmann, Simon Woska, Matthias Migeot, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Whispering-Gallery-Mode resonators are promising building blocks for the realization of photonic devices, such as optical filters, switches or modulators. For a proper performance of these devices, a high tunability of their components is required. To achieve this, we propose resonators made from Liquid Crystal Elastomers (LCEs) as a novel way to tune their resonance wavelength over a wide spectral range.

Their working principle is based on a thermally induced reversible phase transition of LCEs from a nematic to an isotropic phase, which changes the resonator dimension, and therefore the resonance wavelength. LCEs are aligned through a silanization process and LCE resonators are structured using Direct Laser Writing (DLW). To induce the phase transition and the resulting shape deformation, the LCE resonators are doped with an absorber dye. The latter allows heating individual resonators via laser illumination.

To demonstrate reversible tuning of the resonance wavelength, the temperature dependent mode spectra of LCE resonators are evaluated. Heating of the resonators leads to a partly reversible redshift of more than one Free Spectral Range (FSR). The underlying increase in resonator radius can also be used to enable tunable coupling of adjacent resonators in photonic molecules.

KFM 14.3 Wed 16:00 Poster C

Wide Tunability of Coupled WGM Resonators Using Flexible Elastomer Substrates — •Simon Woska, Lukas Mall, Jannis Hessenauer, Carolin Klusmann, Tobias Siegle, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Whispering-Gallery-Mode (WGM) resonators are promising building blocks in photonic devices like optical filters or Coupled Resonator Optical Waveguides (CROWs). Contrary to common implementations of WGM resonators using silica as resonator material, we focus on polymers, which allow for a low-cost and upscalable production.

For plenty of photonic applications a tunable inter-cavity gap between different resonators is highly demanded. These properties can be achieved using flexible substrates, such as elastomers.

Flexible tuning of the inter-cavity gap has been successfully realized in our research group using a mechanically deformable elastomer as substrate. In this contribution, we propose a system based on substrates made from Liquid Crystal Elastomers (LCEs). Due to a phase transition at rather low temperatures, LCE undergoes a fully reversible change in dimension when heated. Thanks to this feature, LCE substrates exhibit several advantages compared to mechanically deformable substrates, including a more adjustable actuation.

We demonstrate the advantages of LCEs over the established mechanically deformable substrates and propose different approaches for the realization of such a tunable system. First results of coupled high-

Q WGM resonators structured on LCE substrates are presented.

KFM 14.4 Wed 16:00 Poster C

Non-Hermitian Defect States from Lifetime Differences — •Marti Bosch — TU Ilmenau, Ilmenau, Germany

The existence of non-hermitian defect states in optical systems is known for systems of coupled resonators with asymmetric backscattering. Here, we demonstrate that defect states in open optical systems can exist due to lifetime differences of counterpropagating modes without the need for asymmetric backscattering within the single resonator. We apply our findings to a finite system of coupled resonators perturbed by nanoparticles, in which we create an interface by inverting the orientation of the resonators in half of the chain. We compare a tight-binding approximation to a full-wave numerical simulation, showing that a system with spectrally isolated defect states can be implemented in a non-hermitian photonic device.

KFM 14.5 Wed 16:00 Poster C

Dielectric properties of P(VDF-HFP)/Ceramic Composites with Respect to Energy Storage Applications — •Marius Falkenstein[1], Tino Band[1], Till Mälzer[1,2], Hartmut S. Leipner[1], Stefan G. Ebbinghaus[1], Kathrin Dörr[1], and Martin Diestelhorst[1] — [1]Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06099 Halle, Germany — [2]enspring GmbH, Weinbergweg 23, 06120 Halle, Germany

Efficient energy storage is necessary for continuous power supply and mobile applications based on alternative energy sources. Because of their high power densities capacitors are interesting for this purpose. Ferroelectric P(VDF-HFP) is a promising storage material, since it exhibits a permittitvity much higher than commonly used polymers.

Within this work, we investigated the pure P(VDF-HFP) as well as nanocomposites of this polymer with powders of TiO_2 and $BaTiO_3$, two ceramics with high permittivities. The dielectric properties of these materials were analyzed with respect to the concrete demands for energy storage.

Besides the frequency dependence of the permittivity and loss at low fields we studied the behavior at high electric fields. Cyclic unipolar D-E-measurements at low frequencies were used to separate conductivity from dielectric properties and to determine the energy-density stored at the capacitors as well as breakdown fields. All these properties were characterized concerning their dependence on the concentration of the fillers and on temperature.

KFM 14.6 Wed 16:00 Poster C

A low cost potassium Prussian blue cathode for potassium ion batteries — •Chenglin Zhang, Yang Xu, Long Liu, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries (PIBs) have attracted increasing attention as a promising alternative to lithium-ion batteries. The hydrated potassium Prussian blue, K0.220Fe[Fe(CN)6]0.805, as a potential cathode material is first demonstrated in PIBs. The cathode exhibits a large reversible capacity within a high and flat potassiation potential of 3.1~3.4 V as well as a great cyclability. Electrochemical reaction mechanism analysis identifies the carbon-coordinated FeIII/FeII couple as redox-active site and proves structural stability of the cathode during charging/discharging. Furthermore, we present a PIB full-cell by coupling the Prussian blue nanoparticles with commercial carbon materials, which confirms the value of practical applications.[1] Considering the low cost and material sustainability, this work is of great significance for the future research and commercial applications of PIBs electrode materials.

[1] Chenglin Zhang, Yang Xu, Min Zhou, Liying Liang, Huishuang Dong, Minghong Wu, Yi Yang, and Yong Lei*[J] Adv. Funct. Mater. (2017):1604307.

KFM 14.7 Wed 16:00 Poster C

Polarization dependent vibrational properties of the ferroelectric $LiNbO_3$(0001) surfaces — •Mike Nico Pionteck, Christof Dues, Kris Holtgrewe, and Simone Sanna — Justus-Liebig-Universität Gießen

The investigation of the vibrational properties has recently become one of the most appealing tools for surface analysis. As Raman frequencies as well as selection rules are strongly related to the surface structure, they represent reliable criteria to identify, validate or rule out competing structural models [1].

In this work, we model the vibrational properties of ferroelectric $LiNbO_3$ surfaces from first principles. The $LiNbO_3$(0001) surfaces are both of technological and academic interest [2], however, the determination of the polarization direction is usually performed by destructive (chemical etching) or elaborate methods that exploit the pyroelectric or piezoelectric properties of the material. Our calculations reveal the presence of surface localized and polarization specific phonon modes of different symmetry in the frequency range between 30 and 960 cm^{-1} both at the positive and at the negative $LiNbO_3$(0001) surface. Calculated Raman intensities demonstrate that most of the surface localized modes are Raman active.

Raman spectroscopy can be thus considered as an easier to implement and non-destructive method to determine the polarity of $LiNbO_3$ surfaces.

