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 TOE 317, HSZ 301; Poster P2/1OG)

Invited Talks

KFM 1.1	Mon	9:30–10:00	HSZ 105	**Doped CVD diamond layers for electronic device applications: Experimental and theoretical study** — •Ken Haenen
KFM 1.2	Mon	10:00–10:30	HSZ 105	**Research and development for fabrication of diamond wafers for industrial use** — •Hideaki Yamada
KFM 1.3	Mon	10:50–11:20	HSZ 105	**Diamond: Material of the future for high power, high frequency devices and quantum applications** — •Shannon Nicley
KFM 2.1	Mon	9:30–10:00	TOE 317	**Novel device integration - combining bottom-up and top-down approaches** — •Artur Erbe
KFM 2.5	Mon	11:20–11:50	TOE 317	**Shapeable materials technologies for high resolution patterning of 3D microelectronic devices** — •Daniil Karnauschenko
KFM 13.5	Thu	11:10–11:40	TOE 317	**3D Printing with Electrons - Advances and Opportunities** — •Harald Plank

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues

SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Sessions

KFM 1.1–1.4	Mon	9:30–11:40	HSZ 105	**Focus: Diamond Technology and Electronics (joint session KFM/DS/HL)**
KFM 2.1–2.8	Mon	9:30–12:50	TOE 317	**Focus: High-resolution Lithography and 3D Patterning (Part I) (joint session KFM/HL/CPP)**
KFM 3.1–3.3	Mon	12:00–13:00	HSZ 105	**Dielectric, Elastic and Electromechanical Properties**
KFM 4.1–4.7	Mon	15:00–17:40	HSZ 105	**Multiferroics (joint session KFM/MA)**
KFM 5.1–5.7	Mon	15:00–17:40	TOE 317	**Microscopy and Spectroscopy with X-rays, Ions and Positrons (joint session KFM/CPP)**
KFM 6.1–6.6	Tue	9:30–11:50	TOE 317	**Diamond**
KFM 7.1–7.5	Tue	12:00–13:40	TOE 317	**Whispering-Gallery-Mode Resonators**
KFM 8.1–8.10	Wed	9:30–12:15	HSZ 401	**Multiferroics and Magnetoelectric Coupling I (joint session MA/KFM)**
KFM 9.1–9.11	Wed	9:30–13:30	TOE 317	**Focus: Polar oxide crystals and solid solutions**
KFM 10.1–10.8	Wed	15:00–17:00	HSZ 401	**Multiferroics and Magnetoelectric Coupling II (joint session MA/KFM)**
KFM 11.1–11.9	Wed	15:00–18:20	TOE 317	**Ferroics - Domains and Domain Walls (joint session KFM/MA)**
KFM 12.1–12.6	Thu	9:30–11:50	HSZ 301	**Materials for Energy Storage (joint session KFM/CPP)**
KFM 13.1–13.7	Thu	9:30–12:20	TOE 317	**Focus: High-resolution Lithography and 3D Patterning (Part II) (joint session KFM/HL/CPP)**
KFM 14.1–14.6	Thu	14:10–16:20	HSZ 301	**TEM-based Nanoanalysis and Microstructure of thin films (joint session KFM/CPP)**
KFM 15.1–15.30	Thu	16:00–18:30	P2/1OG	**Postersession KFM**
KFM 16	Thu	18:30–19:30	TOE 317	**Annual General Meeting of the KFM division**
KFM 17.1–17.8	Fri	9:30–12:30	TOE 317	**Microstructure, Real Structure and Crystal Defects**

Annual General Meeting of the Crystalline Solids and their Microstructure Division

Donnerstag 18:30–19:30 TOE 317

- Bericht
- Verschiedenes

KFM 1: Focus: Diamond Technology and Electronics (joint session KFM/DS/HL)

Time: Monday 9:30–11:40 Location: HSZ 105

Invited Talk KFM 1.1 Mon 9:30 HSZ 105
Doped CVD diamond layers for electronic device applications: Experimental and theoretical study — •Ken Haenen — Institute for Materials Research (IMO), Hasselt University, Diepenbeek, Belgium — IMOMEC, IMEC vzw, Diepenbeek, Belgium

While diamond is considered to be the ultimate wide band gap semiconductor due to its combination of superlative properties, the full understanding of the connection between growth conditions and subsequent layer properties is still lacking. In this presentation, focus is first devoted to the deposition of heavily and lightly B-doped CVD diamond films. Employing microwave plasma enhanced CVD in combination with Ib (100)-oriented high pressure high temperature (HPHT) substrates, the influence of the [C]/[H] ratio on key material properties is presented. This includes the surface morphology, crystal quality, and electrical transport properties by employing a wide range of characterization techniques, i.e.. Hall effect in a wide temperature range, FTIR spectroscopy, Raman spectroscopy, X-ray absorption spectroscopy, XPS, AFM, optical microscopy, and transmission electron microscopy. First principles density functional calculations (DFT) were performed to model the interaction of B with the H-terminated diamond surface, corroborating the observed increase of B-doping incorporation with used methane concentration. The insight offered by the combination of experiment and theory clearly provides a pathway to more efficient doping and enhanced crystal quality. Finally, the use of said layers in Schottky barrier diodes is presented.

Invited Talk KFM 1.2 Mon 10:00 HSZ 105
Research and development for fabrication of diamond wafers for industrial use — •Hideaki Yamada — AIST, Osaka, Japan

Figure of merits of diamond as a candidate material in power electronics are superior to those of other materials, such as Si, SiC, and GaN. Especially, recent increase of the power density in power devices for high-frequency use require extremely high thermal conductivity of diamond. On the other hand, because of its stable quantum state under the standard condition, variety of sensors with wide dynamic-range and quantum computing have been studied. Therefore, in addition to its mechanical and optical applications, use of diamond in spintronics as well as electronics have been attracted researchers for variety of future applications in industry. One of the bottle necks for realization of them is in technique to fabricate diamond wafers with large area and sufficient quality under acceptable cost. We have developed techniques to enlarge seed substrates, and process them to wafers. To understand mechanism of the crystal growth, we simulated the growth environment numerically and compared them with experimental results. Our recent trials, achievement and future prospective to solve above issues aiming at realization of the industrial use of diamond will be presented with the related current state-of-the-art.

20 min. break

Invited Talk KFM 1.3 Mon 10:50 HSZ 105
Diamond: Material of the future for high power, high frequency devices and quantum applications — •Shannon Nicley — Department of Materials, University of Oxford, Oxford, UK

Diamond is an exceptional material in many ways, not only for its well known hardness and highest room temperature conductivity, but also electronic properties like high electron and hole mobilities and a high electronic breakdown field strength. These properties predict that diamond electronic devices should have superior high power and high frequency performance over other semiconductor materials. Diamond is also a promising solid-state host for atomic scale defects for quantum applications. The realisation of diamond electronic devices and the full implementation of diamond quantum applications have both been limited in part by our ability to reliably grow high quality single crystal diamond. Control over the incorporation of dopant atoms such as boron and phosphorus is key for high power applications, and the ability to grow high purity, low-strain diamond as well as precisely place quantum defects remain areas of active investigation. I will give an overview of the growth of synthetic diamond and review recent progress in the control of boron and phosphorus doping. I will also present a very recently developed method for the deterministic and accurate placement of optically coherent NV centres using a laser writing technique. I will discuss the challenges in this field and give an outlook for both extreme electronic device and quantum applications.

KFM 1.4 Mon 11:20 HSZ 105
Preliminary study of diamond based Kinetic Inductance Detectors — •Francesco Mazzocchi, Dirk Strauss, and Theo Andreas Scherer — Karlsruhe Institute of Technology (IAM-AWP), Hermann Von Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen

Kinetic Inductance Detectors (KIDs) have proven themselves as a very versatile cryogenic detector technology capable of applications in various fields due to their flexibility of design, sensibility and ease of production. We have recently proposed a polarization sensitive Lumped Elements KID as sensor for an innovative polarimetric diagnostics based on quantum cascade lasers (QCL) for application in the nuclear fusion. Each detector unit is composed by 4 pixels arranged at the vertices of a square, each pixels being sensible to only one polarization direction. The current system is based on niobium nitride (NbN) superconductor over High Resistivity Silicon (HRSi) substrate. Such material delivers good performances but its relatively high dielectric constant and loss tangent lead to increased substrate losses. Using a transparent substrate may improve this aspect and also the radiation resistance of such devices. Diamond is the substrate of choice, being a material already widely studied and used in the fusion environment as high power microwave window, due its outstanding optical and mechanical performances. In this work we present the preliminary design study and simulations for a diamond based Kinetic Inductance Detector with both single and poly-crystalline diamond (SCD/PCD) substrates taken into account.

KFM 2: Focus: High-resolution Lithography and 3D Patterning (Part I) (joint session KFM/HL/CPP)

Chair: Robert Kirchner (TU Dresden)

Time: Monday 9:30–12:50 Location: TOE 317

Invited Talk KFM 2.1 Mon 9:30 TOE 317
Novel device integration - combining bottom-up and top-down approaches — •Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Scaling electronic devices to smallest structure sizes well below 10nm will require novel developments for the fabrication of single components. Smallest functional devices can be assembled using chemical methods leading to, e.g., single molecules with electronic functionalities. Reliable contacting of single molecules using metallic contacts is, however, an extremely challenging task which has not been solved so far. We have therefore developed techniques which use self-assembly for the creation of conducting nanostructures in order to create small, self-assembled circuits which then can be contacted reliably using standard lithographic methods. In this talk, we demonstrate how single organic molecules can be contacted using mechanically controllable break junctions. In addition, we show how DNA Origamis can be used for the self-assembly of metallic nanowires, which are contacted using electron beam lithography and electrically characterized. Further integration of such nanostructures into standard silicon electronics may be achieved by connecting them with 1d- or 2d-semiconductors. We have therefore developed transistors based on 2d-materials and silicon nanowires using electron beam lithography and dry etching (i.e. using a classical top-down approach), which are reconfigurable. With the combination of these devices with self-assembled nanostructures,

a large variety of electronic nanocircuits can be constructed in future applications.

KFM 2.2 Mon 10:00 TOE 317

Fabrication of NbC Josephson-junction arrays by focused-ion-beam-induced deposition — •Fabrizio Porrati, Felix Jungwirth, Sven Barth, and Michael Huth — Goethe-University, Institute of Physics, Frankfurt a. M.

In this work, a Ga focused-ion-beam is used in combination with the precursor Nb(NMe2)3(N-t-Bu) to fabricate 2D Josephson-junction arrays made of NbC nanodots with typical diameter of 40 nm. Square-arrays with lattice constant between 70 nm and 100 nm are characterized by transport measurements. The ratio Ej/Ec between Josephson coupling energy and the charging energy can be varied by tuning either the dot thickness or the inter-dot distance. As a consequence, a superconductor to insulator transition takes place, as shown by temperature-dependent resistivity measurements. In the Josephson regime, the arrays show magnetic frustration. The resistance as function of the magnetic field exhibits an oscillating behavior with a period of 380 mT for the square-array with lattice constant of 70 nm.

KFM 2.3 Mon 10:20 TOE 317

Avoiding amorphization during semiconductor nanostructure ion beam irradiation — •G. Hlawacek[1], X. Xu[1], W. Möller[1], H.-J. Engelmann[1], N. Klingner[1], A. Gharbi[2], K.-H. Heinig[1], S. Facsko[1], and J. von Borany[1] — [1]Ion Beam Physics and Materials Research, Helmholtz—Zentrum Dresden – Rossendorf, Dresden, Germany — [2]CEA-Leti, Grenoble, France

Ion beam induced amorphization of semiconductor nanostructures limits the applicability of ion beam processing to semiconductor nanostructures. Here, we present an approach that not only avoids this amorphization but in addition allows to tailor the lateral device dimensions of pillars and fins used in modern GAA and Fin-FET designs. Si nanopillars (diameter: 25–50 nm) have been irradiated by either 50 keV broad beam Si^+ or 25 keV focused Ne^+ beam from a helium ion microscope (HIM) at various temperatures using fluences of 2×10^{16} cm^{-2} and higher. While at room temperature strong deformation of the nanopillars has been observed, the pillar shape is preserved above 325°C. This is attributed to ion beam induced amorphization of Si at low temperatures allowing plastic flow due to the ion hammering effect and surface capillary forces. Plastic deformation is suppressed for irradiation at elevated temperatures. Above 325°C, as confirmed by diffraction contrast in BF-TEM, the nanopillars remain crystalline, and are continuously thinned radially with increasing fluence down to 10 nm. This is due enhanced forward sputtering through the sidewalls of the pillar, and agrees well with 3D ballistic computer simulations.

Supported by the H-2020 under Grant Agreement No. 688072.

KFM 2.4 Mon 10:40 TOE 317

Grayscale Lithography: Creating complex 2.5D structures in thick photoresist by direct laser writing — •Dominique Collé — Heidelberg Instruments, Heidelberg, Germany

Heidelberg Instruments's lithography systems make it possible to expose any pattern directly without fabricating a mask, which results in a significantly shorter prototyping cycle. The use of a digital mask also allows some quick modification of the design when necessary. The possibility to modulate the energy of each pixel exposed brings the control over the 3rd dimension. This localized dose modulation can be represented as gray tones in a design between black (no dose / no depth in the resist) and white (highest dose / maximum depth in the resist) with up to 1024 different gray tones. Grayscale lithography opens a new world of application from texturing to micro-optic. Micro lenses array, light diffusers, Fresnel lenses, blazed gratings and diffractive optic elements are some typical micro-structures made with grayscale lithography.

20 min. break

Invited Talk KFM 2.5 Mon 11:20 TOE 317

Shapeable materials technologies for high resolution patterning of 3D microelectronic devices — •Daniil Karnauschenko — Institute for Integrative Nanosciences, Leibniz IFW, Helmholtz str. 20, 01069 Dresden, Germany

Electronic devices are continually evolving to offer improved performance, smaller sizes, lower weight, and reduced costs, often requiring state of the art manufacturing and materials to do so. An emerging class of materials and fabrication techniques, inspired by self-assembling biological systems shows promise as an alternative to the more traditional methods that are currently used in the microelectronics industry. Mimicking unique features of natural systems, namely flexibility and shapeability, the geometry of initially planar microelectronic structures can be tailored. Heavily relying on cylindrical geometry, fabrication of microwave helical antennas, coils, resonators and magnetic sensors is challenging, when conventional fabrication techniques are applied. Involving high resolution lithographic patterning and self-assembly strategies realization of these spatially non-trivial devices in a compact form and with a reduced number of fabrication steps become feasible. This spatial self-assembly process, triggered by an external stimulus, offers a possibility of an improved performance while reducing overall manufacturing complexity of devices and components by harnessing the relative ease in which it can produce microscopic 3D geometries such as a *Swiss-roll* architecture. These benefits can lead to tighter a system integration of electronic components including active electronics with reduced costs fabricated from a single wafer.

KFM 2.6 Mon 11:50 TOE 317

Coupling Single Mode Fibers to Single Quantum Emitters using Femtosecond 3D Printing Technology — •Ksenia Weber[1], Simon Thiele[2], Simon Ristok[1], Sarah Fischbach[3], Jan Hausen[3], Lucas Bremer[3], Mark Saritson[4], Simone Protalupi[4], Alois Herkommer[2], Stefan Reitzenstein[3], Peter Michler[4], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart — [2]Institute for Applied Optics and Research Center SCoPE, University of Stuttgart, Stuttgart — [3]Institute of Solid State Physics, Technische Universität Berlin — [4]Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, University of Stuttgart

We propose a method to efficiently couple single photon quantum emitters to optical single mode fibers. Due to the undirected emission of single photon sources, such as quantum dots or defect centers in crystals, coupling into optical fibers which is essential for long range quantum communication is typically associated with high losses. To overcome this limitation, femtosecond two-photon lithography can be used to directly fabricate a combination of a microlens and an optical fiber holder onto a quantum emitter. A single mode optical fiber is then integrated into the fiber holder. Due to the high precision of the femtosecond 3D printing process, the position of the fiber core can be adjusted with sub-micrometer accuracy to match the focal point of the microlens. Light from the emitter which is focused by the microlens can therefore efficiently be coupled into the fiber. We present a number of different optical layouts and discuss their pros and cons.

KFM 2.7 Mon 12:10 TOE 317

Optical properties of photoresists for femtosecond 3D printing: Refractive index, extinction, luminescence - dose dependence, aging, heat treatment and comparison between 1-photon and 2-photon exposure — •Michael Schmid, Dominik Ludescher, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Femtosecond 3D printing has emerged as an important technology for manufacturing nano- and microscopic optical devices and elements. Detailed knowledge of the dispersion in the visible and near-infrared spectral range is crucial for the design of these optical elements. Here we provide refractive index measurements for different UV-doses, aging times, heat treatment and 2-photon exposed structures for the photoresists IP-S, IP-Dip, IP-L, OrmoComp, IP-Visio, and PO4. We use a modified and automized Pulfrich refractometer setup, utilizing critical angles of total internal reflection with an accuracy of $5{\cdot}10^{-4}$ in the visible and near-infrared spectral range. We compare Cauchy and Sellmeier fits to the dispersion curves. We also give Abbe numbers and Schott Catalog numbers of the almost entirely polymerized resists. Additionally, we provide quantitative extinction and luminescence measurements for all photoresists.

KFM 2.8 Mon 12:30 TOE 317

Acoustic Impedance Matching on Ultrasonic Devices using Additive Manufacturing — •Severin Schweiger, Sandro Koch, Marcel Krenkel, and Marco Kircher — Fraunhofer Institute for Photonic Microsystems, Dresden, Germany

Acoustic impedance matching layers are attached to ultrasonic transducers to increase acoustic energy transmission into the load medium. A capacitive micromachined ultrasonic transducer (CMUT) emits

sound via electrostatic deflection of a flexible electrode. Especially air-coupled CMUTs with protective or focusing layers exhibit a notable impedance mismatch. We propose a new approach to fabricate impedance matching metamaterials with low load-side specific acoustic impedance values, by employing a photolithographic additive manufacturing technology using two photon absorption. It will enable improved impedance matching, which has a beneficiary effect on acoustic bandwidth, efficiency and sensitivity of the CMUT. The center operating frequency of the CMUT can be influenced via this process as well. The technology also allows for direct fabrication of microstructures on the chip, foregoing any adhesion layers that disturb the impedance matching and enabling the protective and/or focusing aspects of the layer. This contribution will show analytic and FEM simulations of CMUTs with matching layers. Fabricated impedance matching layer samples and on chip fabrication will be presented as well. Electric impedance and acoustic measurements are in progress and will be featured accordingly.

KFM 3: Dielectric, Elastic and Electromechanical Properties

Time: Monday 12:00–13:00 Location: HSZ 105

KFM 3.1 Mon 12:00 HSZ 105

High sensitivity characterization of the nonlinear electric susceptibility of a glass ceramic in the microwave range — •Florian Bergmann[1,2,3], Martin Letz[1,2,3], Holger Maune[4], and Gerhard Jakob[1,3] — [1]Johannes Gutenberg Universität Mainz — [2]Schott AG Mainz — [3]MAINZ Graduate School — [4]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). One source of PIM can be the nonlinear electric susceptibility of dielectrics used in the devices. We characterized this nonlinearity of a glass ceramic. To achieve the necessary sensitivity for dielectric nonlinearities, the setup ensures that the measured intermodulation can be ascribed to the material under test while all other intermodulation sources are suppressed. The magnitude is comparable to previously measured high-end sintered ceramics. The power of the intermodulation signal as a function of the input power deviates from the simple 3 dB/dB scaling. This allows new insights into the polarization mechanisms of materials.