[1] B. Halbig et al., Phys. Rev. B 97, 035412 (2018) [2] S. Sanna et al., J. Phys.: Condens. Matter 29, 413001 (2017)

KFM 14.8 Wed 16:00 Poster C

PSF-analysis of ferroelectric domain-walls in tightly focused regimes — •Peter Mackwitz, Kai Spychala, Alex Widhalm, Christof Eigner, Christine Silberhorn, Gerhard Berth, and Artur Zrenner — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

A combined experimental and numerical approach is applied to unravel the second-harmonic generation contrast mechanism of ferroelectric domain structures. The numerical calculation comprises a vectorial model of the imaging process. Experimentally we use a direct imaging technique which records the spatial distribution of the second-harmonic signal in the back focal plane. As the model depends on the optical properties of the material different scenarios of contrast mechanisms can be simulated and compared to the experimental data. With lithium niobate and potassium titanyl phosphate as model systems it turns out that many features of the nonlinear signatures of ferroelectric domain boundaries arise from destructive interference of phase-shifted wavelets. The phase is acquired due to the interaction of the focus with differentially poled domains, whose susceptibility tensor appears rotated by 180°. Another ingredient for the contrast are new tensor elements which do only occur at the domain walls. Furthermore, incoherence due to wall roughness plays an important role. Considering those three phenomena the contrast mechanism can be well described and predictions for other material systems become possible.

KFM 14.9 Wed 16:00 Poster C

Loss tangent mapping measurement on large area diamond discs - An approved quality control method — •Andreas Meier and Theo Scherer — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

As part of electron cyclotron development for heating of several fusion experiments (W7X, Asdex Upgrade, ITER) the characterization on bare and brazed polycrystalline chemical vapour deposition (CVD) diamond discs has been performed. An overview of dielectric properties particularly the loss tangent on about 70 different large area torus and gyrotron windows (Ø80mm - 140mm) realised with low power open resonators is shown. A spherical resonator is used for high-resolution measurements (loss tangent 10E-6) at the centre of the disc. Quality control measuring relating to the homogeneity has been realised with a hemispherical mapping setup (spherical and plane mirror). The results are given in statistic value D10 (10% of analysed area) D50 and D90. An additional optical characterisation method is intended for polished ITER torus discs to identify non-diamond like phase inclusions and cracks. The detection of these defect structures with a microscope is performed by an automatical scale-up mapping in all spatial directions. Size and location of defects are the basis for the quality assurance.

KFM 14.10 Wed 16:00 Poster C

Ultra-cold neutron reflectivity and storage properties of ultra-nanocrystalline diamond films — •Hadwig Sternschulte[1,2], Andreas Frei[2], Peter Geltenbort[3], Christopher Geppert[4], Christian Gorges[4], Petra Müschenborn[2], Stefan Wenisch[2], Stephan Wlokka[2], and Nicolas Wöhrl[5] — [1]Hochschule Augsburg, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Institut für Kernchemie, Johannes Gutenberg-Universität Mainz, Germany — [5]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Ultra-cold neutrons (UCN) have kinetic energies of <300 neV and are used for high precision experiments such as the search for a non zero electrical dipole moment or an accurate determination of the neutron life time. To avoid disturbances the set-up is not located directly at the UCN source and the UCN are transported via total reflection from the source to the experiment. Diamond is an excellent reflector for UCN due to the high atom density in combination with a large bound coherent scattering length and low loss cross sections. Ultra-nanocrystalline diamond (UNCD) films with a very low surface roughness independent of the film thickness can be grown on various 3D shaped substrates by chemical vapour deposition. Therefore they are promising candidates for UCN reflecting layers. In this work we present studies of the UCN reflection and storage properties of UNCD thin films grown on planar 6" Si substrates. The influence of the UNCD film morphology and composition on the reflectivity and storage properties will be discussed.

KFM 14.11 Wed 16:00 Poster C

Abbility of hard metal tools coated with nanocrystalline CVD diamond films to machine ceramic materials — •Jakob Grau[1], Hadwig Sternschulte[1], Nicolas Wöhrl[2], Harald Leiste[3], Sven Ulrich[3], David Gholar[1], Björn Backes-Eckert[1], Achim Rösiger[1], Ralf Goller[1], and Doris Steinmüller-Nethl[4] — [1]Hochschule Augsburg, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [3]KIT, Institute for Applied Materials, Eggenstein-Leopoldshafen, Germany — [4]CarbonCompetence GmbH, Wattens, Austria

Ceramic materials including ceramic composite materials are hard and brittle materials difficult to machine. In principle, milling processes with defined cutting geometries are advantageous to machine materials due the higher removal rates. But hard metal tools do not withstand the abrasion caused by the ceramic material. Protective coatings such as thin nanocrystalline diamond films grown by chemical vapour deposition (CVD) allowing the conformal coating of defined milling tool geometries are an option to enhance the tool life time. In this work hard metal tools in four different geometries coated with nanocrystalline diamond films with measured sp^2/sp^3 C concentration, grain size and stress state were applied to machine C/C-SiC CMC consisting of carbon fibres with SiC as matrix. During the milling process the forces acting on the tool were recorded. It was found that it is in principle possible to machine CMC with CVD diamond coated tools. The influence of the tool geometry on the life time of the tool and especially on the mechanism of the failing process will be discussed.

KFM 14.12 Wed 16:00 Poster C

Effect of synthesis method on properties of multiferroic lead iron niobate — •Nicole Bartek, Vladimir Shvartsman, and Doru Lupascu — Institute for Materials Science and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany

Lead iron niobate, Pb(Fe0.5Nb0.5)O3 (PFN), belongs to multiferroics. That means that at least two types of ferroic order: ferroelectric and antiferromagnetic, coexist. Dielectric and magnetic properties have been studied in PFN powders, ceramics, and thin films, and the phase transitions from paraelectric (PE) to ferroelectric (FE) at around 380 K and from paramagnetic to antiferromagnetic states at around 140 K are well known. There is a certain scattering of data across literature, related to different methods of preparing PFN ceramics. Our work is focused on the synthesis and characterization of PFN ceramics via different methods and the comparison of their properties. Microstructure was analyzed by using X-ray diffraction and scanning electron microscopy. Electric properties and PE/FE phase transition were studied by dielectric spectroscopy and polarization hysteresis loop measurements. Magnetism and magnetoelectric properties were studied by vibrating sample magnetometry. Optical properties and band gap were investigated through Raman and UV-vis spectroscopy in dependence of temperature.

KFM 14.13 Wed 16:00 Poster C

Ba and Mn co-Doped Bismuth Ferrite ($BiFeO_3$) Nanoparticles: Tailoring the Multiferroic Features Through Phase Transformation — •Astita Dubey, Marianela Escobar, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

Multiferroic Bismuth Ferrite (BiFeO3; BFO) Nanoparticles (NPs) are noteworthy suitable materials for spintronics and memory devices due to their advantageous ferroelectromagnetic properties at room temperature. The research on BFO NPs is getting much attention due to enormous magnetic and photocatalytic behavior than their bulk counterparts. We reported systematic study of phase transition and impact on the multiferroic properties due to doping of Ba and Mn in pristine BFO NPs (BixBa1-xFeyMn1-yO3). Crystalline doped NPs sized 30-50 nm exhibit higher crystallographic symmetry from rhombohedral (R3c) to orthorhombic (Pbnm) with enhanced size induced magnetization as well as decrement in impure phases. All NPs were synthesized by wet chemical route (modified sol-gel and hydrothermal) and characterized via UV-VIS absorption spectroscopy, XRD diffraction, TEM, EDX, SEM, Impedance dielectric spectroscopy and Magnetic force microscopy.

KFM 14.14 Wed 16:00 Poster C

Substrate dependant crystalline phases of $TmFeO_3$ thin films — •Sven Becker, Mathias Kläui, and Gerhard Jakob — Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

$TmFeO_3$ (TFO) has orthorhombic structure in bulk and does not show ferroelectric polarization. S.-J. Ahn [1] has demonstrated that TFO grows in a hexagonal phase on Al_2O_3 substrates, which imposes mulitferroic properties. In this work we prepare TFO thin films on various substrates by pulsed laser deposition and observe both orthorhombic as well as hexagonal phase of TFO depending on the choice of substrate material. In a second step we evaluate the possibility to use TFO as a purely antiferromagnetic random access memory. Kosub [2] has shown this approach using Cr_2O_3. The antiferromagnetic state of multiferroic material is read out by anomalous hall effect in a platinum top layer. [1] S.-J. Ahn et al., J. Mater. Chem. C **4**, 4521(2014) [2] T. Kosub et al., Nat. Comm. **8**, 13985 (2017)

KFM 14.15 Wed 16:00 Poster C

Resistive switching of $La_{0.7}Sr_{0.3}MnO_3/PbZr_{0.2}Ti_{0.8}O_3/Pt$ heterostructures — •Tino Band[1], Diana Rata[1], Robert Roth[1], Stefan G. Ebbinghaus[2], and Kathrin Dörr[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06099 Halle, Germany — [2]Institute of Chemistry, Martin Luther University Halle-Wittenberg, Kurt-Mothes-Straße 2, 06099 Halle, Germany

Electric fields in the order of 1-10 $MV\,cm^{-1}$ are often applied at thin ferroelectric films to study electron tunneling through a barrier. An electric field of this magnitude can drive processes which are of electrochemical nature and change the chemical composition in or near the tunnel barrier. Until now, ferroelectric $PbZr_xTi_{1-x}O_3$ (PZT, x=0-0.5) has rarely been studied with respect to ionic-driven resistive switching. We present results on PZT films (x=0.2) grown on $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3(001)$ showing resistive switching like $SrTiO_3$. We have confirmed this for 3 nm thick PZT in nanoscale force microscopy measurements of current-voltage loops at fixed tip positions with subsequent detection of topographic changes. This experimental approach allows one to correlate ionic processes with the features of current-voltage characteristics. As second example, current-voltage characteristics of 10 nm thick PZT with $40\times40\,\mu m^2$ Pt top electrodes have been studied. Both types of measurements reveal resistive switching driven by ionic motion in large electric fields.

KFM 14.16 Wed 16:00 Poster C

Interplay of oxygen vacancies and conductance in $SrMnO_3$ ferroelectric domain walls — •Lokamani Lokamani[1], Peter Zahn[1], and Sibylle Gemming[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany

Strontium manganate ($SrMnO_3$), a perovskite polymorph, exhibits cubic structure at high temperatures, which transforms under tensile strain into a G-type-antiferromagnetic (G-AFM) antiferrodistortive polar phase in the plane parallel to the substrate[1]. Recently, ferroelectric domains have been observed experimentally in 20nm thin films of $SrMnO_3$ under 1.7% tensile strain on (001)-oriented LSAT grown in an oxygen-deficient atmosphere[2]. Strikingly, the individual domains show different conductance features, whereas the domain walls were found to be electrically insulating, rendering the domains to form stable nano-capacitors with high charge retention times.

Here, we present a detailed first-principle investigation of the domain wall formation in strained $SrMnO_3$, the electronic properties and the influence of oxygen vacancies on the 2D-electron gas at the polar domain walls. Preliminary results on the migration energetics of the oxygen vacancies will be presented.

[1] J. H. Lee et al., PRL 104, 207204 (2010)
[2] C. Becher et al., Nature Nanotechnology 10, 661 (2015)
Funding by VI Memriox(VH-VI-422) & Nanonet(VH-KO-606)

KFM 14.17 Wed 16:00 Poster C

Enhancing magnetoelectric coupling in 0-3 composite ceramics — •Doru C. Lupascu[1], Muhammad Naveed-Ul-Haq[1], Shvartsman Vladimir V.[1], Salamon Soma[2], Weber Samira[2], Wende Heiko[2], Labusch Matthias[3], and Schröder Jörg[3] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg- Essen, Universitatsstraße 15, 45141 Essen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [3]Institute for Mechanics, Department of Civil Engineering, University of Duisburg-Essen, Universitatsstraße 15, 45141 Essen, Germany

It is well established that the highest magnetoelectric coupling can be achieved for systems that use a mechanical resonator at or near resonance typically realized as 2-2-layered devices of a magnetostrictive phase and a piezoelectric material. Statically, the coupling must, nevertheless, not be so high, because amplitude enhancement at high mechanical quality factor can be enormous. We show that statically also 0-3 composites show considerable coupling. It is in particular advantageous to seek for a material combination that uses not necessarily large absolute magnetostriction and electrostrictive strain, but rather places the system at external fields, where the largest changes of each arise. A very significant improvement of magnetoelectric coupling was achieved when combining NiFe2O4 with a relaxor ferroelectric system based on (Ba,Ca)(Zr,Ti)O3. [1] M. Naveed-Ul-Haq, et al., Acta Materialia 144 (2018) 305 - 313

KFM 14.18 Wed 16:00 Poster C

The K-edge of Hexagonal Boron Nitride Revisited: Effects of Electron-phonon Coupling on the Absorption Spectrum — •Ferenc Karsai[1], Moritz Humer[2], Georg Kresse[1,2], Espen Flage-Larsen[3], and Peter Blaha[4] — [1]VASP Software GmbH, Sensengasse 8, Vienna, Austria — [2]University of Vienna, Department of Physics, Sensengasse 8, Vienna, Austria — [3]SINTEF Materials and Chemistry, Oslo, Norway — [4]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, Vienna, Austria

The theoretical X-ray absorption near-edge structure for the boron and nitrogen K-edge in hexagonal boron nitride is investigated in great detail employing density-functional theory calculations. Electron-hole interactions are described using the super-cell core-hole method and the Bethe-Salpeter equation. The calculations are carried out with two different codes, the VASP and the WIEN2k code employing the projector augmented wave and the full-potential linear augmented planewave method, respectively. Close agreement between spectra obtained from the two codes is found. However, the boron spectrum obtained in the absence of vibrational effects shows significant deviations from experiment. Particularly the calculated spectrum yields a single 2p sigma peak and hence totally fails to describe the experimentally observed double-peak structure. By the inclusion of electron-phonon interactions the theoretical 2p sigma peak observes a significant splitting. We incorporate these effects in our calculations fully parameter-free and ab initio using a one-shot sampling method and obtain excellent agreement with experiment.