KFM 3.2 Mon 12:20 HSZ 105

Glass ceramics with magnetic crystalline phases for high frequency applications — •Moritz Maximilian Benjamin Krämer[1,2], Martin Letz[1], Martun Hovhannisyan[1], and Martin Jourdan[2] — [1]SCHOTT AG, Mainz, Germany — [2]Johannes Gutenberg University, Mainz, Germany

New generations of mobile data transmittance use higher frequencies to enable significantly higher data rates. The steady frequency increase and especially the step to 5G requires new manufacturing accuracies of high frequency electronic devices. For higher frequencies and smaller wavelengths the requirements to geometric tolerances and material homogeneity increase. Substantially higher accuracies are only accessible by better material homogeneity. Conventional ceramics have a restricted material homogeneity due to pores, thus a new glass ceramic obtained from a true amorphous glassy state possibly enables to reach new applications in the field of mobile data electronic devices. We investigate glass forming regions in the field of crystallization of ferrimagnetic phases. The talk will report on the latest progress in stabilizing the glass as a bulk sample of several cm in order to obtain controlled crystallization.

KFM 3.3 Mon 12:40 HSZ 105

Dilute metallicity in $SrTiO_{3-\delta}$ — •Thomas Schunk-Born[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 $SrTiO_3$ shows comparatively high values of the dielectric constant ε' of ≈ 300 already at room temperature. When cooling the material, these values rise steeply, indicating the vicinity of a ferroelectric phase transition. In $SrTiO_3$, this transition is suppressed by quantum fluctuations, making the compound a quantum paraelectric with saturation values in ε' of the order of 10^4 [1].

While the parent compound is a wide-gap insulator, reduction of the oxygen content introduces free charge carriers in $SrTiO_{3-\delta}$. The result is a conducting and even superconducting material with unusually low charge carrier concentrations, made possible by the large effective Bohr radius caused by the high permittivity of the lattice [2].

While DC-data is available [3], we investigate the conductivity of $SrTiO_{3-\delta}$ depending on frequency and temperature using broadband dielectric spectroscopy. The Drude model is applied to this AC-data to retrieve scattering rate, mobility and effective mass of the charge carriers.

Funded by the DFG 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)
[3] C. Collignon *et al.*, Ann. Rev. Cond. Mat. Phys. **10**, 25-44 (2018)

KFM 4: Multiferroics (joint session KFM/MA)

Time: Monday 15:00–17:40 Location: HSZ 105

KFM 4.1 Mon 15:00 HSZ 105

Magnetoelectric crystals as model systems of quantum optics — •Janek Wettstein[1], Andrei Pimenov[1], Alexander A. Mukhin[2], Artem Kuzmenko[2], Kirill Amelin[3], Toomas Rõõm[3], Urmas Nagel[3], and David Szaller[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia — [3]National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia

The interaction between an ensemble of non-interacting two-level quantum systems and a bosonic field is theoretically described by the Dicke-model which predicts a quantum phase transition in the thermodynamic limit when the strength of the interaction reaches a sufficiently large critical value [1,2]. Here, based on the idea of Ref. [3] we present a method to study the superradiant phase transition in $SmFe_3(BO_3)_4$, where isolated rare-earth quasi-spins (Sm) play the role of the two-level system and the bosonic field is provided by the spin-waves (i.e. magnons) of the antiferromagnetically ordered Fe ions. At low temperatures ($T = 3\,\mathrm{K}$) we observe an avoided crossing of the optically active low-frequency iron magnon and the Sm quasispin excitations with a coupling of about 70% of the critical value needed for the superradiant transition. The strength of the coupling was tuned by varying density and population of the Sm two-level systems.

[1] K. Hepp and E. H. Lieb, Phys. Rev. A 8, 2517 (1973).
[2] Y. K. Wang and F. T. Hioe, Phys. Rev. A 7, 831 (1973).
[3] X. Li et al., Science 361, 794 (2018).

KFM 4.2 Mon 15:20 HSZ 105

Strain-Driven Metal-to-Insulator Transition and Charge Ordering in LiV2O4 — Yu-Mi Wu, Ulrike Niemann, Yi Wang, Y. Eren Suyolcu, Minu Kim, Hidenori Takagi, and •Peter A. van Aken — Max Planck Institute for Solid State Research, Stuttgart, Germany

The coupling of local atomic configurations and electronic degrees of freedom plays a fundamental role in understanding metal-insulator transitions and the formation of charge ordering. In particular, such competing interactions become more pronounced in the geometrically frustrated pyrochlore lattice in the spinel structure, due to fluctua-

tions in the charge, spin and orbital channels. By STEM imaging and electron energy-loss spectroscopy, we have investigated mixed-valence spinel LiV2O4 thin films grown on SrTiO3 and MgO (001) substrates. The epitaxial strain strongly affects the spatial configurations of valence states in LiV2O4, and the local valence distributions are resolved at atomic-scale resolution. Two competing phases are detected in the thin films, a metallic charge-disordered heavy-fermion state on SrTiO3 and an insulating charge-ordered state on MgO. Importantly, our result shows that the out-of-plane lattice compression relieves the charge frustration and induces a Verwey-type-like charge-ordering pattern in LiV2O4. This observation provides atomic-scale insight into the strong charge-order correlation and tuneable electronic-phase transitions in related frustrated systems. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823717 - ESTEEM3.

KFM 4.3 Mon 15:40 HSZ 105

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

Layered perovskite materials, such as $A_3B_2O_7$ Ruddlesden-Popper compounds, are under scrutiny in the search for multiferroics with a strong magnetoelectric coupling and large polarisations at high temperatures. Their crystal structure allows for the implementation of a wide range of magnetic ions and it can be host to geometrically induced ferroelectricity. For $Ca_3Mn_2O_7$, theory predicts a robust magnetoelectric coupling between the improper ferroelectricity and the Mn^{3+} magnetism, mediated by the MnO_6-octahedra tilts. However, experimental evidence is still pending. Here, we investigate such a possible coupling in $Ca_3Mn_{1.9}Ti_{0.1}O_7$. We probe the influence of the magnetic ordering on the ferroelectricity using second harmonic generation (SHG) - a non-invasive, highly symmetry-sensitive laseroptical technique ideal for the study of ferroic order. We observe a strong increase in the SHG signal upon entering the magnetic phase, which indicates a strong influence of the magnetism on the ferroelectricity. Measurements of the SHG spectrum and images of the domain pattern suggest a coupling of the magnetic order to the polarisation mechanism via the octahedral tilts. Our results demonstrate that layered perovskites are promising candidates in search for multiferroics with pronounced magnetoelectric coupling.

KFM 4.4 Mon 16:00 HSZ 105

Magnetic Structure and Magnetoelectricity in Holmium-Doped Langasite — •Lukas Weymann[1], Thomas Kain[1], Lorenz Bergen[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, Vienna, Austria — [2]Prokhorov General Physics Institute of Russian Academy of Sciences, Moscow, Russia — [3]Moscow Institute of Physics and Technology, Dolgoprudny, Moscow region, Russia — [4]Theory of Condensed Matter, Zernike Institute for Advanced Materials, Groningen, The Netherlands

The compounds of the rare-earth langasite family R3Ga5SiO14 were investigated for their striking electromechanical properties in the early 1980s and attracted new scientific attention due to their intriguing magnetic and magnetoelectric properties in the past decade. In this work we present the results of a magnetoelectric effect, i.e. electric polarization induced by an external magnetic field, in the diluted holmium langasite.

This effect has an unusual angular dependence, which can be explained by taking into account the three-fold symmetry of the crystal and its rather complex magnetic structure. The latter was investigated by measurements in a Vibrating Sample Magnetometer and a torque magnetometer. Magnetic and magnetoelectric results can be understood taking into account the interplay between crystal symmetry and the local symmetry of the Holmium ions.

20 min. break

KFM 4.5 Mon 16:40 HSZ 105

Non-invasive study of buried domain patterns in multiferroic bismuth ferrite — •Marvin Müller[1], Yen-Lin Huang[2], Ramamoorthy Ramesh[2], Morgan Trassin[1], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland — [2]University of California, Berkeley, USA

Magnetoelectric (ME) multiferroic materials hosting coexisting and coupled electric and magnetic orders allow for low-energy control of magnetism and thus hold great promise for energy-efficient random-access memories and logic devices. In $BiFeO_3/Co_{0.9}Fe_{0.1}$ heterostructures, room-temperature electric-field-induced reversal of the ferromagnetic magnetization has been recently achieved. Despite extensive studies on the ME coupling in $BiFeO_3$, the switching dynamics remain elusive. The lack of direct experimental access to the ferroic properties of the buried material renders *operando* investigations challenging. Here, we probe the ferroelectric switching in the model system $BiFeO_3/Co_{0.9}Fe_{0.1}$. We use spatially-resolved non-invasive optical second harmonic generation (SHG) to map the net polarization of the buried $BiFeO_3$ layer after voltage application. Our results suggest the emergence of a strong net polarization with the first voltage pulse. Additional scanning probe microscopy is used to correlate this observation with the emergence of stripe-domain patterns with 71° domain walls. This work introduces SHG as an effective tool to non-invasively study buried ferroelectric domain states and thus opens novel pathways towards *operando* electro-optic studies on the dynamics in these coupled systems.

KFM 4.6 Mon 17:00 HSZ 105

B-site doping effects in multiferroic rare-earth hexagonal manganites — •Marcela Giraldo[1], Martin Lilienblum[1], Hasung Sim[2], Lea Forster[1], Je-Geun Park[2], Thomas Lottermoser[1], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland. — [2]Seoul National University, Korea.

Chemical doping is an alternative to tailor the properties of complex oxides. A–site doping in hexagonal $R MnO_3$ with Ca or Zr leads to a conductivity enhancement at the domain walls while preserving the characteristic topological ferroelectric state of the system. Stronger effects on the magnetism in this multiferroic family are expected by doping at the B–site. This is due to the direct perturbation of the magnetic sublattices formed by Mn^{3+} moments. We investigate Al-doping (0-25%) at the B–site in h-$YMnO_3$. We use a combination of second-harmonic generation (SHG) and piezoresponse force microscopy to disclose the effects on antiferromagnetic and ferroelectric domain formation. The later ones, for example, reveal a size decrease with increasing degree of doping. Furthermore, a combination of SHG and X-ray diffraction (XRD) unveils a decreasing trend for magnetic/electric ordering temperatures as a function of doping. This is due to the chemical pressure induced by the distinct ionic sizes of Al and Mn and the progressive decomposition of the long-range order. By tracing the changes in the inherent properties of these ferroic systems, we aim to broaden the understanding for new routes in the manipulation of this important class of multiferroics.

KFM 4.7 Mon 17:20 HSZ 105

Excitations and switching dynamics in RMn2O5 — Louis Ponet[1,2], •Sergey Artyukhin[1], Maxim Mostovoy[3], and Andrei Pimenov[4] — [1]Italian Institute of Technology, Genova, Italy — [2]Scuola Normale, Pisa, Italy — [3]University of Groningen — [4]TU Wien

RMn2O5 manganites have attracted significant attention due to the complex interplay between Mn and rare earth orders, resulting in multiferroic phases and peculiar excitations. Here we perform model and first-principles simulations to analyze excitations and peculiar switching dynamics in these compounds.

KFM 5: Microscopy and Spectroscopy with X-rays, Ions and Positrons (joint session KFM/CPP)

Chair: Enrico Langer (TU Dresden)

Time: Monday 15:00–17:40 Location: TOE 317

KFM 5.1 Mon 15:00 TOE 317

Single-Shot Phase-Contrast Microscopy of Laser-induced Cavitation at MID/EuXFEL — •Johannes Hagemann[1], Malte Vassholz[2], Hannes Höppe[2], Markus Osterhoff[2], Juan Rosello[3], Robert Mettin[3], Andreas Schropp[1], Christian Schroer[1,4], and Tim Salditt[2] — [1]DESY, Notkestraße 85, 22607 Hamburg — [2]Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [3]Drittes Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen — [4]Department Physik, Universität Hamburg,Luruper Chaussee 149, 22761 Hamburg

X-ray free electron lasers offer unique opportunities for imaging of ultra-fast processes on smallest length-scales paired with the penetration power of hard X-rays. One of these processes is laser-induced cavitation in water. The dynamic nature of the processes under study is incompatible to scanning schemes for image acquisition thus we chose propagation-based near-field imaging as full-field imaging scheme. The illumination with high intensity, fs-short X-ray pulses enables imaging with single pulses which yield a still image of the cavitation bubble without motion blur. In this contribution we will present a pump-probe imaging experiment conducted at the MID instrument at the European XFEL. The experiment has been carried out at 14/17.8 keV photon energy. The X-rays have been focused by aberration corrected Be-compound refractive lenses down to 100 nm focus-size. The fluctuating nature of the SASE-process poses some challenges for the data analysis. We present our approach to the data-processing, phase-retrieval and results.

KFM 5.2 Mon 15:20 TOE 317

Latest developments in multi-modal scanning X-ray microscopy — •Michael Stuckelberger — DESY, 22607 Hamburg, Germany

Scanning X-ray microscopy is challenged not only by the ever-smaller structures requiring higher resolution, but also by the increasing complexity of in-situ and operando environments of functional materials. Given that relevant information about micro- and nanostructures is typically extracted from the point-by-point correlation of different properties, the same spot needs to be in the same condition for all measurements. Often, this is not possible without the simultaneous evaluation of all critical measurement modalities.

At the leading X-ray nanoprobe endstations in the US and in Europe, we have set up experiments for multi-modal X-ray microscopy. Involving up to 5 different modalities, the measurements allow the simultaneous evaluation of composition by X-ray fluorescence, structure by X-ray diffraction and ptychography, and of the electrical and optical performance by X-ray beam induced current and X-ray excited optical luminescence.

In this contribution, we will demonstrate the application of multi-modal scanning X-ray microscopy to nanoscale semiconductors and electronic devices, and discuss detector arrangement and compatibility with different scan modes and samples. Beyond state-of-the-art measurements, we will give an outlook to new opportunities and challenges at X-ray nanoprobe endstations of 4th generation synchrotrons that will see light in the coming years.

KFM 5.3 Mon 15:40 TOE 317

Experimental optimization of geometry for propagation based phase contrast X-ray imaging — •Hanna Dierks and Jesper Wallentin — Synchrotron Radiation Research, Lund University, Sweden

Propagation-based phase contrast imaging (PB-PCI) with an X-ray lab source is a powerful technique to study low-absorption samples, e.g. soft tissue or plastics, on the micrometer scale. The choice of the propagation distance and magnification is crucial for the performance, and a trade-off in terms of resolution, contrast and noise is always necessary. Theoretical optimization strategies based on Fresnel propagation have been reported, and here we systematically test these experimentally using a setup with a Cu X-ray tube and a detector with 0.55um effective pixel size. The source-detector distance was between 25 and 40cm and magnification ratios were varied from 1 to 1.3. We verify the key conclusions from the proposed models. The experiments show that the theoretical optimization approach is very sensitive to system parameters such as the X-ray source spot size and detector resolution. Moreover, the energy dependence of the refractive index needs to be taken into account when modelling the polychromatic illumination of an x-ray tube. Finally, the sensitivity of TIE based phase retrieval algorithms on the image noise and contrast are studied.

KFM 5.4 Mon 16:00 TOE 317

Multiscale Mapping and Quantification of Elastic Stress and Domain Size in Bulk Ferroelastic Systems by Dark-Field X-Ray Microscopy — •Jan Schultheiss[1,2], Lukas Porz[1], Lalitha Kodumudi Venkataraman[1], Marion Höfling[1], Semen Gorfman[3], Jürgen Rödel[1], and Hugh Simons[4] — [1]Department of Materials and Earth Sciences, TU Darmstadt, Germany — [2]Department of Materials Science and Engineering, NTNU Trondheim, Norway — [3]Department of Materials Science and Engineering, Tel Aviv University, Israel — [4]Department of Physics, DTU, Denmark

Twinned domains in ferroelastic systems are intimately coupled to local strain fields. Problematically, in complex oxides this coupling often spans over several orders of magnitude of length scale. State-of-the art characterization techniques, however, either lack spatial resolution or their sensitivity is limited to the surface.
Here we use Dark-field X-Ray Microscopy to map and quantify spatial variations of elastic stress and domain size from nm to several μm in a grain of a polycrystalline ferroelectric/ferroelastic (Ba,Ca)(Zr,Ti)O_3 model system as a function of the applied electric field. We find, that the electric field narrows the distribution of elastic stresses by 60%, while the domain size increases by 35%. The suggested methodology can be applied to multiscale correlations in emerging fields in complex oxides and twinned systems.

KFM 5.5 Mon 16:20 TOE 317

Soft X-ray Laminography adds a third dimension to STXM — Katharina Witte[1], •Andreas Späth[2], Simone Finizio[1], Claire Donnelly[1,3], Michal Odstrcil[1], Manuel Guizar-Sicairos[1], Mirko Holler[1], Benjamin Watts[1], Rainer H. Fink[2], and Jörg Raabe[1] — [1]Paul Scherrer Institut, Villigen, Switzerland — [2]FAU Erlangen-Nürnberg, Germany — [3]Department of Physics, University of Cambridge, United Kingdom

Scanning Transmission X-ray microscopy is a powerful tool for spectromicroscopic analysis of nanostructured thin-film specimens. While developments focused on organic soft matter for many years, STXM has meanwhile also contributed to imaging of magnetic nanostructures based on (XMCD) contrast. However, 3D imaging is so far limited to a narrow selection of suitable specimens and constraint experimental conditions. This is especially true for the implementation of tomography, since the full sample rotation perpendicular to the optical axis is usually not possible for geometric reasons. Laminography overcomes this limitation by inclining the sample rotation axis by the laminography angle $\theta < 90°$ so that it is no longer perpendicular to the incident X-ray beam. The major advantage is that the sample (and its support) can be laterally extended without further modification and without risking collisions during rotation. A new setup combines laminography and STXM using soft X-rays. We will present first 3D reconstructions of nanostructured objects from material science, biology and functional magnetic materials. Funding: BMBF grant 05K19WE2 and EU Marie Skłodowska-Curie grant No. 701647.

20 min. break

KFM 5.6 Mon 17:00 TOE 317

Detection system for transmission imaging in helium ion microscope — •Eduardo Serralta[1], Nico Klingner[1], Olivier De Castro[2], Serge Duarte Pinto[3], Cecilia Bebeacua[4], Stefan Findeisen[1], Olivier Bouton[2], Tom Wirtz[2], and Gregor Hlawacek[1] — [1]Helmholz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg — [3]Photonis Netherlands B.V, Ro-

den, Netherlands — [4]Eidgenössische Technische Hochschule, Zürich, Switzerland

Transmission imaging in the helium ion microscope allows to measure mass-thickness contrast and reveal crystallographic information. We recently customized a microchannel plate followed by a delay line readout structure especially for this application. This system can correlate the scanning transmission ion image to the angular distribution of the transmitted ions. An in-vacuum linear support is used to place the detector at different distances from the sample, adjusting the maximum collection angle. Post-processing allows the reconstruction of images for selected scattering angles. The first results show images with nanometer resolution, material contrast, and identification of subsurface features in biological tissues. This work has been supported by the H2020 Project npSCOPE under grant number 720964.