KFM 14.19 Wed 16:00 Poster C

Structural and many-body effects in the linear and nonlinear optical response of $KNbO_3$ from ab initio calculations — •Falko Schmidt, Arthur Riefer, Wolf Gero Schmidt, and Arno Schindlmayr — Universität Paderborn, Paderborn, Germany

Potassium niobate ($KNbO_3$), a perovskite-structure ferroelectric, is widely employed in nonlinear optical applications. Because of its small unit cell, $KNbO_3$ is ideally suited to assess the performance of *ab initio* computational methods for nonlinear optical materials that can be extended to related, more complex materials. After a careful structure optimization, we calculate the linear and nonlinear optical response of $KNbO_3$ in the structurally simple cubic and tetragonal as well as the technologically important orthorhombic phase. While the Kohn-Sham band structure is corrected by GW self-energy shifts, excitonic effects are incorporated by solving the Bethe-Salpeter equation for the linear response. We find a strong dependence on the underlying atomic structure, especially for nonlinear optical spectra. The latter are also strongly affected by the band corrections from the GW approximation.

KFM 14.20 Wed 16:00 Poster C

Influence of quasiparticle and excitonic effects on the optical signatures of polarons and bipolarons in $LiNbO_3$ from *ab initio* calculations — •Falko Schmidt, Uwe Gerstmann, Arno Schindlmayr, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

Lithium niobate ($LiNbO_3$), a perovskite-structure ferroelectric, is widely employed in nonlinear optical applications. A direct comparison between experiment and theory is difficult, however, as this material exhibits a large concentration of intrinsic defects, which strongly influence the optical properties. To reproduce the so-called polaron and bipolaron peaks found in the experimental measurements of the absorption spectrum, we test different possible defect types embedded in a supercell. Starting from density-functional theory, we correct the Kohn-Sham band structure by GW quasiparticle shifts, while excitonic effects are incorporated by solving the Bethe-Salpeter equation. The results shed light on the possible origin of the observed peaks due to the different optical characteristics of the investigated defects.

KFM 14.21 Wed 16:00 Poster C

Quasi particle energies and optical properties of $KTiOPO_4$ calculated by first principles — •Sergej Neufeld, Adriana Bocchini, Uwe Gerstmann, Arno Schindlmayr, and Wolf Gero Schmidt — Universität Paderborn

Potassium titanyl phosphate ($KTiOPO_4$, KTP) is a ferroelectric material that has been utilized in numerous applications based on non linear optics and photonics.

Despite its widespread use, many KPT properties are insufficiently understood. This concerns, e.g. its band gap. Earlier theoretical studies are based on the single-particle picture and report values between 3.0 - 4.0 eV.

In this work, quasiparticle and excitonic effects on the band structure and dielectric function of stoichiometric KTP are studies within the GW0 approximation and by solving the Bethe Salpeter equation (BSE), respectively. It is found that quasiparticle effects open up the band gap to about 5.3 eV. The solution of the BSE yields exciton binding energies of the order of 1.5 eV. Calculations that include both quasiparticle and excitonic effects are found to account for the measured reflectivity.

KFM 14.22 Wed 16:00 Poster C

Transient absorption in iron-doped lithium niobate induced via tailored optical excitation paths — •David Brinkmann, Simon Messerschmidt, Andreas Krampf, Laura Vittadello, and Mirco Imlau — School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany

Doping of lithium niobate (LN) with transition metals, e.g. iron, has a strong impact on the optical properties as well as transport dynamics of optically excited charge carriers. The most of these effects were investigated by the technique of light-induced absorption (LIA) and pump-wavelengths in the visible spectral range preferring a charge transfer from Fe^{2+} to Nb^{5+} (D-band). In this study, we present LIA data measured under three different, tailored experimental conditions, i.e., a combination of different iron concentrations and Fe^{2+}/Fe^{3+} ratios in the crystal and an excitation wavelength in the UV spectral range (355 nm), with the aim to excite the sample via a charge transfer from O^{2-} to Fe^{3+} (C-band) or O^{2-} to Nb^{5+} (LN band-edge). Our results demonstrate clearly the possibility to alter the induced absorption both in the spectral range and relaxation time by order of magnitudes as a function of the excitation paths. All of our observations can be explained straightforwardly by using the excitation and recombination model proposed by Messerschmidt *et al.* [J. Phys.: Condens. Matter (2018) doi: 10.1088/1361-648X/aaf4df] which is based on the presence of both, small polarons as well as self-trapped excitons trapped at different lattice positions. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 14.23 Wed 16:00 Poster C

Temperature-dependent fs-pulse-induced luminescence of lithium niobate — •Janina Ringel, Andreas Krampf, Simon Messerschmidt, and Mirco Imlau — School of Physics, Osnabrueck University, Barbarastr. 7, 49076 Osnabrueck, Germany

Temperature-dependent luminescence of lithium niobate (LN) after fs-pulse illumination is investigated over a large temperature range, i.e., from 10–300 K. As the luminescence intensity decreases exponentially above 100 K, a continuous broadening and shift of the peak position can be observed. Therefore, self-trapped excitons which are accounted for the low-temperature luminescence of LN (Blasse, Mat. Chem. Phys. **14**, 1986) are present at room temperature as well. However, above 200 K an unexpected deviation of the temperature-dependent emis-

sion peak from the well-known Varshni-behavior is found. Expressions based on phonon emission and absorption governed by Bose-Einstein statistical factors fail to describe the observed dependency of the peak position and halfwidth, as well (Viña, Phys. Rev. B **30** (4), 1984). We therefore discuss the presence of a second luminescing center.
Additional time-resolved luminescence data are presented. The decay time decreasing exponentially above 100 K limits the maximum temperature to 180 K. We show that a total of three different decay dynamics are present in heavily Mg-doped samples. Two of them, recently investigated (Kämpfe, Phys. Rev. B **93**, 2016), are lying in the μs–ms and second range, respectively. Here, both are observed for a larger temperature range. Financial support by the DFG (IM37/11-1, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 14.24 Wed 16:00 Poster C

Charge carrier dynamics in $SrTiO_{3-\delta}$ — •Thomas Schunkborn[1], Christoph Grams[1], Kamran Behnia[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Laboratoire Physique et Etude de Matériaux (UMR 8213 CNRS-ESPCI), PSL Research University, Paris, France

Pristine $SrTiO_3$ is a quantum paraelectric insulator with a comparatively high permittivity of $\sim$300 already at room temperature. Upon cooling, its dielectric constant ε' shows a steep rise, usually indicative of a ferroelectric phase transition. In $SrTiO_3$, this transition is suppressed by quantum fluctuations and instead a saturation value of ε' of the order of 10^4 is observed [1].