KFM 5.7 Mon 17:20 TOE 317

Positron Annihilation Studies using a Superconducting Electron Linac — •Maik Butterling[1], Andreas Wagner[1], Maciej Oskar Liedke[1], Eric Hirschmann[1], Ahmed G. Attalah[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 up to 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 6: Diamond

Time: Tuesday 9:30–11:50 Location: TOE 317

KFM 6.1 Tue 9:30 TOE 317

ECRH systems for nuclear fusion reactors — •Dirk Strauss, Theo Scherer, Sabine Schreck, Peter Späh, Andreas Meier, and Gaetano Aiello — Karlsruher Institut für Technologie KIT-IAM-AWP ; D-76344 Eggenstein-Leopoldshafen

A typical ECRH system in fusion devices includes gyrotrons as millimeter wave beam sources, transmission lines with a diamond window as confinement barrier and antennas to inject the beam into the plasma. The electron-cyclotron resonance condition at the required position can be achieved by angular steering or frequency tuning. Apart from heating and current profile shaping the small wavelength allows to suppress MHD instabilities as neoclassical tearing modes. The state of the art ECRH is presented and different variants are discussed with a focus on ultra-low-loss CVD diamond windows.

KFM 6.2 Tue 9:50 TOE 317

Application of CVD Diamond disks for ECRH systems of fusion reactors — •Sabine Schreck, Gaetano Aiello, Andreas Meier, Theo Scherer, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany ,

In fusion reactors, Electron Cyclotron Heating and Current Drive (EC H&CD) systems are used for plasma heating and stabilization. Key components of these systems are diamond windows, which consist of a chemical vapor deposition (CVD) diamond disk (p.c.) joined into a metallic housing. Such windows, employed as gyrotron- or torus windows, allow transmission of high power microwave beams and serve as vacuum boundaries. A very low dielectric loss and a sufficient mechanical stability is thus required.

The ITER EC torus window consists of a diamond disk with a diameter of about 70 mm and a thickness of 1.11 mm (resonance thickness for 170 GHz). The window serves also as confinement barrier for tritium and is classified as "Protection Important Component". A specific test program is required for its qualification, including prototypical activities.

For future fusion machines like DEMO, most likely broadband window solutions as the double disk window or the Brewster window will come into operations. This implies also new requirements for the disks, e.g. large diameters of minimum 180mm for the inclined Brewster-angle disk for a typical aperture of 63.5 mm.

KFM 6.3 Tue 10:10 TOE 317

MPA CVD diamond in nuclear fusion: dielectric characterization and influence of defects — •Gaetano Aiello, Theo Scherer, Andreas Meier, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, D-76021 Karlsruhe, Germany

Microwave Plasma Assisted (MPA) Chemical Vapour Deposition (CVD) diamond is used as window material in the shape of a disk in the heating and diagnostic systems for fusion reactors due to its combination of extraordinary thermal, mechanical and optical properties. CVD diamond polycrystalline disks with central loss tangent lower than 2E-05 allow for transmission of high power microwave beams (1-2 MW). However, the effect on the dielectric losses in diamond of defects like dislocations and nitrogen-vacancy centers introduced by the growing process and/or by subsequent neutrons and gammas irradiation has not fully investigated and understood so far. Investigations by several spectroscopic methods on non-irradiated and irradiated diamond samples are thus planned. In particular, first Elastic Recoil Detection Analysis (ERDA) measurements of small diamond samples have been carried out at the Tandem Laboratory in Uppsala, Sweden, aiming to calculate the sample composition with major focus on nitrogen content. The nitrogen plays an important role in the CVD process as it allows faster growth rates, but it causes greater dielectric losses in diamond.

20 min. break

KFM 6.4 Tue 10:50 TOE 317

Fabrication of Thin Monocrystalline Diamond Membranes — •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

Due to its exceptional physical and chemical characteristics, diamond in a form of thin membranes is a particularly promising material for the fabrication of high quality photonic devices with envisioned applications in quantum information technologies (QIT). In this work we report on the structuring process of thin monocrystalline diamond (MCD) membranes, with a thickness of a few microns and rms roughness values in the range of 0.5-0.6 nm (on a 5 x 5 μm area), by means of inductively coupled plasma reactive ion etching (ICP RIE). A diamond bulk mask was utilized as an etch mask during the fabrication, featuring distinct hole diameters with angled sidewalls to avoid trenches and cracks at the edges of the membrane. Besides an examination of different mask diameters on the resulting morphology and etch quality of the membranes, differing etching mixtures and arrangements were tested to minimize the micro-masking, which can lead to pit structures and hence to an enhanced roughness of the membrane.

KFM 6.5 Tue 11:10 TOE 317

Immobilization of Proteins on Ultrananocrystalline Diamond Surfaces — •Daniel Merker[1], Daniela Bertinetti[2], Katrin Schröder[3], Monika Stengl[3], Friedrich Herberg[2], Johann Peter Reithmaier[1], and Cyril Popov[1] — [1]Institute of Nanostructure Technologies and Analytics, Universität Kassel, Deutschland — [2]Department of Biochemistry, Universität Kassel, Deutschland —

[3]Department of Animal Physiology, Universität Kassel, Deutschland

To investigate the molecular mechanisms of the inner clock in the madeira cockroach the detection of coupling factors is required. These coupling factors are secreted neuropeptides and neurotransmitters necessary to synchronize clock neurons into ensembles which direct the circadian rhythm. In this work we study the possible application of UNCD as a substrate for antibody immobilization to detect these coupling factors. Initially, various covalent coupling routes were investigated to immobilize the green fluorescent protein (GFP). Besides coupling chemistry with functional groups introduced directly on the UNCD surface by plasma, photochemical grafting on H-terminated as-grown UNCD was also investigated. The covalent coupling did not work since the functional groups on the UNCD surface were not reactive enough. In contrast, the photochemical grafting showed successful immobilization of GFP on surfaces with patterned modification (H-terminated squares on O-terminated surface). Since the O-terminated UNCD films have been already successfully applied for long-term cultivation of clock neurons we aim to utilize UNCD as antibody platform and to realize a time-resolved detection of coupling factors.

KFM 6.6 Tue 11:30 TOE 317

Physics of natural and artificial diamond gemstones — •Theo Andreas Scherer — KIT-IAM-AWP, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen

Diamond gemstones were very well appreciated in the antique world. Independent on the purpose of jewelry, diamond is a crystalline solid state material with excellent physical and chemical properties as a high Young modulus or a very high thermal conductivity. By doping the material with boron, electrical conductivity can be observed. This is important for electronic devices. In this talk the wide range of production of gemstones and technical applications like high frequency high power microwave transmission diamond windows for nuclear fusion power plants will be presented. Different diamond classifications, cuts and colors by impurities will be shown. A comparison of natural diamonds and artificial produces ones are topic of the discussion.

KFM 7: Whispering-Gallery-Mode Resonators

Time: Tuesday 12:00–13:40 Location: TOE 317

KFM 7.1 Tue 12:00 TOE 317

Super-directional light emission and emission reversal from micro cavity arrays — Jakob Kreismann, Jaewon Kim, Martí Bosch, Matthias Hein, Stefan Sinzinger, and •Martina Hentschel — Institute for Micro- und Nanotechnologies, Technische Universität Ilmenau, Germany

Optical microdisk cavities with certain asymmetric shapes are known to possess uni-directional far-field emission properties. Here, we investigate arrays of these dielectric microresonators with respect to their emission properties resulting from the coherent behaviour of the coupled constituents. This approach is inspired by electronic mesoscopic physics where the additional interference effects are known to enhance the properties of the individual system. As an example we study the linear arrangement of nominally identical Limaçon-shaped cavities and confirm the increase of directionally emitted light. We find its angular spread to diminish from 20 degrees for the single cavity to about 3 degrees for a linear array of 10 Limaçon resonators, in fair agreement with a simple array model. Moreover, varying the inter-cavity distance we observe windows where the emission directionality is further enhanced (super-directionality), as well as windows with a reversal of the emission direction, another effect that may be interesting for applications like optical sensing or interconnects. We introduce a generalized array factor model that takes the coupling into account.

KFM 7.2 Tue 12:20 TOE 317

Flexible Photonics based on Whispering-Gallery-Mode Resonators and Liquid-Crystal-Elastomers — •Simon Woska, Osman Karayel, Pascal Rietz, Roman Oberle, Jannis Hessenauer, Evelyn Kaiser, Stefan Pfleging, Carolin Klusmann, Tobias Siegle, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Whispering-Gallery-Mode (WGM) resonators confine light due to total internal reflection at their outer rim and feature both high quality factors and low mode volumes. Therefore, they hold huge potential as building blocks for photonic devices or for investigation of topological properties. Many of these applications require a precise tunability of the resonant wavelengths and/or the inter-cavity distance between several resonators. Meeting these requirements, flexible photonics come into play. We include Liquid Crystal Elastomers (LCEs) into our polymeric building blocks in order to exploit their directional, temperature-responsive, and reversible mechanical actuation. Thereby, we are able to tune the optical properties of our systems by precisely controlling their dimensions using temperature as an external stimulus.

In this contribution, we address two different systems: On the one hand, we introduce a pair of rigid WGM resonators mounted on an LCE substrate and show first results of reversible temperature-induced coupling. On the other hand, we present detailed investigations on fully tunable flexible WGM resonators. To this end, the cavities are entirely made from LCE. Hereby, also the effect of the birefringence of LCE on the temperature dependency of different WGMs is discussed.

KFM 7.3 Tue 12:40 TOE 317

Far-field polarization states of 3D-whispering-gallery-mode resonators — •Jakob Kreismann and Martina Hentschel — Technische Universität Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany

We investigate the far-field polarization states of whispering gallery modes in three-dimensional optical cone-shaped cavities. In particular, we study how the inclination angle of the cavity wall influences the polarization state of the far field. We show that the far-field lobes separate the helicities of light as a consequence of the spin-orbit coupling of light present in the cavity due to strong transverse confinement. Furthermore, the polarization states depend on the viewing angle, the opening angle of the conical cavity and the axial mode number. This is accompanied by a transition from linear to circular polarization without utilizing anisotropic or inhomogeneous materials.

KFM 7.4 Tue 13:00 TOE 317

Nonhermitian defect states from lifetime differences — •Marti Bosch[1,2], Simon Malzard[2,3], Martina Hentschel[1], and Henning Schomerus[2] — [1]TU Ilmenau, Ilmenau, Deutschland — [2]Lancaster University, Lancaster, UK — [3]Imperial College London, London, UK

Nonhermitian systems provide new avenues to create topological defect states. An unresolved general question is how much the formation of these states depends on asymmetric backscattering, be it nonreciprocal as in the nonhermitian skin effect or reciprocal as encountered between the internal states of asymmetric microresonators. Here, we demonstrate in a concrete, practically accessible setting of a lossy coupled-resonator optical waveguide that nonhermitian defect states can exist in open optical systems due to lifetime differences, without the need for asymmetric backscattering within or between the individual resonators. We apply our findings to a finite system of coupled circular resonators perturbed by nanoparticles, following the concept of creating an interface by inverting the position of the nanoparticles in half of the chain. We compare a coupled-mode tightbinding approximation to full-wave numerical simulations, showing that spectrally isolated defect states can indeed be implemented in this simple nonhermitian photonic device.

KFM 7.5 Tue 13:20 TOE 317

Splitting and combining of exceptional points — •Jaewon Kim[1] and Jung-Wan Ryu[2] — [1]Technische Universität Ilmenau, Germany — [2]Institute for Basic Science, Daejeon, South Korea

At Exceptional point(EP) of non-Hermitian system, not just eigenvalue of Hamiltonian but also its eigenfunctions are degenerated. For the sensor application of microcavity, it was shown that EP can be used to increase its sensitivity and it actually demonstrated experimentally. Since then, interests on higher order EP, where more than 3 eigenfunctions are degenerated, naturally arose.

We studied splitting and combining of higher order EPs. The results of splitting are depend on the form of perturbation. For instance, EP3

can break into 2 EP2 or 3 EP2. Also we interpreted that many EP2, as an analogy of atom, can combine to make higher order EPs. By studying how they combine we can classify higher order EP.

KFM 8: Multiferroics and Magnetoelectric Coupling I (joint session MA/KFM)

Time: Wednesday 9:30–12:15 Location: HSZ 401

KFM 8.1 Wed 9:30 HSZ 401

High Temperature THz study of conical phase of BiFeO3 — •Dániel Gergely Farkas[1,2], Boglárka Tóth[1], Kirill Amelin[3], Toomas Rõõm[3], Urmas Nagel[3], Toshimitsu Ito[4], and Sándor Bordács[1] — [1]Department of Physics, Budapest University of Technology and Economics — [2]Condensed Matter Research Group of the Hungarian Academy of Sciences, 1111 Budapest, Hungary — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — [4]National Institute of Advanced Industrial Science and Technology (AIST), Tokyo, Japan

Multiferroics, materials with coexisting ferroelectric and magnetic order, are one of the most intensively studied systems in modern solid-state physics. BiFeO3 is one of the most studied multiferroic material since its multiferroic phase persists also at room temperature [1].

A recent theoretical model [2] predicted a conical phase between the cycloidal and canted AFM phase in BiFeO3. Magnetization measurements up to 300K have already confirmed the existence of this intermediate phase [3].

We performed THz absorption measurements at temperatures between 5-350K, and observed the magnon spectrum of the conical phase. The phase transitions and their hysteresis were observed at 300 and 350K.

[1] J. Moreau, et al., J. Phys. Chem. Solids 32, 1315 (1971).
[2] Z. V. Greeva, et al., Phys. Rev. B 87, 214413 (2013).
[3] S. Kawachi, et al., Phys. Rev. Mat. 1, 024408 (2017).

KFM 8.2 Wed 9:45 HSZ 401

Metastable transverse conical state in multiferroic BiFeO3 — •Boglarka Toth[1], Daniel Gergely Farkas[1], Jonathan S. White[2], Istvan Kezsmarki[3], Toshimitsu Ito[4], and Sandor Bordacs[1] — [1]Budapest University of Technology and Economics, Physics Department — [2]Paul Scherrer Institute — [3]University of Augsburg — [4]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8562 Ibaraki, Japan

Magnetoelectric multiferroic materials with coexisting ferroelectric and magnetic orders have received much attention as they may find applications in low power consumption magnetoelectric memories and data storage devices. Among these materials, $BiFeO_3$ is a unique compound as it is multiferroic even at room temperature, which is essential for future applications. Although $BiFeO_3$ is the most studied multiferroic material, its magnetic phase diagram is not fully understood. Due to the ferroelectric distortion, the so-called Dzyaloshinskii-Moriya interaction is allowed, which, competing with the Heisenberg interaction, results in a cycloidal structure below T_N = 640 K in zero field. We investigated the magnetic phases above room temperature using magnetization measurements and small-angle neutron scattering (SANS) and found a transverse conical state between the zero-field cycloidal state and the high field canted antiferromagnetic phase. Furthermore, the conical state with large magnetoelectric effect remains (meta)stable in zero-field after decreasing the magnetic field.

KFM 8.3 Wed 10:00 HSZ 401

Magneto-electric properties and low-energy excitations of multiferroic $FeCr_2S_4$ — •Ana Strinic[1], Stephan Reschke[1], Zhe Wang[1], Michael Schmid[1], Alois Loidl[1], Vladimir Tsurkan[1,2], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86159 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chisinau, Republic of Moldova

$FeCr_2S_4$ is under investigation for over four decades and shows remarkable magnetic as well as electronic properties. While a paramagnetic state is present at room temperature, for low temperatures long-range ferromagnetic order stets in and is followed by an incommensurate magnetic structure. Below $T = 10$ K a multiferroic ground state with orbital ordering is reached and IR phonons indicate a loss of inversion symmetry [1][2][3]. We report on the low-frequency optical excitations measured by THz spectroscopy. We measured the magnetic field dependence within the temperature range of orbital ordering and the temperature dependence of the different phases within the H-T-phase diagram for several polarizations of the THz-radiation in relation to the applied magnetic field. We will discuss the origin of the low-energy excitations and their relation with multiferroic properties of $FeCr_2S_4$.

[1] J. Bertinshaw *et al.*, Scientific Reports, 4, (2014).
[2] L. Lin *et al.*, Scientific Reports, 4, (2014).
[3] J. Deisenhofer *et. al.*, Physical Review B, 100, (2019).

KFM 8.4 Wed 10:15 HSZ 401

Evidence for existence of electromagnon in the multiferroic phase of Cu(II)O: A novel type polarized neutron scattering study at the thermal triple-axis spectrometer PUMA@FRM II — •Avishek Maity[1,2], Steffen Schwesig[1], Fabian Ziegler[1], Oleg Sobolev[1], and Götz Eckold[1] — [1]Institute for Physical Chemistry, Georg-August-University of Göttingen, 37077 Göttingen, Germany — [2]Heinz Maier-Leibnitz Zentrum (FRM II), Technical University of Munich, 85748 Garching, Germany

Since the spontaneous electric polarization was discovered in one of its anti-ferromagnetic (AFM) phases AF2 with T_n = 230 K [1], Cu(II)O regained the focus of research as a model compound for high-temperature type-II multiferroics. The ferroelectricity in the AF2 phase is induced by the cycloidal spin arrangement due to an anisotropic super-exchange interaction (DM) leading to an interesting coupling between spinwave and optical phonon namely electromagnon which is the elementary excitations involving in the magnetoelectric coupling [2]. Here we present the results from polarized neutron scattering to characterize low-energy magnetic excitations in the multiferroic phase of CuO using a novel type of polarization analysis available at the thermal triple-axis spectrometer PUMA@FRM II allowing the simultaneous detection of spinflip and non-spinflip scattering. We have determined energy gaps of several magnon modes and evidenced the signature for the existence of electromagnons near 3 and 13 meV [3].

Refs: [1] Kimura *et al.*, Nat. Mat. 7, 291 (2008). [2] Cao *et al.*, Phys. Rev. Lett. 114, 197201 (2015). [3] Maity *et al.* 2019 (submitted).

KFM 8.5 Wed 10:30 HSZ 401

Quantifying multiferroic domain population by nuclear magnetic resonance spectroscopy — •Thomas Gimpel[1], Markus Prinz-Zwick[1], Caroline Steinbrecht[1], Norbert Büttgen[1], Vladimir Tsurkan[1,2], and István Kézsmárki[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, Academiei strada 5, Chisinau, Republic of Moldova

We demonstrate that nuclear magnetic resonance spectroscopy can be used to measure the volume fraction of multiferroic domains. This new technique is applicable to anisotropic magnets where the different multiferroic domains are characterized either by different orientations of the magnetization or by different forms of the hyperfine coupling or the quadrupole interactions. The latter case is realized, e.g., in type-I mutliferroics where the ferroelectric domains have non-collinear polar axes. We carried out a proof-of-concept study on GaV_4Se_8 which has recently gained interest due to its multiferroic behavior and for hosting Néel-type magnetic skyrmions. This material becomes ferroelectric below 42 K - where four polar domains with polar axes along the cubic <111>-type axes emerge - and orders magnetically below 18 K. Its multiferroic domain population can be controlled either by magnetic or by electric fields. By our new method we can directly quantify the volume fraction of each of the four domains.

15 min. break.