By reducing the oxygen content, charge carriers are introduced in $SrTiO_{3-\delta}$. Due to the large effective Bohr radius caused by the high permittivity, the material becomes conducting and even superconducting at unusually low charge carrier densities [2].

Using broadband dielectric spectroscopy, we investigate the conductivity of samples with different charge carrier densities depending on frequency and temperature to show an evolution from insulating ($\sigma' \approx 0$), to variable-range-hopping ($\sigma' \propto \omega^s$), to Drude-metal ($\sigma' \propto \omega^{-2}$) behavior.

Funded by the Deutsche Forschungsgemeinschaft via CRC 1238 and HE3219/6-1.

[1] R. Viana *et al.*, Phys. Rev. B **50**, 601 (1994)
[2] X. Lin *et al.*, Phys. Rev. X **3**, 021002 (2013)

KFM 14.25 Wed 16:00 Poster C

Time-resolved multicolor emission of harmonic nanoparticles via nonlinear frequency mixing — •Jan Klenen[1], Christian Kijatkin[1,2], Bjoern Bourdon[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Osnabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

Harmonic nanoparticles (HNPs) attract growing interest owing to their unique nonlinear optical (NLO) properties such as loosened phase-matching conditions. Motivated by applications in the fields of multiphoton microscopy and holography, thorough investigations on harmonic generation have been sparked. Nevertheless, reports on three-wave mixing processes in HNPs are scarce, especially with respect to temporal evolution, even though this approach may pave the way towards ultrafast sub-ps time-resolved microscopy and fluorescence upconversion spectroscopy (FLUPS). Using two nondegenerate femtosecond pulses, transient nonlinear frequency mixing (FM) processes are studied comprehensively in nanoscaled lithium niobate powder plaques and thin particle layers using NLO diffuse reflectometry [C. Kijatkin *et al.*, *Photonics* **2017**, *4*(1), 11]. A particular focus is given to the spectrotemporal analysis of multicolor emission exceeding the visible spectral range. Further assessment is performed in regard to FLUPS through upconversion of a picosecond pulse in order to test the viability of HNP powders as an alternative to crystalline media as a flexible material for different scalings and wavelengths. Financial support (DFG INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 14.26 Wed 16:00 Poster C

Investigation of an inline detection system for conversion coatings on aluminum alloys by means of specular reflectance — •Yannic Toschke[1], Jörg Rischmüller[1], Mirco Imlau[1], Simon Podendorf[1], Mareike Schlag[2], Kai Brune[2], and Hauke Brüning[2] — [1]School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany — [2]Fraunhofer IFAM, Wiener Strasse 12, 28359 Bremen, Germany

In accordance with Europe*s REACH agreements 2017 (Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals) restrictions of conversion coatings for metallic surfaces containing Cr^{+6} have further led to investigations of suitable alternatives. Reasoning behind those restrictions were the confirmed carcinogenic properties of hexavalent Chromium. One possible approach comparable in its corrosion inhibition and function as adhesion agent consists of Cr^{+3} and Zr^{+4}. Precise control of the process parameters is crucial for the performance of any kind of coating. Therefore, an additional method for inline quality control is desired. In this study a reliable and non-destructive method based on specular reflectance will be discussed matching those requirements. Five different qualities of the given conversion coat (20-70 nm) were applied on two different aluminum alloys (AA3003 and AA6060) and investigated with REM, LIBS and corrosion tests. Differentiation between each coating and the uncoated substrate are shown. Correlation between the gathered measurements suggests that an affordable method for inline quality control was found. Prime influence seems to arise from the morphology of the coating.

KFM 14.27 Wed 16:00 Poster C

Zone-plate based soft X-ray microscopy with sub-10 nm resolution — Rainer H. Fink[1,2], Joshua Loroña Ornelas[1], •Andreas Späth[1], Jörg Raabe[3], Christian David[3], and Benedikt Rösner[3] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]CENEM, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland

Soft X-ray scanning transmission microspectroscopy (STXM) using Fresnel zone plates (FZPs) as focusing elements has developed into a routine technique for the investigation of semi-transparent thin film specimens. Routine operation of STXMs uses spatial resolution of around 30 nm, determined by the outermost zone width of the FZP. An elegant method to fabricate high-resolution FZPs has been introduced by doubling the line density obtained from the lithography step utilizing atomic layer deposition (ALD). We have recently prepared FZPs with line structures to about 7 nm, thus pushing the resolution limits into the sub-10 nm regime. We will report on the resolution tests of specific test samples, but also on technologically relevant specimens where the improvement in lateral resolution becomes inevitable. Determination of the spatial resolution was conducted using a two-dimensional Fourier shell correlation of two independent data sets. This yielded a real space resolution of $<$ 8 nm considering the half-bit criterion. The project achieved funding by the BMBF (project 05K16WED), within the EU-H2020 Research and Innovation Programme, No. 654360 NFFA-Europe, and by Marie Skłodowska-Curie grant No. 701647.

KFM 14.28 Wed 16:00 Poster C

Efficient Iterative Phase Reconstruction for X-Ray Near Field Holography — •Johannes Hagemann[1], Silja Flenner[2], and Imke Greving[2] — [1]DESY, Notkestraße 85, 22607 Hamburg — [2]HZG, Notkestraße 85, 22607 Hamburg

An iterative solver has always a drawback compared to a single step solution: it takes more time to compute. For large data sets as they occur for example in x-ray propagation-based phase-contrast tomography, this can be a hindering factor. On the other hand an iterative scheme can be the only way to get a meaningful reconstruction of the object under survey [1].

In this contribution we demonstrate an algorithmic improvements on the alternating projection algorithm for better convergence. With this algorithm we were able to recover the phases of a strongly phase shifting and absorbing multi material specimen. This specimen has been ivory which was partly coated with Gallium during the FIB preparation process for the measurement. The measurements were obtained at the nano-imaging endstation of beamline P05 at PETRA III, DESY.

[1] J. Hagemann, M. Töpperwien and T. Salditt, "Phase retrieval for near-field X-ray imaging beyond linearisation or compact support," Appl. Phys. Lett., 113 (2018)

KFM 14.29 Wed 16:00 Poster C

μ lenses in Silicon Carbide — •Fiammetta Sardi — 3 pysics institute, Stuttgart, Germany

Silicon carbide(SiC) is an appealing material due to its properties in the applications of quantum technologies. Its wide-band gap and highly developed fabrication techniques show great potential as a resource in quantum technology evolution.

Silicon Vacancy Defects hosted in the crystalline structure of SiC exhibit a long relaxation time at room temperature and a manageable coherence control on a single spin. Nevertheless, the high refractive index of the material leads to strong refraction and total internal reflection ending in deviation of the defects* photoluminescence at SiC-air interface.