KFM 8.6 Wed 11:00 HSZ 401

Revealing the antiferromagnetic spin density in multiferroic $Ba_2CoGe_2O_7$ — •Henrik Thoma[1], Vladimir Hutanu[2], Manuel Angst[3], Georg Roth[4], and Thomas Brückel[3] — [1]Jülich Centre for Neutron Science JCNS at MLZ, 85747 Garching, Germany —

[2]Institute of Crystallography, RWTH Aachen and Jülich Centre for Neutron Science JCNS at MLZ, 85747 Garching, Germany — [3]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institute PGI, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [4]Institute of Crystallography, RWTH Aachen, 52056 Aachen, Germany

Polarized neutron diffraction (PND) is a powerful method which provides direct access to the scattering contribution from nuclear-magnetic interference and thus reveals the phase difference between the nuclear and magnetic structure. Generally limited to the case of centrosymmetric structures in the paramagnetic state, this information can be used to construct spin density maps and local susceptibility tensors in order to study the anisotropy between magnetic interactions. Introducing an advanced approach in the maximum-entropy method for a model-free reconstruction of spin densities, these limitations were overcome. PND was applied to study the magnetic anisotropy in the non-centrosymmetric unconventional multiferroic $Ba_2CoGe_2O_7$. Using the new approach, a detailed 3D spin density distribution in the unit cell was obtained for the first time both in the paramagnetic and antiferromagnetic ground state. The obtained results clearly show the 2D character of the magnetic interactions in the title compound and are compared to the results of regular magnetic structure refinement.

KFM 8.7 Wed 11:15 HSZ 401

In situ electric and magnetic control of conductive domain walls in multiferroic GaV_4S_8 — •Somnath Ghara, Korbinian Geirhos, Vladimir Tsurkan, Peter Lunkenheimer, and István Kézsmárki — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

GaV_4S_8, the lacunar spinel compound, has recently attracted interests due to the presence of different modulated magnetic phases, including Néel-type skyrmions and multiferroic properties. This compound undergoes a transition to the polar rhombohedral ($R3m$) state at T_{JT} = 45 K and a subsequent magnetic transition at T_C = 13 K. In the present work, by polarization and magnetic susceptibility studies, we demonstrate that the population of the four polar domains, with polarization along the four cubic < 111 >-type directions, can be controlled in situ both by electric and magnetic fields. Most interestingly, the dc conductivity of the polar multi-domain state is 10^6 times higher than that of the mono-domain state, indicating the presence of conductive domain walls. Correspondingly, when tuning the domain wall density by magnetic fields, we could achieve a giant magnetoresistance as high as 10^8 %. Furthermore, the conductivity of the domain walls shows a strong non-linearity, in contrast to the bulk.

KFM 8.8 Wed 11:30 HSZ 401

Dielectric loss in spiral magnets — •Francesco Foggetti[1,2], Andrei Pimenov[3], and Sergey Artyukhin[1] — [1]Istituto Italiano di Tecnologia, Genova, Italy — [2]Università di Genova, Genova, Italy — [3]Institut für Festkörperphysik, Wien, Austria

Magnetic frustration often results in non-trivial spin textures. Spiral spin structures are common in magnetic perovskites due to competing exchange interactions and may give rise to ferroelectric polarization via inverse Dzyaloshinskii-Moriya mechanism. Here we model chiral domain walls in the spiral magnetic order and characterize the excitation spectrum using a model Hamiltonian describing spins interacting with polar ionic displacements. Results suggest that high dielectric constant in spiral multiferroics (i.e. $TbMnO_3$, $MnWO_4$) originates from contributions of soft domain wall-localized electromagnons and that spiral order may play a fundamental role in the giant magneto-electric effect, observed in proximity of a phase transition from collinear antiferromagnetic order to a conical spiral in Ni_3TeO_6.

KFM 8.9 Wed 11:45 HSZ 401

Depth-resolved magnetism in La0.67 Sr0.33 MnO3/PMN-PT as a function of applied electric field — •Tanvi Bhatnagar[1,2], Anirban Sarkar[1], Emmanuel Kentzinger[1], Andras Kovács[2], Qianqian Lan[2], Patrick Schöffmann[3], Annika Stellhorn[1], Markus Waschk[1], Brian Kirby[4], Alexander Grutter[4], Rafal Edward Dunin-Borkowski[2], and Thomas Brückel[1] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institute (PGI-4), JARA-FIT, 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute (PGI-5), 52425 Jülich, Germany — [3]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at MLZ, 85747 Garching, Germany — [4]NIST Center for Neutron Research, NIST, Gaithersburg, MD

The magnetic depth profile of an epitaxially-grown artificial multiferroic ferromagnetic/ (ferroelectric, piezoelectric) La0.67Sr0.33MnO3/0.7(Pb(Mg1/3Nb2/3)O3)-0.3(PbTiO3)(001) heterostructure is studied using polarized neutron reflectometry, revealing changes in interfacial magnetism when a voltage is applied between the layers. For a better understanding of the results, structural characterization of the interfacial morphology is performed using transmission electron microscopy.

KFM 8.10 Wed 12:00 HSZ 401

Polarized neutron reflectometry of magneto-electric coupling in Fe_3O_4/PMN-PT(011) artificial multiferroic heterostructures — •Patrick Schöffmann[1], Anirban Sarkar[2], Tanvi Bhatnagar[2,3], Mai Hussain Hamed[4], Stephan Geprägs[5], Emmanuel Kentzinger[2], Annika Stellhorn[2], Brian Kirby[6], Alexander Grutter[6], Sabine Pütter[1], Martina Müller[4], and Thomas Brückel[2] — [1]Forschungszentrum Jülich GmbH, JCNS@MLZ, Garching, Germany — [2]Forschungszentrum Jülich GmbH, JCNS-2 and PGI-4, JARA-FIT, Jülich, Germany — [3]Forschungszentrum Jülich GmbH, ER-C-1 and PGI-5, Jülich, Germany — [4]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [5]Walther-Meißner Institute, BAdW, Garching, Germany — [6]NIST Center for Neutron Research, NIST, Gaithersburg, USA

Magnetoelectric coupling phenomena in artificial thin film heterostructures have attracted attention because of the rich application possibilities in data storage and novel devices. Growing a ferrimagnetic Fe_3O_4 thin film on a ferroelectric $[Pb(Mg_{1/3}Nb_{2/3})O_3]_{0.7}$-$[PbTiO_3]_{0.3}$ (PMN-PT) substrate in (011) orientation constitutes a heterostructure that allows for control of magnetic properties via an applied out-of-plane voltage. Using SQUID magnetometry and polarised neutron reflectometry, a clear change in magnetisation strength and orientation through the sample depth can be observed, upon the application of voltage. The effects are different along the in-plane axes (100) and $(01\bar{1})$.

KFM 9: Focus: Polar oxide crystals and solid solutions

Time: Wednesday 9:30–13:30 Location: TOE 317

KFM 9.1 Wed 9:30 TOE 317

On the Growth of Lithium Niobate-Tantalate Solid Solution Single Crystals — •Steffen Ganschow[1], Detlef Klimm[1], Michael Rüsing[2], Benjamin Kirbus[2], Zeeshan Amber[2], and Lukas M. Eng[2] — [1]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany — [2]Institut für Angewandte Physik, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

Lithium niobate ($LiNbO_3$, LN) and lithium tantalate ($LiTaO_3$, LT) belong to the most widely used ferroelectric materials, with applications that range from novel electronic and micro-mechanical devices to (integrated, nonlinear) optics. Recently, lithium niobate-tantalate solid-solution ($LiTa_xNb_{1-x}O_3$, LNT) single crystals have been demonstrated. LNT potentially might outperform pure LN and LT applications, since offering superior material properties such as the tailored birefringence combined with large temperature stability.

Crystallization of LNT solid solutions from the melt is characterized by a strong segregation leading to a pronounced macro-distribution of components and, occasionally, to cellular growth [1,2]. In this contribution here, we critically review previous attempts to manufacture LNT single crystals, and discuss novel approaches that promise LNT single crystals of enhanced chemical homogeneity. A phase diagram of the quasi-binary system based on a thermal analysis will be presented along with the results of our first crystal growth experiments.

[1] T. Fukuda and H. Hirano, J. Crystal Growth 33, 127 (1976).
[2] A. Bartasyte et al., Mater. Chem. Phys. 134, 728 (2012).

KFM 9.2 Wed 9:50 TOE 317

Poling of lithium niobate tantalate mixed crystals: Lessons learned from lithium niobate and tantalate — •Lukas M. Eng[1], Steffen Ganschow[2], Henrik Beccard[1], Ekta Singh[1], Zeeshan Amber[1], Benjamin Kirbus[1], and Michael Rüsing[1] — [1]Institut für Angewandte Physik, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

The ability to structure ferroelectric domains is the key ability for the functionalization of ferroelectric materials leading to their broad palette of applications, ranging from novel electronics, micromechanical devices, to (integrated, nonlinear) optics. Lithium niobate ($LiNbO_3$, LN) and lithium tantalate ($LiTaO_3$, LT) belong to the most widespread used materials for these applications. Recently, lithium niobate-tantalate ($LiTa_xNb_{(1-x)}O_3$, LNT) mixed crystals have been fabricated, that potentially promise advantages over the boundaries of bare LN or LT, such as an improved temperature stability, or the tailoring of material properties such as the birefringence. Furthermore, LNT presents a model system for testing the impact and relevance of several effects (doping, poling, temperature, etc.) on their technological performance. In this work we discuss and analyze the poling of the model systems LN and LT and present first observations of domains in this mixed crystal system. The fabrication and analysis of poled domains in the model system LNT presents a key step towards realizing novel devices for a broader range of applications.

KFM 9.3 Wed 10:10 TOE 317

High fidelity periodic poling of x-cut thin film lithium niobate for integrated optics analyzed with second harmonic microscopy — •Michael Rüsing[1], Jie Zhao[2], Shayan Mookherjea[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany — [2]University of California, San Diego, 9500 Gilman Dr, La Jolla, CA-92093-0407, USA

Nonlinear optics in periodically-poled thin film lithium niobate (TFLN) promises superior performance and conversion efficiencies compared to their bulk counterparts. The keys to high nonlinear conversion efficiency are high fidelity periodic poling of waveguides with a homogenous domain duty cycle, and long poling length (at least for several mm). Recently observed conversion efficiencies are limited by poling length or by inhomogeneous domain duty cycles. In this work we demonstrate periodic poling of TFLN using a single poling pulse with a tailored waveform. The poling process is analyzed in detail with Second Harmonic (SH) microcopy which provides nondestructive information about the poling quality, such as the poling depth of inverted domains measured with a 10 nm depth resolution. This enables us to produce near-perfect poling of domains over the entire length of up to 5 mm with a periodicity as small as 3 μm. Such devices are shown to possess a high SH conversion efficiency, as well as high-quality and narrow-band entangled photon-pair generation at telecommunication wavelengths.

KFM 9.4 Wed 10:30 TOE 317

Ion Transport in LiNbO3 - An Overview — Johanna Uhlendorf[1], Peter Fielitz[1], Erwin Hüger[1,2], Lars Dörrer[1,2], Steffen Ganschow[3], Klaus-Dieter Becker[4], Holger Fritze[5], Günter Borchardt[1], and •Harald Schmidt[1,2] — [1]TU Clausthal, Institut für Metallurgie — [2]TU Clausthal, Clausthaler Zentrum für Materialtechnik — [3]Leibniz-Institut für Kristallzüchtung, Berlin — [4]TU Braunschweig, Institut für Physikalische und Theoretische Chemie — [5]TU Clausthal, Institut für Energieforschung und Physikalische Technologien

Lithium niobate (LN) is one of the most technologically important polar metal oxides with an extraordinary combination of ferroelectric, piezoelectric, acoustic, optical as well as ion conducting properties. The self-diffusion of the ionic constituents and the underlying point defects of LN are of high importance for the overall conductivity, structural disorder, stability of defect clusters, ferroelectric domain wall pinning, high temperature stability and optical applications. We present a comprehensive overview of the state-of-the-art knowledge on the diffusion of Li, Nb, and O in LN as investigated in our laboratories during the last years. The experiments were carried out with stable tracers in combination with secondary ion mass spectrometry, neutron reflectometry and high-temperature optical spectroscopy.

10 min. break

KFM 9.5 Wed 11:00 TOE 317

Oxygen transport in single crystalline Li(Nb,Ta)O3 solid solutions at high temperatures — •Bujar Jerliu[1], Yuriy Suhak[1], Dmitry Roshchupkin[2], Boris Red'kin[2], Steffen Ganschow[3], Harald Schmidt[1], Günter Borchardt[1], Klaus Dieter Becker[4] und Holger Fritze[1] — [1]Clausthal University of Technology, Goslar, Germany — [2]Institute of Microelectronics Technology and High Purity Materials, RAS, Chernogolovka, Russia — [3]Leibnitz Institute for Crystal Growth, Berlin, Germany — [4]Braunschweig University of Technology, Braunschweig, Germany

Single crystalline lithium niobate-tantalate (LiTaxNb(1-x)O3, LNT) solid solutions are expected to overcome the problems of thermal instability of lithium niobate (LiNbO3, LN) and low Curie temperature of lithium tantalate (LiTaO3, LT). This work focuses on study of transport mechanisms in LNT crystals with different Nb/Ta ratio, grown by the Czochralski technique. The oxygen transport kinetics are investigated in the temperature range from 850°C to 1200°C using the stable isotope 18O as the tracer. Subsequently, the diffusion profiles are acquired by secondary ion mass spectrometry. The oxygen diffusion coefficients for LiNb0.88Ta0.12O3 single crystals at annealing temperatures of 850°C and 1000°C equal about 4.5 x 10-18 m2/s and 1.5 x 10-16 m2/s, respectively. Our previous 18O tracer experiments carried out on stoichiometric LN revealed a local maximum on the depth profiles, which was explained by the Li-diffusion out of the crystal structure. Such a maximum is not observed for LNT compound, which could possibly indicate an improved stability of the material.

KFM 9.6 Wed 11:20 TOE 317

Electrical and electromechanical properties of single crystalline Li(Nb,Ta)O3 solid solutions at elevated temperatures — •Yuriy Suhak[1], Bujar Jerliu[1], Dmitry Roshchupkin[2], Boris Red'kin[2], Steffen Ganschow[3], Günter Borchardt[1], Klaus-Dieter Becker[4], and Holger Fritze[1] — [1]Clausthal University of Technology, Goslar, Germany — [2]Institute of Microelectronics Technology and High Purity Materials, Chernogolovka, Russia — [3]Leibniz Institute for Crystal Growth, Berlin, Germany — [4]Braunschweig University of Technology, Braunschweig, Germany

Piezoelectric materials with high piezoelectric coefficients that can be operated above 500 °C are in high demand for industrial actuating applications. Lithium niobate (LiNbO3) and lithium tantalate (LiTaO3) possess high piezoelectric coefficients, however their usage is limited by thermal instability (LiNbO3) and low Curie temperature (LiTaO3). This work focuses on the electrical and electromechanical properties of Li(Nb,Ta)O3 crystals that are expected to overcome the mentioned restrictions of individual compounds. The electrical and electromechanical properties are investigated by means of impedance spectroscopy and resonant ultrasound spectroscopy, respectively. The experiments are performed in a gas-tight tube furnace, which allows working temperatures up to 1000 °C. The investigations revealed, that Li(Nb,Ta)O3 solid solutions show lower conductivity than LiNbO3 at high temperatures and low oxygen partial pressures (pO2). At 930 °C and pO2 of 10-15 bar the conductivity of LiNb0.29Ta0.71O3 sample is almost two orders of magnitude lower than that of LiNbO3.

KFM 9.7 Wed 11:40 TOE 317

Photoconductivity of strontium barium niobate revisited: spectral features, long-term relaxation, current-voltage hysteresis — •Elke Beyreuther[1], Julius Ratzenberger[1], Liudmila I. Ivleva[2], Pavel A. Lykov[2], and Lukas M. Eng[1,3] — [1]Institute of Applied Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Prokhorov Institute of General Physics, Russian Academy of Sciences, Moscow, Russia — [3]Cluster of Excellence 2147 – Complexity and Topology in Quantum Matter (ct.qmat)

Here, we report on the large photoconductive response (PCR) of strontium barium niobate ($Sr_{0.61}Ba_{0.39}Nb_2O_6$, SBN61) single-crystals grown by the modified Stepanov technique. We analyzed the PCR for both z- and x-cut SBN61 samples, using two different electrical wiring setups for each, by gradually varying the intensity and spectral composition of the incident photons. The crystals show a pronounced PCR already under diffuse daylight. Apart from a huge resistance decrease by three orders of magnitude upon super-bandgap illumination (370 nm), we observe in all four samples (i) distinct spectral features upon sub-bandgap excitation (800-390 nm) that clearly hint towards in-gap states beyond the one- and two-center models discussed in conjunction with doped SBN61 so far, as well as (ii) an extremely slow long-term relaxation for both light-on and light-off transients in the

range of hours (after sub-bandgap excitation) and days (after super-bandgap excitation). Moreover, a strong phototunable I-V hysteresis (tested with 500-nm and 380-nm illumination) along the polar axis of the z-cut sample is measured.

KFM 9.8 Wed 12:00 TOE 317

Superposed picosecond luminescence kinetics in lithium niobate — •Andreas Krampf, Simon Messerschmidt, and Mirco Imlau — University of Osnabrueck, Department of Physics, Barbarastrasse 7, 49076 Osnabrueck, Germany

Various manifestations of small polarons strongly affect the linear and nonlinear optical properties in the oxide crystal lithium niobate ($LiNbO_3$, LN). Whereas related transient-absorption phenomena in LN have been studied extensively in the last decades, a sound microscopic picture describing the blue-green (photo)luminescence of lithium niobate single crystals is still missing. In particular, nearly nothing is known about: (i) the luminescence build-up and (ii) its room temperature decay. We here present the results of our systematic experimental study using nominally undoped and Mg-doped LN crystals with different Mg concentration. Picosecond luminescence was detected by means of femtosecond fluorescence upconversion spectroscopy (FLUPS) extended to the inspection of oxide crystals in reflection geometry.

Taking the recently proposed microscopic model into account, which describes luminescence decay in LN by local radiative self-trapped exciton recombination and/or migration and subsequent pinning on defect sites, a detailed analysis of the kinetic traces reveals, that the picosecond luminescence decay represents the superposition of exponential and stretched-exponential decay paths.

We critically discuss the data considering the interplay with small polaron transport. Financial support by the DFG (IM37/11-1, INST 190/165-1 FUGG) is gratefully acknowledged.

10 min. break

KFM 9.9 Wed 12:30 TOE 317

A high-temperature optical spectroscopy study of lithium niobate, $LiNbO_3$ — •Klaus-Dieter Becker[1], Jianmin Shi[1], Holger Fritze[2], Günter Borchardt[2], and Steffen Ganschow[3] — [1]TU Braunschweig, Institute of Physical and Theoretical Chemistry, 38106 Braunschweig, Germany — [2]Clausthal University of Technology, 38640 Goslar, Germany — [3]Leibniz Institute for Crystal Growth, 12489 Berlin

Optical absorption spectra of chemically reduced LN are dominated by broad bands in the visible and NIR region which have been attributed to various types of electron small polarons, see e.g. Ref. [1]. At 1000 °C, spectra measured under such conditions are dominated by an absorption band centered at about 0.9 eV due to free small polarons, i.e. due to electrons localized on niobium ions on regular sites. Band intensity has been found to follow a power law dependence on oxygen partial pressure P_{O2} of the form $(P_{O2})^m$ with m = 0.23 ± 0.01. This m-value is in excellent agreement the value of 1/4 predicted on the basis of point defect thermodynamics for the proposed chemical reduction model of LN. The experimental kinetics of reduction and oxidation processes upon oxygen activity jumps have been found to provide a non-conventional route to diffusion of lithium vacancies as well as to lithium ions in c-LN.

[1] O.F. Schirmer, M. Imlau, C. Merschjann, B. Schoke, J. Phys. Condens. Matter, 21 (2009) 123201.

KFM 9.10 Wed 12:50 TOE 317

Tunable conductive domain wall switches in 200-μm-thick lithium niobate single crystals — •Henrik Beccard, Benjamin Kirbus, Ekta Singh, Zeeshan Amber, Michael Rüsing, Elke Beyreuther, and Lukas M. Eng — Institut für Angewandte Physik, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

In the ferroelectric model material lithium niobate (LNO), state-of-the-art techniques allow the targeted poling of ferroelectric domains, as well as the robust enhancement of domain wall (DW) conductivity over several orders of magnitude [1]. Imaging and analyzing these properties can be elegantly performed with piezoresponse force microscopy (PFM) and confocal 3D second harmonic generation (SHG) microscopy [2]. The correlation between DW geometry and electrical DW conductivity is well established both theoretically and experimentally. Moreover, it can be adequately simulated e.g. using a resistor network model [3].

Therefore, an increasing focus in the ferroelectrics community is set on the realization of DW-based nanoelectronic devices. Recently, tunable DW switches have been reported for LNO thin films [4]. On the contrary, we report on tunable DW switches inside of 200-μm-thick LNO single crystals, relying purely on solid electrodes [5].

[1] C. Godau et al. ACS Nano 11, 4816 (2017)
[2] T. Kämpfe et al. Phys. Rev. B 8, 035314 (2014)
[3] B. Wolba et al. Adv. Electron. Mater. 4, 1700242 (2018)
[4] H. Lu et al. Adv. Mater. 1902890 (2019)
[5] B. Kirbus et al. ACS Appl. Nano Mater. 2, 5787 (2019)

KFM 9.11 Wed 13:10 TOE 317

$LiNbO_3$: Model ferroelectric oxide or unique compound? — •Simone Sanna[3], Andreas Krampf[1], Yuriy Suhak[2], Mirco Kai Imlau[1], and Holger Fritze[2] — [1]Universität Osnabrück — [2]Technische Universität Clausthal — [3]Justus-Liebig-Universität Gießen

After five decades of dedicated research, $LiNbO_3$ has become one of the most intensively investigated ferroelectrics. The effort of the ferroelectric community has lead to unprecedent deep insight (and open issues) in the physical mechanisms that determine the materials properties. It is however still to be settled whether the knowledge collected on $LiNbO_3$ is generally valid, or strictly material specific. In order to answer this question, we investigate and compare (theoretically and experimentally) fundamentally different aspects of $LiTaO_3$ and $LiNbO_3$. First principles calculations reveal the existence of point defects in $LiTaO_3$ compatible with the polaronic picture established in $LiNbO_3$. Luminescence and absorption spectroscopy measurements show very similar dynamics and spectral features in $LiNbO_3$ and $LiTaO_3$. Electrical conductivity measurements demonstrate the existence of a low temperature and a high temperature regime for the two materials, from which rather similar activation energies can be extrapolated. The results suggest that the knowledge of the physical mechanisms gathered on $LiNbO_3$ can be transferred to other ferroelectric oxides such as $LiTaO_3$ and related solid solutions.

KFM 10: Multiferroics and Magnetoelectric Coupling II (joint session MA/KFM)

Time: Wednesday 15:00–17:00 Location: HSZ 401

KFM 10.1 Wed 15:00 HSZ 401

Switching of magnetoelectric states in Y-type hexaferrite single crystals — •Vilmos Kocsis[1], Taro Nakajima[1], Masaaki Matsuda[2], Akiko Kikkawa[1], Yoshio Kaneko[1], Junya Takashima[1,3], Kazuhisa Kakurai[1,4], Taka-hisa Arima[1,5], Yusuke Tokunaga[1,5], Yoshinori Tokura[1,6], and Yasujiro Taguchi[1] — [1]RIKEN CEMS, Wako-shi, Japan — [2]Oak Ridge National Laboratory, Tennessee, USA — [3]Venture Lab TOKYO, Tokyo, Japan — [4]CROSS, Tokai, Japan — [5]Department of Advanced Materials Science, University of Tokyo, Kashiwa Japan — [6]Tokyo College and Department of Applied Physics, University of Tokyo, Tokyo, Japan

In Y-type hexaferrites, magnetic interactions result in a complex phase diagram with non-collinear magnetic phases. The magnetoelectric (ME) properties are mainly dominated by a multiferroic FE3 phase [1,2]. The FE3 phase has been observed both as a metastable and stable phase close to room temperatures [3,4,5] and offers an ideal candidate to study the stability of ME phases and ME states. Here we explore the direct and converse ME effects in Y-type hexaferrites with different Sr doping levels. We demonstrate the isothermal switching between ME states, and discuss these new results as a possible way to measure the stability of the ME state in multiferroic materials. [1] T. Kimura, Ann. Rev. Condens. Matter Phys. 3, 93-110 (2012) [2] T. Kimura et. al., PRL 94, 137201 (2005) [3] S. Hirose et. al., APL 104, 022907 (2014) [4] T. Nakajima et. al., PRB 94 195154 (2016) [5] V. Kocsis et. al., Nat. Comm. 10, 1247 (2019)

KFM 10.2 Wed 15:15 HSZ 401

Low-frequency magnetic resonances of the polar ferrimagnet Mn2Mo3O8 — •Dávid Szaller[1], Lukas Weymann[1], Alexey Shuvaev[1], Andrei Pimenov[1], Johan Viirok[2], Urmas Nagel[2], Toomas Room[2], Sándor Bordács[3], Krisztián Szász[3], Vladimir Tsurkan[4], and István Kézsmárki[4] — [1]Institute of Solis State Physics, TU Wien — [2]National Institute of Chemical Physics and Biophysics, Tallinn — [3]Department of Physics, Budapest University of Technology and Economics — [4]Experimental Physics V, University of Augsburg

The polar M2Mo3O8 crystals with M=Fe,Co,Mn, exhibit various magnetic orders coupled to the electric polarization of the material. In the static limit, this magneto-electric coupling opens a new path for data storage[1], while in the dynamical range the spin-wave excitations offer a model system to study axion physics[2]. However, the microscopic description of the spin-wave resonances and the magneto-electric coupling in these material family is still an open task.

We followed the magnetic field dependence of the spin-wave resonances of the ferrimagnetic Mn2Mo3O8 in three magnetic phases by combining far-infrared optical spectroscopy and backward-wave oscillators. Both the observed resonance frequencies and the field dependence of the magnetization were quantitatively reproduced by a relative simple anisotropic two-sublattice antiferromagnetic model.

[1]Y. Wang et al, Sci. Rep. 5, 12268 (2015).
[2]T. Kurumaji et al, Phys. Rev. Lett. 119, 077206 (2017).

KFM 10.3 Wed 15:30 HSZ 401

Signatures of electric dipoles in zig-zag spin chain β-$TeVO_4$ — Martina Dragičević[1], Željko Rapljenović[1], David Rivas Góngora[1], Mirta Herak[1], •Tomislav Ivek[1], Matej Pregelj[2], Andrej Zorko[2], Helmuth Berger[3], and Denis Arčon[2,4] — [1]Institute of Physics, Zagreb, Croatia — [2]Jožef Stefan Institute, Ljubljana, Slovenia — [3]Ecole polytechnique fédérale de Lausanne, Lausanne, Switzerland — [4]Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia

Even though non-composite magnetoelectric materials appear to be rare, one promising way to achieve magnetoelectric effect is through spiral magnetic orders which can break the space inversion symmetry and allow electric dipoles to form. In this work we present the dielectric response of single crystal quasi-1D quantum magnet β-$TeVO_4$ at low temperatures and in the presence of external magnetic field. This zig-zag spin chain system with frustrated anisotropic interactions has a complex phase diagram: at $T_{N1} = 4.65\,K$ the paramagnetic phase gives way to an incommensurate spin-density wave; below $T_{N2} = 3.28\,K$ a superposition of two spin-density waves is observed with differing wave vectors, the so-called spin stripe phase; finally, at the low temperature of $T_{N3} = 2.28\,K$ their two wave vectors coincide and a vector chiral ground state is established. Most interestingly, at T_{N3} there are tantalizing experimental indications of emergent electric dipoles. The magnetic phase diagram will be discussed in the context of dielectric properties and of ground state as a potentially multiferroic phase.

KFM 10.4 Wed 15:45 HSZ 401

In-plane magnetoelectric response in bilayer graphene — •Paul Wenk[1], Michael Kammermeier[2], and Ulrich Zülicke[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, P.O. Box 600, Wellington 6140, New Zealand

A graphene bilayer shows an unusual magnetoelectric response whose magnitude is controlled by the valley-isospin density, making it possible to link magnetoelectric behavior to valleytronics. Complementary to previous studies, we consider the effect of static homogeneous electric and magnetic fields that are oriented parallel to the bilayer's plane. Starting from a tight-binding description and using quasidegenerate perturbation theory, the low-energy Hamiltonian is derived, including all relevant magnetoelectric terms whose prefactors are expressed in terms of tight-binding parameters. We confirm the existence of an expected axion-type pseudoscalar term, which turns out to have the same sign and about twice the magnitude of the previously obtained out-of-plane counterpart. Additionally, small anisotropic corrections to the magnetoelectric tensor are found that are fundamentally related to the skew interlayer hopping parameter γ_4. We discuss possible ways to identify magnetoelectric effects by distinctive features in the optical conductivity.

[PRB **100**, 075421 (2019)]

KFM 10.5 Wed 16:00 HSZ 401

In-situ switching of the magnetoelectric domain states in the cubic spinel Co_3O_4 — •Maximilian Winkler, Somnath Ghara, Korbinian Geirhos, Peter Lunkenheimer, Stephan Krohns, Vladimir Tsurkan, and István Kézsmárki — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

We report a strong linear magnetoelectric effect in the collinear antiferromagnetic state of Co_3O_4 single crystals. Co_3O_4 crystallizes in the cubic spinel structure, with magnetic Co^{2+} at the A-sites, tetrahedrally surrounded by oxygen, and non-magnetic Co^{3+} at the B-sites in an octahedral environment [1]. In this work, we investigate all components of the magnetoelectric tensor and found that the largest value of is $\alpha = 14$ ps/m. We showed that the magnetoelectric monodomain state can be obtained by magnetoelectric poling across the Néel-temperature, $T_N = 30$ K. For the mono-domain state the sign of α depends on the sign of the product of the external electric and magnetic fields, E and H. We also demonstrated, that after the magnetoelectric poling below T_N the magnetoelectric domain state can be controlled in-situ by reversing either the external electric or magnetic field. The dynamics of this switching process leads to a deeper understanding of the linear magnetoelectric coupling in Co_3O_4.

[1] W. Roth, *J. Phys. Chem. Solids* **25**, 1-10 (1964)

KFM 10.6 Wed 16:15 HSZ 401

Magnetoelectricity in Itinerant-Electron Paramagnets, Ferromagnets and Antiferromagnets — •Roland Winkler[1,2,3] and Ulrich Zülicke[4,2] — [1]Physics, Northern Illinois University, USA — [2]Materials Science Division, Argonne National Laboratory, USA — [3]Materials Science and Engineering, University of Illinois at Urbana-Champaign, USA — [4]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, New Zealand

We present a detailed theory for magnetoelectricity in itinerant-electron paramagnets, ferromagnets and antiferromagnets, whereby an electric field can induce a magnetization and a magnetic field can induce a polarization. Accurate numerical calculations are complementd by analytical models that provide a detailed microscopic understanding of magnetoelectricity in itinerant-electron systems. Our realistic calculations suggest that an electrically induced magnetization can be as large as one Bohr magneton per charge carrier.

This work was supported by the NSF under Grant No. DMR-1310199. Research at UIUC was supported by the Illinois MRSEC, NSF Grant No. DMR-1720633. Work at Argonne was supported by DOE BES under Contract No. DE-AC02-06CH11357.

KFM 10.7 Wed 16:30 HSZ 401

Voltage-controlled on switching and manipulation of magnetization via redox transformation of beta-FeOOH nanoplatelets — •Martin Nichterwitz[1,2], Sabine Neitsch[1], Stefan Röher[1], Daniel Wolf[1], Kornelius Nielsch[1,2], and Karin Leistner[1] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany

Voltage control of magnetism by ionic approaches, such as the metal/metal oxide transformation in gated architectures, presents a promising pathway to low-power magnetic devices or magnetic actuation. Such magneto-ionic manipulation has been reported mainly for ultrathin films and nanoporous metal alloy structures so far.

We investigate electrodeposited porous beta-FeOOH nanoplatelets as starting material, known as active material from catalysis research. The FeOOH is polarized in 1M LiOH solution at room temperature. The voltage-induced structural and morphological changes are probed and correlated to the magnetic changes measured in an in situ anomalous Hall effect setup. This approach, starting from paramagnetic FeOOH, enables complete and non-volatile ON switching of ferromagnetic layers at a low voltage and large reversible magneto-ionic effects.[1] During the first reduction step, we transform FeOOH into a rough granular Fe layer. This high surface Fe layer is then switched reversibly via a redox transformation. As a result, large voltage-induced changes in magnetization are achieved, which exceed those obtained for sputtered Fe films and Fe nanoislands.[2]

[1] Nichterwitz et al., J. Phys. D (2019), accepted;
[2] Duschek et al., J. Mater. Chm. C 6 (2018) 8411

KFM 10.8 Wed 16:45 HSZ 401

Magneto-ionic tunable hysteresis, magnetic domains and exchange bias in ironoxide/iron surface layers — •Jonas Zehner[1], Rico Huhnstock[2], Steffen Oswald[1], Sebastian

Schneider[1], Ivan Soldatov[1], Sebastian Fähler[1], Rudolf Schäfer[1], Arno Ehresmann[2], Kornelius Nielsch[1], Dennis Holzinger[2], and Karin Leistner[1] — [1]IFW Dresden — [2]Uni Kassel, Institut für Physik und CINSaT

The ubiquity and rise in the use of electronic devices demands low power operation modes. Voltage assisted ionic displacement and electrochemical processes offer large magnetic changes at room temperature. This so called magneto-ionic (MI) control shows promising characteristics to enable energy efficient spintronics, actuation and neuromorphic computing. In the current study, MI effects on coercivity and exchange bias (EB) are demonstrated for sputter deposited and natively oxidized FeOx/Fe films of up to 13 nm in thickness. In FeOx/Fe films, the uniaxial anisotropy constant Ku increases upon an electrochemical transformation of the oxide layer to metal iron. At the same time, consistent with the anisotropy change, the equilibrium magnetic domain size increases. This effect enables voltage-induced 180° magnetization switching. In a next step, this tunable FeOx/Fe layer is combined with an underlying antiferromagnet. Non-volatile and reversible changes in the EB are achieved this way. The mechanism is revealed via X-ray photoemission spectroscopy and links the observed changes to an increase in the Fe layer thickness. These results are exciting for designing EB systems and magneto-electric devices in general.

KFM 11: Ferroics - Domains and Domain Walls (joint session KFM/MA)

Time: Wednesday 15:00–18:20 Location: TOE 317

KFM 11.1 Wed 15:00 TOE 317

Ferroelectric Domain Structure In Hexagonal Yttrium Manganite Thin Films - A Phase Field Study — •Amadé Bortis, Manfred Fiebig, and Thomas Lottermoser — Department of Materials, ETH Zurich, Zurich, Switzerland

The topologically protected vortex domains in hexagonal rare-earth manganites exhibit rich physics, both from a fundamental and application point of view. In thin films, however, the nanoscale domain size has thus far hindered the experimental investigation of domain patterns - the existence of vortex domains remains elusive. Here, we use a phase-field model based on a known Landau expansion of the free energy and incorporate boundary conditions for a thin film. With this model, we investigate up to which thickness a thin films retains the bulk-like vortex-string network - closed loops of connected vortices. We simulate the evolution of the structural domains for different thicknesses. In the ultrathin regime, we find straight lines of vortices emerging perpendicular to the films surface, similar to stacked 2D vortex patterns. As the thickness increases, we find an intermediate regime where the vortex lines start bending and merging, while still not being connected into closed loops. Finally, the bulk-like vortex-strings are recovered for a thickness of about 50 unit cells. Our work shows an effective 2D to 3D transition in rare-earth manganite thin films, revealing the impact of confined dimensionality on the domain topology.

KFM 11.2 Wed 15:20 TOE 317

Dielectric nonlinearity in $0.5(Ba_{0.7}Ca_{0.3})TiO_3$–$0.5Ba(Zr_{0.2}Ti_{0.8})O_3$ ferroelectric thin film capacitors — •Maximilian Becker[1,2], Claus Burkhardt[1], Reinhold Kleiner[2], and Dieter Koelle[2] — [1]NMI Natural and Medical Sciences Institute at the University of Tübingen, Reutlingen, Germany — [2]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, University of Tübingen, Germany

We use the recently developed Rayleigh analysis based on impedance spectroscopy to investigate dielectric nonlinearity caused by irreversible motion of domain walls in lead-free ferroelectric $0.5(Ba_{0.7}Ca_{0.3})TiO_3$–$0.5Ba(Zr_{0.2}Ti_{0.8})O_3$ (BCZT) thin films. Impedance spectra from 10 Hz to 1 MHz were collected at different excitation fields on pulsed laser deposited polycrystalline and epitaxial BCZT thin film capacitors. Rayleigh plots were created by fitting the measured complex impedance to an equivalent-circuit model containing the Rayleigh element. For a polycrystalline film, we observed nonlinear behavior in good agreement with the Rayleigh law at a threshold field $E_T \approx 55\,\mathrm{kV/cm}$ with Rayleigh constant $\alpha' = 0.407 \pm 0.035\,\mathrm{cm/kV}$. For the epitaxial counterpart, we found Rayleigh-like behavior which is not in full agreement with the Rayleigh law at $E_T \approx 3.75\,\mathrm{kV/cm}$ with $\alpha' = 1.836 \pm 0.031\,\mathrm{cm/kV}$, indicating a significantly higher domain wall mobility. Our results demonstrate the superiority of Rayleigh analysis based on impedance spectroscopy over the commonly used single-frequency approach.

This work was partly funded by the BMBF (Grant No. 13GW0123E).

KFM 11.3 Wed 15:40 TOE 317

Soft modes and effective Hamiltonian for the antiferroelectric NaNbO3 — •Niloofar Hadaeghi and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

To understand the antiferroelectric(AFE) phase transition in prototype $NaNbO_3$, we carried out detailed symmetry analysis and first-principles calculations. The primary modes have been identified together with the coupling terms up to the fourth order based on symmetry. The corresponding energy landscape is obtained by constraint calculations with specific mode(s) frozen-in, and is further fitted to get the effective Hamiltonian. It is observed that there are three dominant modes for the AFE phase of $NaNbO_3$; R_5^-, T_2, and Δ_5. Our results reveal that it is not possible for the system to adopt the coupling of R_5^- and T_2 modes, since there is a strong mutual repulsion between them. However, coupling of both R_5^- and Δ_5, and T_2 and R_5^- are essential in the reduction of energy. Theses couplings are cooperative to stabilize the AFE phase. That is, the trilinear coupling is essential for the occurrence of the AFE phase. We also investigated the unfolded band structure to understand the effects of such soft modes on the electronic structure.