A possibility to decrease this effect is the fabrication of shallow Solid immersion lenses (SIL) of a few micrometres in size on a SiC wafer, resulting in refractionless transmission of light along the SIL surface. Defects are supposed to be placed in the centre of the SIL for maximum enhancement of collected photoluminescence .

In this work, a scalable method for the fabrication for SILs in SIC is presented, using photo-lithography and reaction ion etching(RIE) to transfer SILs from the photoresist to SiC. For lenses with an NA=0.7, enhancements higher than 2.5 in the photoluminescence of defects has been achieved.

KFM 14.30 Wed 16:00 Poster C

On the effect of high current densities on thin iron-carbon alloy films — •Thomas Brede, Christine Borchers, Reiner Kirchheim, and Cynthia Volkert — Institut für Materialphysik, Georg-August-Universität, Göttingen, Deutschland

The recently discovered flash sintering method for preparing high quality oxide materials can be applied to the preparation of high performance nanocrystalline metals as well. Just as for the oxide materials, it is possible to use electric fields and currents to enhance densification of metal powders while limiting grain growth, however, the exact mechanism is still under discussion. The goal of our study is to understand how electric currents effect impurity redistribution and grain growth in fine grained metals.

Thin nanocrystalline iron films with high carbon concentrations are prepared as a model system and to compare with the behavior of nanocrystalline bulk samples. The thin film samples are heated and exposed to high current densities comparable to those experienced during the sintering process of bulk materials and the evolution of the microstructure, morphology and carbon concentration are investigated using electron microscopy. Extensive effects of the electrical current on C redistribution and grain growth are observed, including strong coupling between grain growth and C content and the formation of grains that are elongated along the direction of the current. The various microstructural observations will be summarized and possible explanations will be discussed.

KFM 14.31 Wed 16:00 Poster C

Mask-less, high aspect ratio, high resolution electron-beam-induced etching of diamond — •Vasilis Dergianlis, Martin Geller, Dennis Oing, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Diamond has attracted significant attention as a promising material for a broad range of emerging applications, such as host material for NV-centers in future quantum information technologies [1], or as ultrasensitive nano-sensors [2]. Structuring this extremely stable material is, however, highly challenging. First attempts have shown the possibility to use water vapor in combination with an electron beam [3], however only with a strong anisotropy of the etching process and a low-resolution in the μm-range.

In this contribution, we report on high-resolution etching of undoped, hydrogen-terminated, single crystalline diamond layers of <100> orientation without anisotropy in the etching process. We used a Scanning Electron Microscope (SEM) in a dual beam Focused Ion Beam (FIB) together with water vapor, which was injected directly onto the sample surface. Using this versatile and non-invasive technique, trenches with widths of only 10 nm were precisely etched into the diamond sample. Our results show the possibility of high-resolution mask- and resistless patterning of diamond for nano-optical and electronic applications.

[1] Dutt et al., Science **316**, 1312 (2007)
[2] Maze et al., Nature **455**, 644 (2008)
[3] Martin et al., Phys. Rev. Lett. **115**, 255501 (2015)

KFM 14.32 Wed 16:00 Poster C

Improved automatic proton beam writing — •Lukas Jäger, Alrik Stegmaier, and Hans Hofsäss — II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen Germany

Proton beam writing is a maskless lithographic technique using a focused high energy proton beam to pattern materials and create high aspect-ratio 3D structures. At the II. Institute of the University Göttingen a tandem accelerator with a beam line for proton beam writing is available. To control the beams position on the sample, the sample-holder can be moved by two piezo stages. First the beam shape is measured via a PIXE measurement on a Ni-grid. The beam shape can be used by a program to compute the near optimal movement of the sample-holder during irradiation. Instead of rasterizing the desired pattern, the program optimizes the irradiation pattern to enable the irradiation of more complex patterns. Recent advances in the software development improved stability, fail safety and accuracy of the irradiation process, including a newly automatic blanking system.

KFM 14.33 Wed 16:00 Poster C

Cu-poor region of the CuI phase diagram: An ab initio study — •Stefan Jaschik, Mário Rui Gonçalves Marques, and Miguel A. L. Marques — Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, D-06099 Halle (Saale), Germany

We studied the Cu-poor region of the phase diagram of CuI using both global structural prediction methods and cluster expansion techniques. We found that, at the level of the Perdew-Burke-Ernzerhof approximation to the exchange-correlation functional, there are ordered-defect compounds that are energetically favored with respect to pristine CuI. This may explain the large number of Cu vacancies that is usually found in experimental samples.

KFM 14.34 Wed 16:00 Poster C

Small bound polarons in $LiTaO_3$ — •Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

The optical response of many oxide crystals including the electro-optic material $LiNbO_3$ has been successfully explained by the presence of small polarons. The latter are quasiparticles formed when the interaction of a charge carrier with the surrounding lattice is strong enough to trap the charge carrier at essentially one lattice site. While different kind of small polarons have been described [1] and demonstrated [2] in $LiNbO_3$, much less is known concerning the isomorphic and isoelectronic $LiTaO_3$. Although the existence of small bound polarons might be expected due to the high lattice polarizability, the verification of this assumption is still missing. In this work we provide the atomistic description of small bound polarons $Ta_{Li}^{5+/4+}$ in $LiTaO_3$. The calculations performed within density functional theory with Hubbard corrections predict the large lattice relaxation of the oxygen ligands associated to the electronic capture at the antisite center, which can be interpreted as due to the polaron formation. The charge distribution is localized within essentially one unit cell and resembles the atomic Fe d_{z^2} orbitals, suggesting a scarce hybridization the Ta d orbitals.

[1] O. F. Schirmer et al., J. Phys.: Condens. Matter 21, 123201 (2009). [2] F. Freytag et al., Nature Scientific Reports 6, 36929 (2016).

KFM 14.35 Wed 16:00 Poster C

Plastic deformation in polycrystalline $BaTiO_3$ — •Marion Höfling[1], Pengrong Ren[2], Stefan Lauterbach[1], Xijie Jiang[1], Jurij Koruza[1], Till Frömling[1], and Jürgen Rödel[1] — [1]Department of Earth and Materials Science, Technische Universität Darmstadt, 64287 Darmstadt — [2]School of Materials Science and Engineering, Xi'an University of Technology, Xi'an, P.R. China

Oxides can exhibit dislocations with charged cores and charge-compensating surrounding layers. These dislocations are in general considerably more temperature stable than point defects and have been described as one-dimensional dopants. Some recent publications have demonstrated that changing the dislocation density can be used to tune individual material's properties, for example the ionic conductivity in TiO2 [1]. In this study we investigated the plastic deformation of polycrystalline BaTiO3 as a possible means to introduce dislocations into ceramics. The creep mechanisms of BaTiO3 were determined at different temperatures and stresses based on the power law exponents obtained from high-temperature uniaxial compression experiments and a first approximation for a deformation mechanism map was created. Several samples were successfully plastically deformed on the border of the diffusion-dislocation creep regime and the resulting effects on the ferroelectric and dielectric properties were examined. Transmission electron microscopy (TEM) and piezo force microscopy (PFM) were carried out to identify the influence of the creep experiments on the microstructure and the domain evolution.