KFM 11.4 Wed 16:00 TOE 317

Dimerized phases in IrTe2: phase diagram from a first-principles-derived model — Gabriele Saleh and •Sergey Artyukhin — Italian Institute of Technology, Genova, Italy

Materials with strong spin-orbit coupling have attracted recent interest due to their non-trivial magnetism and topological properties. IrTe2 combines some of the strongest spin-orbit-coupled cations and anions, and shows below 220 K a puzzling sequence of ordered phases with different patterns of short Ir-Ir bonds (dimers), some of which break the inversion symmetry. In spite of active efforts of the community, first principles simulations have struggled to describe the energetics of these phases, especially when the spin-orbit coupling is accounted for. Here we discuss a simplified model that captures dimer energetics, and use it to calculate the phase diagram and discuss the structure of domain walls. The choice of the model parameters is guided by first-principles simulations.

KFM 11.5 Wed 16:20 TOE 317

Robust In-Plane Ferroelectricity in Ultrathin Epitaxial Aurivillius Films — •Elzbieta Gradauskaite[1], Marco Campanini[2], Banani Biswas[3], Christof W. Schneider[3], Manfred Fiebig[1], Marta D. Rossell[2], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, Empa, Switzerland — [3]LMX, Paul Scherrer Institut, Switzerland

Layered ferroelectrics exhibit functionalities beyond those of the classical ferroelectric perovskite compounds due to their highly anisotropic structure. Unfortunately, the layered architecture has been impeding their growth as single crystalline thin films, and thus their integration into oxide-electronic devices. We show that deposition of layered ferroelectric $Bi_5FeTi_3O_{15}$ (BFTO) thin films on a lattice-matching $NdGaO_3$ (001)-oriented orthorhombic substrate supports the epitaxial single-crystal form of this Aurivillius compound. Layer-by-layer growth is demonstrated, permitting in-situ control of thickness with sub-unit-cell accuracy and resulting in atomically flat surfaces. The achievement of twin-free films significantly enhances their uniaxial ferroelectric properties. In the ultrathin regime, such films exhibit in-plane polarization with a periodic arrangement of ferroelectric domains, which, in conjunction with uniaxial ferroelectric anisotropy, results in nominally charged domain walls. Hysteresis measurements reveal a remnant polarization of 16.5 μC cm^{-2} with a remarkable endurance after 10^{10} switching cycles. The uniaxial in-plane ferroelectricity of Aurivillius thin films breaks new ground for alternative device

paradigms less susceptible to the depolarizing-field effects.

20 min. break

KFM 11.6 Wed 17:00 TOE 317

Ferroelectric domain wall imaging by focused ion beam — •Erik Roede[1], Aleksander Mosberg[1], Donald Evans[1], Theodor Holstad[1], Zewu Yan[2], Edith Bourret[3], Antonius van Helvoort[1], and Dennis Meier[1] — [1]NTNU, Trondheim, Norway — [2]ETH, Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Charged ferroelectric domain walls (DWs) have received much attention for their functional properties and potential applications [1]. The orientation of a DW relative to the ferroelectric polarization determines the charge state and electronic properties of the wall. Therefore, the propagation of DWs through a crystal has drastic effects on the properties measured at the surface. Still, research on DWs has so far been dominated by surface techniques.

In this work, we introduce the use of focused ion beam (FIB) techniques [2] for 3D domain and DW imaging in ErMnO3[3] with nanoscale resolution. This enables relating the measured surface properties to the 3D domain wall geometry, enabling a move towards a comprehensive knowledge of the intrinsic properties of charged ferroelectric domain walls and their application in future nanoelectronic devices.

[1] D. Meier et al., Nature Materials, 11, 284-288 (2012) [2] A. Mosberg et al., Appl. Phys. Lett. 115, 122901 (2019) [3] Z. Yan et al., J. Cryst. Growth, 409, 75-79 (2015)

KFM 11.7 Wed 17:20 TOE 317

Functional bubble domains in ferroelectric superlattices — •Anna Grünebohm[1] and Claude Ederer[2] — [1]ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Materials Theory, ETH Zürich, 8093 Zürich, Switzerland

In this contribution we revisite the phase diagram of $BaTiO_3$–$SrTiO_3$ superlattices by means of ab initio based molecular dynamics simulations [1]. We discuss the stabilization of domain walls by epitaxial strain and the interplay of depolarization and anisotropy energy. Excitingly, transitions between stripe and bubble domains can be induced by an electrical field in close analogy to stray-field stabilized skyrmions in magnetic films. The local and global properties of the superlattices differ considerably in the vicinity of this transition. Thus exceptional functional responses such as negative capacitance may be realized.

[1] T. Nishimatsu et al., Phys. Rev. B **78**, 104104 (2008).

KFM 11.8 Wed 17:40 TOE 317

Tracing domain formation in ferroelectric PZT films in-situ — •Martin Sarott, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zurich, Switzerland

The pronounced impact of growth conditions on the formation of domains in ferroelectric thin films obstructs the effective design of devices based on ferroelectrics that require controlled polarization states and deterministic switching dynamics. Here, we overcome this notorious difficulty by tracking in-situ, during growth, the emergence of domains in ultrathin ferroelectric layers. We use a combination of in-situ optical second harmonic generation (ISHG) and reflection high energy electron diffraction to directly observe the formation of in-plane oriented a-domains in an otherwise c-domain matrix in technologically relevant PZT films. By monitoring ISHG, we correlate the signal to the domain structure and identify a signature of mixed in-plane/out-of-plane domain patterns. Furthermore, we reveal the impact of epitaxial strain on the emergence of a-domains in a c-domain matrix. Our in-situ approach allows us to disentangle the influence of various growth parameters on the domain structure and thus enables the design of thin films with predefined domain states for reliable ferroelectric properties in the ultrathin regime.

KFM 11.9 Wed 18:00 TOE 317

Photovoltage from ferroelectric domain walls in $BiFeO_3$ — •Sabine Körbel[1,2], Stefano Sanvito[1], and Jirka Hlinka[2] — [1]School of Physics & CRANN, Trinity College Dublin, Ireland — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Ferroelectric domain walls are objects capable of creating local electric fields in ferroelectric materials, and therefore in principle allow for a domain-wall driven photovoltaic effect. However, up to now the magnitude of such a domain-wall photovoltage was never measured nor calculated directly: experimentally it is hard to distinguish between domain-wall and bulk photovoltaic effect; first principles calculations used only an indirect approach based on the ionic polarization in the dark state, neglecting the electronic polarization. In order to directly calculate the domain-wall photovoltage in $BiFeO_3$, we modeled the excitonic charge density upon light irradation from first principles and determined the potential variations at the domain walls and consequently the domain-wall photovoltage. We find indeed that excitons form an electric dipole layer at the domain walls resulting in a domain-wall driven photovoltage, and that the excitonic dipole moment is aligned parallel to the net polarization, not, as previously assumed, antiparallel. By comparing the calculated domain-wall photovoltage to the total photovoltage measured in experiment, we conclude that the domain-wall effects are relatively small and cannot account for the major part of the measured photovoltage. This indicates that bulk effects, not domain-wall effects, dominate the photovoltage in $BiFeO_3$.

KFM 12: Materials for Energy Storage (joint session KFM/CPP)

Time: Thursday 9:30–11:50 Location: HSZ 301

KFM 12.1 Thu 9:30 HSZ 301

Investigation of Li diffusion mechanisms in V_2O_5 — •Fabian Dietrich and Eduardo Cisternas Jara — Núcleo Milenio Multi-Mat & Departamento de Ciencias Físicas, Universidad de La Frontera, Temuco, Chile

Vanadium pentoxide (V_2O_5) is a promising candidate for the use as cathode material in lithium ion batteries (LiB) due to its layered structure. For the use as electrode material, it is necessary to understand fundamental aspects of its structure as well as mechanisms during the charging and discharging process. Hence, we investigate the diffusion of lithium ions in that material, paying attention to vanadium pentoxide species with different amount of inserted lithium.

The investigations are done by simulation of the processes using density functional theory (DFT) in the periodic boundary condition, also in combination with plane-wave basis sets and dispersion correction. Diffusion pathways are calculated using the nudged-elastic band (NEB) method. Resulting barrier heights are used for subsequent Monte-Carlo simulations. Frequency calculations are used to estimate the diffusion coefficients, which are also used in the MC simulations.

We assumed different diffusion mechanisms for the pure V_2O_5 and the lithiated species LiV_2O_5. While in V_2O_5 a quite free diffusion of Li ions is possible, the occupation of distinct lattice positions by Li ions leads to a blocking of certain pathways. Thus, the knock-off mechanism is proposed for LiV_2O_5. This assumption could be confirmed by the calculations, comparing different mechanisms for the diffusion in LiV_2O_5.

KFM 12.2 Thu 9:50 HSZ 301

Evaluation of the Applicability of the Brick Layer Model for Describing the Electrical Transport within Ceramic Materials — •Janis K. Eckhardt[1,2], Markus S. Friedrich[2,3], Matthias T. Elm[2,3,4], Peter J. Klar[2,3], and Christian Heiliger[1,2] — [1]Institute for Theoretical Physics, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [4]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

In literature, the transport properties of ceramics such as the active cathode material within lithium ion batteries are commonly described by making use of the so called Brick Layer Model (BLM). The BLM cannot account for percolation effects. However, the microstructure of real devices, e.g. secondary materials of cathodes or thin films is such that disorder will lead to percolation effects. In order to account for these effects and to validate the applicability of the BLM an impedance

network model based on Kirchhoff's current law has been developed. With its help it is possible to compute impedance spectra and current density distributions of defined or random structures that mimic the properties of the real microstructure. Comparing the computational result to the prediction of the BLM, it becomes obvious that an additional semicircle(s) and signal(s) respectively in the impedance and distribution of relaxation times spectra may occur. This effect can be attributed to the multidimensional transport mechanism within the structures which is not accounted for in the commonly used BLM.

KFM 12.3 Thu 10:10 HSZ 301

First principles calculation on intrinsic defects properties of Sodium Niobate — •Lorenzo Villa — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, TU Darmstadt, Otto-Berndt-Straße 3, D-64287 Darmstadt, Germany

In recent years extended research has been focusing on improving the properties of capacitors for energy storage applications. In this context, lead-free antiferroelectric materials (AFE) are excellent candidates due to their ability of displaying high energy density, high energy efficiency and low environmental impact. In this class of compounds, $NaNbO_3$ (NN) is amongst the most promising materials, due to the possibility to obtain double P-E loops at room temperature. One of the mostly used methods to obtain narrower antiferroelectric P-E loops is via doping. Intrinsic defects can interact with the dopants and therefore can have an impact on AFE properties. In order to investigate the interaction of intrinsic defects with dopants, we have studied the contribution of vacancies to intrinsic electron and hole conductivity and their interaction with different types of dopants (Sr, Ca, Mn). All calculations were performed in the framework of Density Functional Theory using Hybrid functionals. In particular, we have investigated the formation energies of all vacancy types considering all possible charge states in five different regions of the stability diagram.

20 min. break

KFM 12.4 Thu 10:50 HSZ 301

Glass ceramics with proton conducting crystalline phases — •Laura Weisshoff[1,2], Martin Letz[1,2], Martin Jourdan[1], and Martun Hovhannisyan[2] — [1]Johannes Gutenberg Universität Mainz — [2]Schott AG Mainz

Proton conducting crystal phases such as the perovskite type have their application in proton conducting fuel cells (PCFC), sensors and hydrogen separation. A reduction of the operating temperature due to highly efficient inorganic proton conducting materials is an important development target. For this, a proton-conducting electrolyte is a key component and an optimized material is required. Standard ceramic solutions show high sintering temperature and pores. A non-gas tight material can lead to a catastrophic failure of the PCFC. Therefore, we develop pore free glass ceramics with lower sintering temperature. The present talk reports the progress of glass ceramics with proton conducting crystalline phases.

KFM 12.5 Thu 11:10 HSZ 301

Rapid, clean and scalable synthesis of microporous functional MOFs and their non-conventional forms via mechanochemistry — •Krunoslav Užarević — Ruder Boskovic Institute, 10000 Zagreb, Croatia

Here we present the application of mechanochemical reactions,[1] i.e. reactions between solid reactants induced by mechanical force, for a rapid, green and room-temperature transformation of environmentally safe metal precursors, oxides or hydroxides into most relevant microporous MOFs, such as HKUST-1, MOF-74[5] or zirconium-based MOFs of UiO[3] and NU- families, and also their multi-metal or amorphous derivatives not accessible from solution. We show here how the milling produces high-quality MOFs quantitatively in multigram quantities by using only a catalytic amount of *green liquids, such as methanol or water.

In situ synchrotron X-ray powder diffraction monitoring[8] revealed that the mechanochemical formation of MOFs often proceeds through intermediate phases, most of which are inaccessible from solution procedures. It is possible to isolate and characterize these intermediates, and also use them for the controllable synthesis of multi-metal MOFs, such as various bimetal MOF-74 materials, with interesting magnetic properties and strong potential for new catalytic reactivity.

[3] James et al, Chem. Soc. Rev. 2012, 42, 7638. [2] Julien et al, J. Am. Chem. Soc., 2016, 138, 2929. [3] Užarević et al., Chem. Commun. 2016, 52, 2133. [8] a) Užarević et al., J. Phys. Chem. Lett, 2015, 6, 4129.

KFM 12.6 Thu 11:30 HSZ 301

Actuation and electrostriction of composite films with heteregenous filler clustering — •Elshad Allahyarov — Duisburg-Essen University, Theoretical Chemistry

Controlled actuation of electroactive polymers with embedded high dielectric nanoparticles is theoretically analyzed. If the inclusions are placed randomly in the elastomer body, the composite always contracts along the direction of the applied field. For a simple cubic distribution of inclusions, contraction occurs if the applied field is directed along the [001] direction of the lattice. For inclusions occupying the sites of other lattice structures such as body-centered or face-centered cubic crystals, the composite elongates along the field direction if it is applied along the [001] direction. The stability of the elongation against the imperfectness of the lattice site positions and the distortion ratio of the initial structures are examined. Finite elongation windows show up for the initially distorted body-centered cubic and face-centered cubic crystals as a function of the distortion ratio of the initial structure. The existence of these elongation windows are also predicted from the analysis of the electrostatic energy of the distorted body-centered cubic and face-centered cubic lattice structures. Our results indicate that the electrostriction effect, which is the main contribution to the actuation of low aspect-ratio composites, strongly depends on the geometry of the spatial distribution of nanoparticles, and can thereby largely be tuned.

KFM 13: Focus: High-resolution Lithography and 3D Patterning (Part II) (joint session KFM/HL/CPP)

Chair: Robert Kirchner (TU Dresden)

Time: Thursday 9:30–12:20 Location: TOE 317

KFM 13.1 Thu 9:30 TOE 317

Curvilinear Magnetism: Fabrication and characterization — •Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Extending 2D structures into 3D space has become a general trend in multiple disciplines including electronics, photonics, and magnetics. This approach provides means to enrich conventional or to launch novel functionalities by tailoring curvature and 3D shape. We realize 3D curved magnetic thin films where new fundamental effects emerge from the interplay of the geometry of an object and topology of a magnetic sub-system [1]. The application potential of 3D magnetic architectures is explored for the realization of mechanically shapeable magnetoelectronics [2] for virtual and augmented reality appliances [3,4]. To advance in this research field, we develop novel theoretical methods [5-7], fabrication [1,8,9] and characterization techniques [8-11]. These topics will be addressed in the presentation.

[1] R. Streubel et al., J. Phys. D: Appl. Phys. 49, 363001 (2016). [2] D. Makarov et al., Appl. Phys. Rev. 3, 011101 (2016). [3] S. Cañón et al., Nature Electronics 1, 589 (2018) & Science Adv. 4, eaao2623 (2018). [4] J. Ge et al., Nature Comm. 10, 4405 (2019). [5] O. Volkov et al., PRL 123, 077201 (2019). [6] O. Volkov et al., Sci. Rep. 8, 866 (2018). [7] V. P. Kravchuk et al., PRL 120, 067201 (2018). [8] K. S. Das et al., Nano Let. 19, 6839 (2019). [9] M. Nord et al., Small 1904738 (2019). [10] R. Streubel et al., Nature Comm. 6, 7612 (2015). [11] T. Kosub et al., Nature Comm. 8, 13985 (2017).

KFM 13.2 Thu 9:50 TOE 317

3D printing of complex submillimeter-sized wide angle objectives — •Zhen Wang[1], Ksenia Weber[1], Simon Thiele[2], Alois

Herkommer[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Institute of Technical Optics and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

Compact image sensors with a variety of focal lengths, fields of view, and other optical parameters, will be the enabling technology of integrated devices for industry 4.0. In order to miniaturize the imaging devices from currently several mm^3 to below 1 mm^3, and to achieve diameters of the optics below 1 mm, 3D printing with femtosecond laser pulses is the method of choice. Here, we present several multi-lens designs as well as printed objectives with fields of view that range from 60° to 95°, and focal lengths in the range of 200-300 μm, with diameters around 800 μm, which allow for wide-angle imaging. We characterize their performances and report how to overcome some issues when printing such challenging designs. In the future, those objectives can be directly printed onto CMOS imaging chips which will enable very compact image sensors.

KFM 13.3 Thu 10:10 TOE 317

Additive technology for X-ray optical applications — •Adam Kubec, Frieder Koch, and Christian David — Paul Scherrer Institut

X-ray optics are used in many setups connected to materials analysis. Due to very different properties of X-rays as compared to visible light different challenges, have to be tackled in order to manufacture optics. The refractive index has only a small difference to unity. This results in a relatively small optical power. This makes it challenging to manufacture refractive lenses. A successful concentration of X-ray using refractive lenses could only been shown in 1996 using a set of individual refractive lenses.

Today refractive lenses for X-rays are commercially available and are widely used in many synchrotron radiation sources. However, it is still challenging to manufacture aberration free lenses for X-rays. Therefore, custom-made radially symmetric corrector phase plates are used to reduce the aberrations. Spiral phase plates can generate X-ray beams carrying orbital angular momentum of various topological charges.

Additive technology can now also used in order to manufacture refractive lenses directly. Due to the versatility of 3D printed geometries, it is possible to manufacture lenses adapted specifically to improve measuring techniques, such as Ptychography.

We will also see further applications of 3D printing for X-ray applications such as 3D resolution pattern (Siemens Star). These can be can be used to quantify the quality of X-ray tomography setups.

KFM 13.4 Thu 10:30 TOE 317

Mass-producible microoptical elements by injection compression molding and focused ion beam structured titanium molding tools — •Simon Ristok[1], Marcel Röder[2], Simon Thiele[3], Mario Hentschel[1], Thomas Günther[2], André Zimmermann[2], Alois Herkommer[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Hahn-Schickard, Stuttgart, Germany — [3]Institute of Applied Optics and Research Center SCoPE, University of Stuttgart, Germany

Injection molded polymer is the material of choice for micro-optics used in mass producible devices such as smartphones or optical sensors. For feature sizes on the micrometer scale the molding tools are usually fabricated by nickel electroplating on a silicon master, which was previously structured by electron beam lithography and subsequent etching. In total, two inversion steps are necessary to transfer the structure from the silicon master to a plastic polymer part. Here, we introduce an alternative method that requires only a single inversion step. An extremely robust titanium molding tool is directly structured with high precision by focused ion beam milling. We demonstrate the fabrication of Fresnel lenses with 100 μm diameter and a maximum structure height of 1 μm. The inverse Fresnel lens structured into the titanium is transferred to polymer by injection compression molding, enabling rapid mass replication. We show that the optical performance of the molded Fresnel lenses is in good agreement with simulations, rendering our approach suitable for applications which require compact and high quality optical elements in large numbers.

20 min. break

Invited Talk KFM 13.5 Thu 11:10 TOE 317

3D Printing with Electrons - Advances and Opportunities — •Harald Plank — Institute of Electron Microscopy, Graz University of Technology, Graz, Austria

Since the advent of additive manufacturing, this technology class made tremendous progress. While achievable feature sizes continuously decreased from cm's over mm's towards the sub-micron range their 3D possibilities became increasingly powerful. Naturally, there is a strong interest to push 3D printing into the nano-scale, to take advantage of nanoscale effects. Within the small pool of relevant technologies at that scale, Focused Electron Beam Induced Deposition (FEBID) is a highly promising candidate, as it allows additive, direct-write manufacturing of even complex 3D architectures with feature sizes down to 20 nm on most materials and practically any given surface morphology. Together with an increasing availability of precursors with different functionalities, 3D-FEBID has advanced from a trial-and-error laboratory method to a predictable 3D nano-printing technology. In this talk, the audience is first introduced to the basic principles of 3D-FEBID, complemented by recent advances, which strongly increased precision, predictability and reliability. We then present software solutions for the comfortable upfront design of 3D objects and review several application examples, which strongly benefit from the here presented 3D nanofabrication appraoch. To highlight the industrial relevance of 3D-FEBID, we present concepts of advanced nano-probes for application in scanning probe microscopy. We close the talk with a view on current activities, remaining challenges and future opportunities.

KFM 13.6 Thu 11:40 TOE 317

Perfluorinated amidinate compounds for focused electron beam induced deposition (FEBID) — •Katarzyna Madajska and Iwona Szymańska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

FEBID is a direct maskless nanolithography technique, based on the local dissociation of adsorbates upon the irradiation with electrons.[1][2] Silver pentafluoropropionate was applied in the FEBID process yielding 2D and 3D deposits containing up to 70 at. % Ag. [3][4]

Here we report on our study of silver and copper complexes with perfluorinated amidines (CnF2n+1C(=NH)NH2), which are similar in structure to carboxylates but they differ in donor atoms (N,N-donor).

Thermal analysis, EI MS spectrometry, sublimation experiments and temperature variable infrared spectra analysis were carried out to determine the volatility of compounds and their thermal decomposition mechanism. The compounds selected, as based on the results of the volatility, were examined for their sensitivity to the electron beam, using an electron microscope (SEM, TEM).

[1] Utke and A. Gölzhäuser, Angewandte Chemie Int. Ed. 49 (2010) 9328-9330. [2] D. Belić, M. M. Shawrav, E. Bertagnolli, H. D. Wanzenboeck, Beilnstein J. Nanotechnol, 2017, 8, 2530-2543. [3] L. Berger, K. Madajska, I. B. Szymanska, K. Höflich, M. N. Polyakov, J. Jurczyk, C. Guerra-Nuñez, I. Utke, Beilstein J. Nanotechnol., 2018, 9, 224-232. [4] K. Höflich, J. M. Jurczyk, K. Madajska, M. Götz, L. Berger, C. Guerra-Nuñez, C. Haverkamp, I. Szymanska, I Utke, Beilstein J. Nanotechnol., 2018, 9, 842-849.

KFM 13.7 Thu 12:00 TOE 317

Synthetic strategies towards FEBID precursors — •Iwona Szymańska and Katarzyna Madajska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

The choice of the precursor is crucial for the success of focus electron beam induced deposition (FEBID) because its physicochemical features determine the composition of the deposit.[1] The applied compounds should effectively generate volatile metal carriers, which can be transport over a surface substrate. In the next stage adsorbed molecules should clearly decompose upon electron beam irradiation forming nanostructures. Additionally, the FEBID precursors should be air stable, easy handling, low cost, and safe. Research was focused on the coordination compounds of copper(II) and copper(I), silver(I) and rhenium(III) with N- and O-donor ligands, which seems to be promising for a FEBID process. The influence of structural features such as: 1) the kind of the central atom and its oxidation state; 2) the coordination sphere composition, 3) the modifications of the ligand substituents by fluorination or branching, were observed. [2,3]

Acknowledgements: Nicolaus Copernicus University in Toruń (Statute Research no.103) for the financial support.

References [1] I. Utke et al., J. Vac. Sci. Technol. B, 2008, 26, 1197. [2] L. Berger et al., Beilstein J. Nanotechnol., 2018, 9, 842. [3] K. Höflich et al., Beilstein J. Nanotechnol., 2018, 9, 842.

KFM 14: TEM-based Nanoanalysis and Microstructure of thin films (joint session KFM/CPP)

Chair: Bernd Rellinghaus (Dresden Center for Nanoanalysis, TU Dresden)

Time: Thursday 14:10–16:20 Location: HSZ 301

KFM 14.1 Thu 14:10 HSZ 301

The effect of dynamical scattering in ferroelectrics on the measurements of internal electric fields by momentum-resolvedSTEM — •Achim Strauch[1,2], Andreas Rosenauer[3], Andrei Sokolov[4], Evgeny Tsymbal[4], and Knut Müller-Caspary[1,2] — [1]Forschungszentrum Jülich — [2]RWTH Aachen University — [3]IFP Universität Bremen — [4]University of Nebraska-Lincoln

Ferroelectric tunnel junctions (FTJs) are one focus of next-generation memories. With these non-volatile memories, the energy consumption can be reduced. Devices with $BaTiO_3$ tunnel junctions cannot be reversibly polarised at ferroelectric thickness below approximately 3 nm [1]. For investigations, a STEM method would be desirable to map the ferroelectric domain structure in ferroelectric nanofilms exploiting the recently accessible four-dimensional data sets from momentum-resolved STEM [2]. In this contribution, we address the impact of systematic errors arising from dynamical scattering, violated inversion symmetry, sample tilt, and redistributions of electrons due to chemical bonding in a simulation study accompanied by experiments on $BaTiO_3$ and $PbZr_xTi_{1-x}O_3$. The effects of dynamical scattering can lead, depending on thickness, to a systematic error [3] in the order of the expected unit-cell averaged electric fields. Finally the influence of surfaces charges will be discussed.

[1] Garcia et al., Nature Comm. 5, 4289 (2014)
[2] K. Müller et al., Nature Commun. 5, 5653 (2014)
[3] K. Müller et al., Phys. Rev. Lett. 122 (2019)

KFM 14.2 Thu 14:30 HSZ 301

A Novel High-Pressure Tin Oxynitride Sn_2N_2O — •Philipp Gollé-Leidreiter[1], Shrikant Bhat[2], Leonore Wiehl[1], Ute Kolb[1], and Ralf Riedel[1] — [1]Technische Universität Darmstadt — [2]Photon Science DESY

The crystal structure of a novel high pressure high temperature tin oxynitride phase (Sn_2N_2O) was solved via Automated electron Diffraction Tomography (ADT) [1]. The new phase was synthesized from a Sn-N-O precursor at 20 GPa and 1200-1500°C. Due to strong overlaps of symmetrically non-equivalent reflections, the unknown structure could not be solved based on X-ray powder diffraction data. Using the ADT method three dimensional electron diffraction data from a single nanocrystal can be collected in a TEM [2]. The crystal is tilted in 1° steps and diffraction patterns are measured sequentially. Thereby, the reconstructed reciprocal space delivers the unit cell as well as the space group. The intensities of the reflections can be extracted and used to solve the crystal structure via approaches like *direct methods*. The new phase crystallizes in space group Pbcn with the unit cell parameters: a=7.8Å, b=5.53Å, c=5.54Å. The crystal structure could be solved and refined applying kinematic and dynamic theory. It is a Rh_2S_3 type structure where the Sn atoms are sixfold coordinated by O and N atoms. The refined structure compares very well with DFT calculations. This shows the value ADT can provide for the structure solution of high pressure and high temperature materials.

[1]Bhat S, et al. (2019) Chem. Eur. J. 10.1002/chem.201904529
[2]Kolb U, et al. (2019) doi.org/10.1107/S2053520619006711

KFM 14.3 Thu 14:50 HSZ 301

The role of spatial coherence for the creation of and imaging with atom size electron vortex beams — •Darius Pohl[1,2], Stefan Löffler[4], Sebastian Schneider[2,3], Peter Tiemeijer[5], Sorin Lazar[5], Kornelius Nielsch[2], and Bernd Rellinghaus[1,2] — [1]Dresden Center for Nanoanalysis, TU Dresden, D-01062 Dresden, Germany. — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany. — [3]Institute for Solid State Physics, TU Dresden, D-01062 Dresden, Germany. — [4]University Service Centre for Transmission Electron Microscopy, TU Wien, 1040 Wien, Austria. — [5]Thermo Fisher Scientific, PO Box 8066, 5600 KA Eindhoven, The Netherlands.

Recently discovered electron vortex beams (EVBs), which carry quantized orbital angular momenta (OAM), are envisioned to be used in combination with measurements of the electron magnetic circular dichroism (EMCD) to determine the magnetic properties of a material in transmission electron microscopes. Since EVBs can be easily focused down to sub-nanometer diameters, this novel technique bears enormous potential for the quantification of spin and orbital magnetic moments with unrivalled lateral resolution. We use specially designed condenser apertures to generate isolated atom size EVBs with user-selectable OAM. Since the "purity" of the beam regarding the chosen OAM depends on the coherence of the electron source, we have used the monochromator in a double aberration corrected FEI Titan[3] 80-300 microscope to control the degree of this coherence. It will be presented, how a likewise improved coherence will affect the quality of the EMCD measurements.

10 min. break

KFM 14.4 Thu 15:20 HSZ 301

Ferroelectric and structural properties of epitaxial NaxBi1-xTiO3 and BaxSr1-xTiO3 based thin films for electrocaloric studies — •Bruno Magalhaes[1,2], Stefan Engelhardt[1,2], Christian Molin[3], Sylvia Gebhardt[3], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [2]Institute of Material Science, TU Dresden, Dresden, Germany — [3]Fraunhofer IKTS, Fraunhofer Institute for Ceramic Technologies and Systems, Winterbergstraße 28, D-01277 Dresden, Germany

The purpose of our study is to investigate the electrocaloric effect in lead-free epitaxial NaxBi1-xTiO3 (NBT) and BaxSr1-xTiO3 (BST) based thin films. We are focusing on microstructural changes to identify the basic mechanisms of the caloric effects, which might enable a further optimization. Our aim is to investigate the influence of the deposition parameters as well as the functional properties in these material systems. Therefore, NBT and BST based thin films were grown on different single crystalline substrates by pulsed laser deposition. The structural characterization verifies an epitaxial growth of both materials with an additional tetragonal distortion. Temperature and frequency dependent measurements of the dielectric properties as well as polarization were used to determine the temperature of maximum permittivity and the ferroelectric properties, respectively. Finally, we will discuss the impact of the deposition parameters on the structural and functional properties of the grown films. This work is supported by the DFG priority program 1599 Ferroic cooling.

KFM 14.5 Thu 15:40 HSZ 301

Uncloaking structural information of ultra-thin oxide films by surface enhanced Raman spectroscopy — •Mads C. Weber[1], Sebastian Heeg[2], Roman Wyss[3], Martin Sarott[1], Morgan Trassin[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Department of Information Technology and Electrical Engineering, ETH Zurich — [3]Department of Mechanical and Process Engineering, ETH Zurich

Strained oxide thin films are a source for properties nonexistent in bulk form such as ferrelectricity in $SrTiO_3$ or altered conductivity in nickelates. These physical properties result commonly from subtle structural distortions. Unfortunately, subtle distortions and specifically oxygen displacements are chronically difficult to probe hindering an in-depth understanding of the phenomena. Here, we introduce surface enhanced Raman spectroscopy (SERS) – a technique so far restricted to molecules and carbon-nanostructures – to scrutinize the structure of oxide thin films. A porous gold membrane deposited on the sample acts as antenna and amplifies the Raman signal of the outer layers only. Using this method, we set the Raman spectra of our model thin film $LaNiO_3$ apart from the substrate giving the important structural insight. Beside information on the strain state of $LaNiO_3$, we identify an ultra-thin surface layer structurally different from the rest of the film. Such a surface layer was so far only theoretically predicted, however, never observed. In general, we anticipate that the introduction of SERS to reign of complex oxides films will help to understand the link between novel physical phenomena and structural distortions.

KFM 14.6 Thu 16:00 HSZ 301

Characterizing self-assembled nanostructures in a hierarchical-structured film by coherent two-dimensional microscopy — •Donghai Li[1], Evgenii Titov[1], Maximilian

Roedel[2], Verena Kolb[2], Sebastian Goetz[1], Roland Mitric[1], Jens Pflaum[2,3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Lehrstuhl für Experimentelle Physik VI, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), Magdalene-Schoch-Str. 3, 97074 Würzburg, Germany

Self-assembled nanostructures facilitate the development of functional materials with widely tunable properties. Hierarchical architectures consist of nanoscale building blocks spatially modulated by microscale patterns. Despite its relevance for applications and devices, characterization is demanding with existing methods because typically the local molecular-scale assembly pattern within the nanostructure cannot be resolved. Here, we determine nanostructure morphology in a hierarchically structured organic film using coherent two-dimensional (2D) micro-spectroscopy in combination with theoretical modelling of excitonic spectra. We obtain local 2D spectra with diffraction-limited spatial resolution of 260 nm. Using first principles calculations of exciton spectra for model aggregates we connect the experimentally observed signal to the characteristic lengthscale of the nanocrystallites. Thus we obtain a spatial map of nanoscale self-assembly size and confirm it to be correlated with the local slope of the microstructured film surface.

KFM 15: Postersession KFM

Time: Thursday 16:00–18:30 Location: P2/1OG

KFM 15.1 Thu 16:00 P2/1OG

Defect physics in $LiTaO_3$ — •Mike N. Piontek and Simone Sanna — Insitut für Theoretische Physik und Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

While the defect physics of $LiNbO_3$ has been object of many investigations, the nature of point defects in the isomorphic and isoelectronic $LiTaO_3$ is much less known. Although the existence of small bound polarons [1,2] in $LiTaO_3$ 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 $LiTaO_3$ and of many other point defects such as Ta and Li vacancies. 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 relative formation energies of the investigated defects closely mirror those of corresponding defects in $LiNbO_3$ [3], suggesting a rather similar defect physics in the two materials. [1] O. F. Schirmer et al., J. Phys.: Condens. Matter **21**, 123201 (2009). [2] F. Freytag et al., Nature Scientific Reports **6**, 36929 (2016). [3] Y. Li, W. G. Schmidt, S, Sanna, Phys. Rev. B **89**, 094111 (2014).

KFM 15.2 Thu 16:00 P2/1OG

Optimizing the electrocaloric effect in $BaSrTiO_3$ with molecular dynamics simulations — •Aris Dimou, Ankita Biswas, and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Germany

The electrocaloric effect (ECE) is the adiabatic temperature change of a material in a varying external electrical field which is promising for novel cooling devices [1]. We use ab initio based methods to optimize the ECE in $BaSrTiO_3$ solid solutions. Using coarse grained methods we show how the optimal operation temperature may be adjusted with the concentration of Sr [2]. As the next step we focus on the impact of the atomistic structure using DFT and core-shell potentials [3].

[1] X. Moya *et al.*, Nature Mater. **13**, 439 (2014).
[2] T. Nishimatsu *et al.*, J. Phys. Soc. Japn. **85**, 114714 (2016).
[3] S. Tinte *et al.*, J. Phys.: Condens. Matter **16**, 3495 (2004).

KFM 15.3 Thu 16:00 P2/1OG

Spatially resolved excitation of luminescing self-trapped excitons in lithium niobate — •David Brinkmann, Andreas Krampf, and Mirco Imlau — School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany

Light-induced luminescence in lithium niobate, $LiNbO_3$ (LN), is based on the excitation of self-trapped excitons (STE) [Blasse, G. *et al.* Z. Phys. Chem 57 (1968) doi: 10.1524/zpch.1968.57.3_6.187]. These quasi-particles can be efficiently excited optically by a fs-pulse and recombine radiatively in the blue-green spectral range. Using a spatially modulated light pattern for excitation, i.e., a pump pulse interference pattern, STEs are generated in sharp, spatially separated parts of the crystal. Whereas similar holographic gratings based on the excitation of small polarons have previously only been studied indirectly by diffraction experiments based on the nonlinear change of the refractive index and absorption coefficient caused by the polarons, we can now, for the first time, perform a digital read-out of such gratings via detection of the luminescing STEs by means of a CMOS camera. The impact of these findings both for the analysis of recorded grating patterns, for the transport physics of STEs and for visionary applications in digital holography is discussed. Financial support by the DFG (IM 37/11-1, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 15.4 Thu 16:00 P2/1OG

Enhancement of grating recording with sub-ps, near-infrared laser pulses at $1.6\,\mu$m in iron-doped lithium niobate — •Janina Ringel[1], Bjoern Bourdon[1], Felix Freytag[1], Mirco Imlau[1], Alexandr Shumelyuk[2], and Serguey Odoulov[2] — [1]Department of Physics, Osnabrueck University, Osnabrueck, Germany — [2]Institute of Physics, National Academy of Sciences, Kyiv, Ukraine

Recording of long-lived photorefractive gratings in the near-infrared, e.g. at a wavelength of $\lambda = 1.6\,\mu$m, is commonly highly inefficient in Fe:$LiNbO_3$, but can be sufficiently enhanced by means of temporally and spatially synchronized gate pulses. However, nothing is known about the underlying photophysical mechanism that enables diffraction efficiencies of up to 25 % so far. Here, we adress this question by studying the role of the gate light photon energy using trains of sub-ps-pulses (100 fs, 1 kHz) that can be tuned all over the VIS and NIR spectral range. We find two distinct efficiency maxima in the VIS and NIR spectral range and a pronounced dependence on the light polarization. Our findings are discussed within two excitation mechanisms: (1) The spatial modulation of the NIR recording pattern is imprinted onto the homogeneous gate light distribution via a one-photon-absorption process. (2) The photon energies of recording and gating light add-up via a two-photon process. Despite these new paths for carrier excitation, the further development of the grating follows the steps of the well-known photorefractive process. Financial support (DFG INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 15.5 Thu 16:00 P2/1OG

Clocking nonlinear optical frequency-mixing in disordered, polar nanoparticles — •Jan Klenen[1,2], 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) are of increasing importance due to their extended nonlinear optical (NLO) properties resulting from loosened phase matching conditions [C. Kijatkin, PhD thesis **2019**] thereby enabling visionary applications in biomedicine or material science, for instance. Significant effort has been devoted to the investigation of light-matter interactions in nanoscaled media [D.S. Wiersma, *Nature Photonics* **2013**, *7*(3)]. However, the physical processes governing the temporal evolution in such media have not been fully quantified yet. Based on this premise, we present a time-resolved numerical study on pulsed laser light propagation in HNP powders using a random-walk model with Monte-Carlo based Mie calculations and evaluate its implications on NLO processes. In addition, experimental investigations of the temporal evolution of NLO sum frequency generation are performed via pump-probe spectroscopy to validate the model and to predict the behavior for different systems. We are able to analyze the effect of different particle sizes on the temporal pulse profile and discuss the potential of HNPs as a flexible alternative to crystalline media for determination of the instantaneous frequency distribution of (sub-) ps pulses. Financial support (DFG INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 15.6 Thu 16:00 P2/1OG

Light-induced absorption in Fe:LN by means of ns-pump supercontinuum-probe spectroscopy — •Bjoern Bourdon,

Simon Messerschmidt, David Brinkmann, Andreas Krampf, Laura Vittadello, and Mirco Imlau — Department of Physics, Osnabrueck University, Osnabrueck, Germany

Pulse-induced transient absorption (TA) phenomena in iron doped lithium niobate, such as green-induced infrared absorption or green-induced blue-absorption, play an important role in laser-induced damage and are commonly attributed to the absorption features of small polarons. However, only recently, *Messerschmidt* [S. Messerschmidt, *J. Phys. Condens. Matter*, **31** (2019)] has proposed a revised model taking the presence of long-lived excitonic states bound to Fe_{Li} centers into account. We here investigate the pulse-induced TA by means of ns-pump supercontinuum-probe spectroscopy in the time range from $10^{-7} - 10^{2}$ s with the goal to control and probe the blue absorption feature related with these excitonic states. For this purpose, three distinct experimental configurations are investigated that enable targeted optical injection of electron-hole-pairs at Nb^{5+}–O^{2-}-octahedra in direct vicinity of Fe_{Li} and a clear separation from the well-known small polaron absorption bands. As a result, the optical fingerprint of the $Fe_{Li}^{2+} - O^{-} - V_{Li}$ excitonic state is deduced revealing a broadband absorption feature (total width: 1.2 eV) with two peaks at 2.2 eV and 3.0 eV and a maximum absorption cross-section of up to $\sigma(2.85\,\mathrm{eV}) = (4 \pm 2) \cdot 10^{-22}\,\mathrm{m}^2$. Financial support (DFG INST 190/165-1 FUGG, DFG IM37/11-1) is gratefully acknowledged.