[1] Adepalli et al. Phys. Chem. Chem. Phys., 2014, 16, 4942

KFM 14.36 Wed 16:00 Poster C

Pressure-induced amorphization of dynamically compressed and heated minerals by X-ray diffraction and electron microscopy — •Christoph Otzen[1], Hanns-Peter Liermann[1], and Falko Langenhorst[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institut für Geowissenschaften, Jena, Germany

Large planetary meteorite/asteroid impacts play a crucial role in the history of the Earth, traces of which can still be found in minerals today and provide important information about past impact events. The most significant impact indicator is the amorphization of many minerals and many studies have been performed to constrain the conditions for amorphization as a function of pressure and compression rate. The effects of temperature and grain sizes, however, have not yet been investigated accurately and *in-situ*, due to experimental limitations and the extreme conditions attained during shock compression.

In this study, we carried out dynamic compression experiments and simultaneously measured *in-situ* X-ray powder diffraction of abundant rock-forming minerals. We use membrane-driven diamond-anvil cells to rapidly compress the samples to high pressures and are in the process of developing a new setup for simultaneous pressure and temperature increase. We aim at creating the thermodynamic conditions that can be found in natural impacts in an effort to constrain the conditions for amorphization more precisely. We will present initial results of these diffraction experiments and the analyses on the recovered samples by transmission electron microscopy.

KFM 15: Annual General Meeting of the KFM division

Time: Wednesday 18:30–19:00 Location: PHY 5.0.21

KFM 16: Multiferroics and Magnetoelectric coupling II (joint session MA/KFM)

Time: Friday 9:30–11:45 Location: H39

KFM 16.1 Fri 9:30 H39

Reversible magnetoelectric interconversion of ferroic domain patterns in (Dy,Tb)FeO_3 — •Ehsan Hassanpour[1], Mads C. Weber[1], Yusuke Tokunaga[2], Yasujiro Taguchi[3], Yoshinori Tokura[3], Thomas Lottermoser[1], and Manfred Fiebig[1,3] — [1]ETH Zurich, Switzerland — [2]University of Tokyo, Japan — [3]RIKEN CEMS, Japan

Multiferroic materials can show a variety of exquisite effects due to hosting coexisting and complex magnetic and electric orders. Recently it was reported that a ferroelectric domain pattern from one layer is transfered to a ferromagnetic layer in a multiferroic heterostructure[1]. Here we show that we can reversibly interconvert magnetic and ferroelectric domain patterns in a single phase of multiferroic bulk system $Dy_{0.7}Tb_{0.3}FeO_3$. In this material, it was shown that a ferroelectric polarization is induced as a result of interaction of two magnetic sublattices of iron Fe^{3+} and rare-earth (Dy,Tb) R^{3+} via exchange forces. The strong coupling of these three order parameters creates a variety of composite domains and domain walls. Using magnetooptic imaging, we show that electric field pulses of specific speeds and amplitudes can generate and tune those domains/domain walls. Ultimately, by imprinting a domain pattern in the rare-earth's antiferromagnetic order, we transfer it from the ferromagnetic order of iron to the ferroelectric order and vice versa using magnetic and electric fields, respectively.

[1] De Luca *et al. Phys. Rev. Applied* **10**, 054030 (2018)

KFM 16.2 Fri 9:45 H39

Coupled electric and magnetic domains and domain walls in h-*R*MnO_3 at the microscale — •Marcela Giraldo, Thomas Lottermoser, and Manfred Fiebig — ETH Zurich, Switzerland.

Fundamental understanding of the cross-coupling between ferroic orders at the level of domains and domain walls is crucial for the manipulation of multiferroics. It was shown for the first time on h-$RMnO_3$ that coupling between ferroelectricity and antiferromagnetism –with order parameters P and l, respectively– occurs in a type-I multiferroic where ferroic orders emerge independently. At the macroscopic scale, it was observed that the antiferromagnetic domain pattern (l) is defined by two independent domain patterns formed by P and the multiferroic order parameter Pl [1]. Albeit, coupling on the microscopic regime, on the level of the ferroelectric vortex domains which are characteristic for these materials has remained under debate. For the first time, we investigate the coupling between electric and magnetic domains in h-$RMnO_3$ on the microscopic scale using second-harmonic microscopy. We reveal that two of the three order parameters (P, l and Pl) change their sign simultaneously at every domain wall while the third one retains its sign. This confirms the earlier observation [1] that P and Pl form independent domain patterns. In addition, we show a new type of domain wall where P and Pl change their sign, while l remains constant. Our observations solve the open debate about coupling of domains and domain walls at the microscale and add new findings to understand the unique coupling nature in a type-I multiferroic.

[1] M. Fiebig *et al.*, Nature **419**, 818 (2002).

KFM 16.3 Fri 10:00 H39

Magnetoelectric Polarizability in Magnetic Insulators — •Maximilian Merte[1,2], Frank Freimuth[1], Stefan Blügel[1], and Yuriy Mokrousov[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

In the field of spintronics, the interaction of insulators with external electromagnetic fields plays a crucial role for future prospects related to fundamental understanding and technological applications of magnetic oxides. In a situation of reduced symmetries, magnetic insulators can exhibit a finite electric polarization. Recently, a semiclassical approach describing the positional shift of Bloch electrons due to interband mixing induced by an external electromagnetic field was proposed [1]. These shifts can be computed via response matrices, which are constructed from interband velocity elements and band energies. Here we want to report on the implementation of this approach by means of Wannier interpolation, which can be applied as a postprocessing step to first-principles calculations performed with the Jülich DFT code FLEUR [2], an implementation of the FLAPW method. We apply the developed method to the study of magnetoelectric polarizability to selected magnetic insulators.

[1] Qian Niu *et al.*, Phys. Rev. Lett. 112, 166601 (2014).
[2] www.flapw.de .

KFM 16.4 Fri 10:15 H39

Artificial multiferroic domain walls in oxide heterostructures — •Elzbieta Gradauskaite, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zurich, Switzerland

Ferroelectric domain walls possess symmetry-dependent functional properties enabled by confinement. Enhanced conductivity, for instance, is observed in charged domain walls. Regrettably, domain walls of this type are very scarce in nature due to energetically unfavourable electrostatics, which hinders technological development of domain wall nanoelectronics. We propose ferroic thin film oxide interfaces as an alternative. The polar state of $BaTiO_3$ and $BiFeO_3$ ferroelectrics can be manipulated via atomically precise surface termination control and monitored with in-situ second harmonic generation (ISHG) during the growth. Using this approach, stable head-to-head and tail-to-tail polarization-oriented configurations of ferroelectric layers can be created. Their interfaces are charged and can be regarded as artificial domain walls. By inserting an ultrathin $La_{1-x}Sr_xMnO_3$ ferromagnetic film at the junction we design a magnetoelectric multiferroic interface. Using a combination of ISHG and SQUID magnetometry, we show that the interlayer magnetic moment can be enhanced or diminished when the artificial domain wall has a head-to-head or tail-to-tail configuration, respectively. Our work provides new insights into electrical control of magnetism in multiferroic oxide heterostructures.

KFM 16.5 Fri 10:30 H39

Complex magnon spectrum of the simple collinear antiferromagnet $Co_2Mo_3O_8$ — •Stephan Reschke[1], Dániel Farkas[2], Sandor Bordács[2], Vladimir Tsurkan[1], and István Kézsmárki[1] — [1]University of Augsburg, Augsburg, Germany — [2]Budapest University of Technology and Economics, Budapest, Hungary

$Co_2Mo_3O_8$ belongs to a family of hexagonal lattice type-I multiferroics, showing peculiar magnetoelectric effects. In this compound the magnetic Co^{2+} ions are in either tetrahedral or octahedral oxygen coordination and form honeycomb layers in the ab plane. Based on neutron powder diffraction, $Co_2Mo_3O_8$ is a 4 sub-lattice collinear easy-axis antiferromagnet below $T_N = 42$ K. By THz time-domain spectroscopy measurements the magnon excitation spectra of differently oriented single crystals were investigated in magnetic fields up to 7 T. Interestingly, we observed magnon spectra far more complicated than expected for the proposed simple antiferromagnetic structure, with more than 20 magnon modes. Most of these modes show a splitting for magnetic fields applied along the c axis, which supports the predominantly easy-axis character of the antiferromagnetic state. Furthermore, we also observed directional dichroism for some of the modes, a consequence of the dynamic magnetoelectric effects.

KFM 16.6 Fri 10:45 H39

Vacuum encapsulated high frequency magnetic field sensors based on the ΔE effect — •Benjamin Spetzler[1], Florian Niekiel[2], Fabian Lofink[2], Bernhard Wagner[2], and Franz Faupel[1] — [1]Kiel University, Kiel, Germany — [2]Fraunhofer ISIT, Itzehoe, Germany

Investigations into the ΔE effect of magnetoelastic materials have revealed the exciting promise of detecting low frequency and small amplitude magnetic fields [1]. Typical approaches are based on electrically exciting a resonator by applying an alternating voltage to a magnetoelectric composite structure with soft magnetic properties [2]. Previously presented sensors are operated either in the first or second bending mode with resonance frequencies in the lower kHz regime [3]. Due to the low resonance frequencies and comparatively large quality factors, the bandwidth of these sensors is too small for many biomedical applications. Here, we present vacuum encapsulated cantilever resonators operating at high frequency modes with bandwidths in the kHz regime. In addition to common bending modes, longitudinal and more complex modes are also used. The various modes are analyzed experimentally and theoretically for sensitivity, detection limit, mechanical properties and loss mechanisms with a comprehensive magneto-electromechanical model. Important consequences for future sensor designs are derived.

[1] B. Gojdka, et al., APL, 99 (22), (2011)
[2] S. Zabel, et al., APL, 107 (15), (2015)
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KFM 16.7 Fri 11:00 H39

High magnetic field phases of magnetoelectric LiFePO4 and LiNiPO4 — •Botond Forrai[1], Atsuhiko Miyata[2], Dávid Szaller[3], Vilmos Kocsis[4], Yasujiro Taguchi[4], Yoshinori Tokura[4], István Kézsmárki[5], and Sándor Bordács[1] — [1]Department of Physics, Budapest University of Technology and Economics, Budapest 1111, Hungary — [2]Laboratoire National des Champs Magnetiques Intenses, Toulouse 31400, France — [3]Institute of Solid State Physics, Vienna University of Technology, Vienna 1040, Austria — [4]RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan — [5]Zentrum für Elektronsiche Korrelation und Magnetismus, Institut für Physik, Universität Augsburg

Olivine-type orthophosphates has been attracting much attention due to their strong linear magnetoelectric effect. The low-field magnetic phases giving rise to the magnetoelelctric effect are well charachterized, however, their high field phase diagrams have not been fully explored. Therefore, we studied the magnetic phases of LiFePO4 and LiNiPO4 at 5K by magnetization measurements till their magnetization reach the saturation. The competing exchange interactions leads to several phase transitions in LiNiPO4, while in LiFePO4 a single spin-flop transition is detected due to the strong anisotropy. The magnetic phase diagrams are interpreted in a classical mean-field model, which allowed us to identify the key terms in spin Hamiltonian.

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Electric field control of the nonreciprocal light absorption in $Ba_2CoGe_2O_7$ — •Jakub Vít[1], Toomas Rõõm[2], Urmas Nagel[2], Johan Viirok[2], Vilmos Kocsis[1,3], Yoshinori Tokura[3], István Kézsmárki[1,4], and Sándor Bordács[1] — [1]Budapest University of Technology and Economics, Hungary — [2]National Institute Of Chemical Physics And Biophysics, Estonia — [3]RIKEN CEMS, Japan — [4]Experimental Physics 5, University of Augsburg, Germany

In crystalline solids where space inversion and time-reversal symmetries are simultaneously broken, the propagation of (quasi)particles can be different when the wave vector is reversed. Strong nonreciprocal light absorption has been observed on spin-wave excitations of multiferroics, i.e. ferroelectric and magnetic materials, where the sign and the magnitude of the effect were controlled by an external magnetic field. Here, we report an electric-field control of the nonreciprocal light absorption on THz excitations of $Ba_2CoGe_2O_7$. In the canted antiferromagnetic phase, we demonstrate that an electric field can be used to switch between low- and high-absorption states of magnetoelectric excitations. Our finding can facilitate the use of multiferroics in low-power consumption switchable optical diodes.

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Manipulating Coercivity and Mangetization Reversal in Bulk Ferromagnetic Metals with Small Voltages — •Xinglong Ye, Robert Kruk, and Horst Hahn — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Germany

Voltage control of magnetic properties in ferromagnetic metals is usually restricted to the scale of atomic layer due to their strong electric-field screening. Here we show that magnetic properties of bulk ferromagnetic metals can be hugely and reversibly tuned by small voltages through charging and discharging of hydrogen atoms. We manipulated the coercivity of micrometer-sized ferromagnetic metals by an amplitude of 2500 Oe with voltages only around 1 volt. Through this effect voltage-assisted and -gated magnetization reversal have been demonstrated. Experimental and density functional theory simulation results suggest that this phenomenon originates from the change of magnetocrystalline anisotropy at the surface layers with absorption and desorption of hydrogen atoms, which changes the nucleation field of reversed domains. This work may open up a new route for voltage control of magnetic properties in bulk metals, and voltage-assisted magnetization reversal also has implications for magnetic recording.