KFM 15.7 Thu 16:00 P2/1OG

Wide-field real-time nonlinear optical microscope in living organism — •Niklas Bethke[1,2], Dustin Dzikonski[1,2], Laura Vittadello[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Osnabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

Nonlinear optical microscopy have emerged as a successful tool within the bio-medical research field enabling the possibility to do imaging in intact-live organism. In particular this type of microscope have to enable (i) high peak intensity to exploit non-linear effect, (ii) a field of view in the millimeter regime to ensure a proper imaging of the organism and (iii) the possibility to do time resolved experiment in the millisecond regime, where the most interesting biological effect occur. To embeded all this requirement in a single setup, the combination of an appropriate marker and the development of a non-conventional microscope setup is required. In this respect a femtosecond laser is coupled to an confocal laser scanning microscope, enabling the unique possibility (i) to control the non-linear effect by means of repetition rate (single shot - 80 MHz) and pulse duration (30 fs - 10 ps); (ii) to image living organism with a field of view up to about 1 mm and (iii) acquire images with an exposure time in range of tens of millisecond. Furthermore, niobate nanoparticles, such as $KNbO_3$, are examined as marker candidate. They are of increasing importance as multimodal nanophotonic probes in biological environments due to their biocompatibility and pronounced nonlinear optic (NLO) properties. Financial support (DFG INST 190/179 FUGB) is gratefully acknowledged.

KFM 15.8 Thu 16:00 P2/1OG

Fs-pump-supercontinuum-probe absorption spectroscopy of small polarons in polar oxide crystals — •Anton Pfannstiel, Andreas Krampf, and Mirco Imlau — University of Osnabrueck, Department of Physics, Barbarastrasse 7, 49076 Osnabrueck, Germany

Spectroscopy of small polaron absorption on the sub-ns timescale is commonly performed using probe pulses at distinct wavelengths. As small polaron absorption bands in polar oxide crystals with a rich defect structure are very broad and often superpose, transient absorption kinetic traces can usually not unambiguously be assigned to individual small polaron species. Furthermore, their distinct absorption bands naturally remain unresolved.

We thus have developed a fs-pump-supercontinuum-probe spectrometer enabling the investigation of small polaron absorption from the visible (VIS) to the near-infrared (NIR) spectral region with sub-ps temporal resolution. As a unique feature different crystals for supercontinuum probe generation and a joint VIS-NIR-spectrometer are combined.

Using the setup, we successfully studied transient absorption of various polar oxide crystals such as $LiNbO_3$, $LiTaO_3$ and $LiNb_{1-x}Ta_xO_3$, etc. We discuss our findings in the well-established framework of small polaron absorption. Financial support by the DFG (IM37/11-1) is gratefully acknowledged.

KFM 15.9 Thu 16:00 P2/1OG

NV-center formation after femtosecond-laser pulse excitation — •Marie Kempkes, Tobias Zier, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Recent studies showed that colour centers, like, NV-centers in diamond are a promising candidate for technological applications, since they could operate as single-photon emitter in the visible range. Unfortunately, due the fabrication process of NV-centers by artificial growth or ion bombardment the number of NV-centers is not well defined and not sufficiently controllable. Another disadvantage is the fact, that the sample has to be heated intensively in order to increase the vacancy and nitrogen mobility, which is necessary that NV-centers can form anyway. During this heating process other defects could appear within the crystalline structure that could decrease the efficiency of the NV-center. Therefore, we simulated the formation of a NV-center driven by femtosecond-laser excitation by ab initio methods. For this we first performed ab initio molecular dynamics simulations of diamond with a defect density of 3.1% and analyzed their impact on ultrafast phenomena, like, nonthermal melting and thermal phonon squeezing. We used this knowledge to perform simulations of the case that the nitrogen atom and the vacancy were not nearest neighbours in the beginning. Our results indicate, that femtosecond-laser pulses could be used to controllably produce NV-centers nonthermally on a timescale less than 200 fs with smallest possible impact on the surrounding crystal.

KFM 15.10 Thu 16:00 P2/1OG

Loss tangent measurements on an extremely large diamond disc for Brewster angle windows — •Andreas Meier[1], Gaetano Aiello[1], Theo Scherer[1], Sabine Schreck[1], Dirk Strauss[1], Christoph Wild[2], and Eckhard Wörner[2] — [1]Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Diamond Materials GmbH, Hans-Bunte-Straße 19, 79108 Freiburg, Germany

Advanced Electron Cyclotron heating systems for future fusion reactors, such as DEMO, are designed for multi-frequency operation. The favored output window concept of the high power microwave beam is the brewster angle setup, but it requires a disc diameter of 180 mm for the 67.2° angle and the 63.5 mm waveguide. In addition, a thickness of approximately 2 mm is needed to achieve the proper mechanical stability. State of the art microwave plasma reactors are not capable of growing discs of such a size. The maximum available diameter of a polycrystalline CVD diamond disc suited to microwave applications is currently 140 mm.

An extremely large diamond disc with a diameter of 180 mm for RF transmission application was produced by the industrial partner Diamond Materials GmbH. High-resolution loss tangent measurements for several areas of this disc have been realized by using a spherical resonator.

KFM 15.11 Thu 16:00 P2/1OG

Integration of physics instruments of the ITER EC Upper Launcher — •Peter Späh, Gaetano Aiello, Andreas Meier, Theo Scherer, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Hermann-von-Helmholtz-Platz 1, Germany

Physics instruments installation often causes challenging mechanical design requirements and components must be protected properly from harsh environmental conditions. This is particularly the case for fusion plants like ITER, where sensitive applications shall operate under severe conditions in terms of heat, mechanical loads and radiation. For ITER an EC Heating and Current Drive System has been designed where delicate components like microwave reflectors (mirrors), corrugated waveguides, mirror actuators, dielectric transmission devices (CVD Diamond windows) and shutter valves were precisely integrated into heavy system components, designed to sustain substantial mechanical loads and equipped with powerful cooling systems and radiation shielding.

This poster presents the mechanical integration of physics instruments of the ITER EC Upper Launcher and their connection to appropriate cooling systems.

KFM 15.12 Thu 16:00 P2/1OG

Flexible Liquid Crystal Elastomer Substrates for Coupling of Whispering-Gallery-Mode Resonators — •Pascal Rietz, Simon Woska, Osman Karayel, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Whispering-Gallery-Mode (WGM) resonators confine light due to total internal reflection in a rotationally symmetric structure. They are promising elements of versatile photonic devices like filters or switches. A reversible tuning of the inter-cavity gap between several resonators is thereby beneficial for various applications. In this context, we propose mechanically flexible photonic devices completely made from polymers. We fabricate substrates out of liquid crystal elastomers (LCEs) onto which the resonators are structured by Direct Laser Writing.

LCEs are cross-linked but flexible polymers that change their conformation when heated over a moderate temperature range. By doing so, the dimension along a previously ordered direction is reduced. This fully reversible transformation allows the tuning of the inter-cavity gap of WGM resonators structured onto these substrates.

In this contribution, we demonstrate a process for the fabrication of substrates made from LCE. The necessary parallel alignment of the LCE monomers is achieved by a rubbing process of sacrificial layers which is adapted from the liquid crystal technology. To achieve a reliable and enhanced ordering of the LCE monomers and hence a better actuation of the substrates we also present a method and first results to quantify this actuation.

KFM 15.13 Thu 16:00 P2/1OG

Photoluminescence Spectroscopy of Zinc Oxide based Ring Resonators — •Timo Vullhorst, Nils Weber, and Cedrik Meier — Department Physik, Uniersität Paderborn, 33098 Paderborn

Due to its UV emission at around 375 nm, its strong photoluminescence and nonlinear optical properties, the wide-gap semiconductor zinc oxide (ZnO) is a current subject in photonics research. ZnO based ring resonators (RR) are a novel concept that promise to be small scale, tunable devices capable of filtering and emitting light in the UV-VIS range, allowing for the application as optical modulators, mechanical strain sensors and biosensors. Here, we demonstrate numerical results on optimized devices, fabrication via electron beam lithography and subsequent characterization via photoluminescence spectroscopy of ZnO RRs. ZnO RRs on SiO_2 with heights ranging from 300 to 500 nm were successfully realized with outer radii between 2-4 μm and ring widths between 0.1-1.5 μm, together with full disk resonators. The highest quality factors of Q$\sim$3000 were achieved in a 400 nm high ZnO ring resonator with 4 μm outer radius and 1.5 μm ring width. The findings substantiate the viability of ZnO for application in RR devices and form the starting point for further development and implementation of ZnO RRs.

KFM 15.14 Thu 16:00 P2/1OG

Tunable coupling of Whispering Gallery Mode resonators by temperature regulated contraction of Liquid Crystal Elastomers — •Osman Karayel, Simon Woska, Roman Oberle, Pascal Rietz, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Applications in various fields of optics like communications or sensors can be realized using Whispering Gallery Mode (WGM) resonators, which grant in particular on micron scales exceptionally high quality factors. Evanescent fields in the surrounding medium allow for coupling of WGM resonators in close proximity. Coupling of WGM resonators and especially the ability to vary their coupling strength by tuning the gap between them is essential for advanced applications.

We present WGM resonators processed by Direct Laser Writing on Liquid Crystal Elastomer (LCE) substrates to achieve adjustable coupling gaps. LCE has the ability to reversibly contract in one direction for rising temperature, which can be utilized to move resonators placed on top of the LCE towards each other. It is possible to produce LCE substrates on sub-millimeter scales matching the dimensions of the WGM resonators, which potentially allows for on-chip applications.

We demonstrate tunable coupling of two WGM resonators purely by temperature variation of the LCE substrate. In fiber-based transmission-spectroscopy measurements of the resonators the effects of coupling are reflected by modifications of the spectral features. These changes get more pronounced with rising temperatures due to observably smaller gaps between the resonators.

KFM 15.15 Thu 16:00 P2/1OG

Raman micro-spectroscopy of x-cut thin film lithium niobate periodically poled with high fidelity for integrated optics — •Sven Reitzig[1], Michael Rüsing[1], Benjamin Kirbus[1], Joshua Gössel[1], Zeeshan Amber[1], Jie Zhao[2], Shayan Mookherjea[2], and Lukas Eng[1] — [1]Institut für Angewandte Physik, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany — [2]University of California, San Diego, 9500 Gilman Dr, La Jolla, CA-92093-0407, USA

Periodically poled thin film lithium niobate (TFLN) promises high performance for integrated nonlinear and quantum optics. Aside the long poling lengths, a homogenous domain duty cycle is desired in order to achieve high nonlinear conversion efficiencies and narrow band-spectra. However, most works are lacking reliable imaging techniques that allow assessing the homogeneity of poling over both larger structure sizes and within individual domains. [1,2] Complementing recent SHG microscopy investigations [3], we apply here Raman micro-spectroscopy to inspect the domain formation in TFLN. By carefully analyzing the E(TO) and A1(TO) phonon modes, we are able to map intriguing material properties such as internal electric fields that show distinct variations between poled domains and domain walls. Raman spectroscopy hence provides unique domain analysis possibilities as needed for device fabrication with improved integrated nonlinear optical characteristics.

[1] A. Rao et al., OE 27, 25920 (2019). [2] L. Chang et al., Optica 3, 531 (2016). [3] M. Rüsing et al., JAP 126, 114105 (2019).

KFM 15.16 Thu 16:00 P2/1OG

Mapping of Conductivity at Ferroelectric Domain Walls using Alternating Voltages — •Jan Schultheiss[1], Erik Lysne[1], Jakob Schaab[2], Edith Bourret[3], Zewu Yan[3,2], Stephan Krohns[4], Donald M. Evans[1], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU Trondheim, Norway — [2]Department of Materials, ETH Zurich, Switzerland — [3]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [4]Experimental Physics V, University of Augsburg, Germany

Ferroelectric domain walls (DWs) are natural interfaces that separate domains with different orientation of the electric polarization. Using conductive atomic force microscopy (cAFM), it was found that DWs can exhibit completely different electronic conduction properties than the bulk domains. The characterization of the intrinsic transport behavior, however, remains a challenging task as conventional cAFM is inherently susceptible to contributions from contact resistance.
Here, we study the electrical conduction at ferroelectric domain walls under alternating voltages (a.c.) in the frequency range 0.2-20 MHz. We compare spatially resolved current maps with standard d.c. cAFM and highlight differences for different types of DWs in a hexagonal manganate ($ErMnO_3$). We find that domain- and DW-related conduction contrasts drop at distinctly different frequencies, correlating with the polarization configuration at the DWs. Quantification of the characteristic frequencies provides new insight into the intrinsic transport mechanism at functional DWs.

KFM 15.17 Thu 16:00 P2/1OG

3D Chemical Mapping of Nanostructural Features in Ferroelectrics by Atom Probe Tomography — •Kasper A. Hunnestad, Jan Schultheiss, Theodor S. Holstad, Antonius T. J. van Helvoort, and Dennis Meier — Norwegian University of Science and Technology, Trondheim, Norway

The functional properties of materials are intimately related to the atomic-scale structure and chemistry in all three dimensions. While conventional high-resolution electron microscopy (HREM) techniques enable visualization of the atomic structure, they lack depth resolution of the chemical composition. Atom Probe Tomography (APT) is an advanced analytical method that allows 3D quantitative mapping of the chemical composition with better than 100 ppm sensitivity and sub-nanometer spatial resolution. Combining the two techniques, both atomic structure and chemical composition of nanoscale features become accessible.

Here, we apply correlated HREM and APT measurements to ferroelectric domain walls (DWs) to understand the origin of their complex nanoscale properties. Using a Focused Ion Beam DWs are extracted into APT specimens from a model ferroelectric single crystalline system (hexagonal manganite, ErMnO3). Subsequently, HREM is used to locally identify and characterize the DWs in the specimens and provide information about the exact DW geometry and atomic structure. Based on first APT test measurement 3D chemical maps of up to 100x100x550 nm^3 are gained, providing insight into the local chemistry at ferroelectric DWs with unprecedented precision.

KFM 15.18 Thu 16:00 P2/1OG

Ferrimagnetic oxide substrates in the synthesis of multiferroic heterostructures — •Thomas Ruf and Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie,

Universität Leipzig, Linnéstraße 2, D-04103, Leipzig

The aim of this work is to deposit ferroelectric $BaTiO_3$ thin films on single crystalline ferrimagnetic oxide substrates Fe_3O_4 and $Y_3Fe_5O_{12}$ (YIG) to couple both ferroic properties.

X-ray Photoelectron Spectroscopy (XPS) investigations with different YIG samples have been conducted. Single crystalline YIG on $Gd_3Ga_5O_{12}$ and single crystal YIG exhibit enhanced stoichiometric ratio of Y/Fe, whereas polycrystalline nano powder YIG is close to the structural formula. Additionally, the epitactically grown sample reveals a reduced surface (enhanced content of Fe(II)). The observed stoichiometric deviations could be correlated to specific aspects of XPS, like high surface sensitivity of XPS (approx. 2 - 5 nm) and photoelectron diffraction.

Pulsed Laser Deposition of $BaTiO_3$ on single crystalline Fe_3O_4 can be performed at room temperature in oxygen environment. In this way, the chemical integrity of the substrate is preserved, e.g. oxidation at higher temperatures to alpha-Fe_2O_3 is prevented. The crystallisation of the resulting amorphous material could be achieved by heating in ultra-high vacuum (UHV). Samples with different intended film thicknesses of deposited $BaTiO_3$ precursor on Fe_3O_4 have been heated up to 650 °C in UHV. Segregation of Ti^{4+}-ions from the surface to the substrate has been monitored by XPS and X-ray Diffraction (XRD).

KFM 15.19 Thu 16:00 P2/1OG

Thermal investigation of nonlinear crystals for high power ultrashort MID-IR OPCPA pumped at 1 micrometer — Mahesh Namboodiri[1], •Gregor Indorf[2], Torsten Golz[2], Jan H. Buss[2], Michael Schulz[2], Robert Riedel[2], Tim Laarman[1,3], and Mark J. Prandolini[2] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]Class 5 Photonics GmbH, Notkestraße 85, 22607 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging CUI, Luruper Chaussee 149, Hamburg 22761, Germany

Mid-Infrared (Mid-IR) OPCPA lasers delivering ultrashort, high reprate and high-power levels are of considerable interest for vibrational spectroscopy, label-free microscopy and ultrafast vibrational dynamics by directly addressing the electronic ground state of the system under investigation. These high power lasers require nonlinear crystals (NLC) having a high nonlinear susceptibility and transparency in the Mid-IR range. We have therefore selected a few NLCs for the present study and compare their linear and nonlinear absorption coefficients along with nonlinear refractive index pumped at 1 micrometer. In particular, we have used the crystal LGS for high power laser studies at 8 micrometer.

KFM 15.20 Thu 16:00 P2/1OG

Current induced insulator-metal transition in Ca_2RuO_4 — •Konstantin Dietrich, Christoph Grams, Kevin Jenni, Markus Braden, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Germany

Ca_2RuO_4 is a Mott insulator with a first order metal insulator transition at a critical temperature of $T_C = 357$K [1]. The change in conducting behavior is accompanied by a change in crystal structure of the layered ruthenate. The conducting phase above T_C has an elongated c-axis ($c = 12.26$Å) compared to the non-conducting phase ($c = 11.77$Å) below T_C [2].

This phase transition can not only be induced by a change in temperature but also by application of an electrical field [3]. At temperatures below 50K the application of small currents can even induce very strong diamagnetic behavior [4].

Using pulsed spectroscopy, we investigate the dynamics of this field-induced switching process. We are able to discriminate heating effects by separating the time-scales for temperature and field induced transitioning and we can identify the signatures of inner contacts due to the coexistence of metallic and insulating phases.

Funded by the Deutsche Forschungsgemeinschaft via CRC 1238.

[1] C. S. Alexander *et al.*, Phys. Rev. B **60**, 12 (1999)
[2] O. Friedt *et al.*, Phys. Rev. B **63**, 174432 (2001)
[3] F. Nakamura *et al.*, Sci. Rep. **3**, (2013)
[4] C. Sow *et al.*, Science **358**, 1084 (2017)

KFM 15.21 Thu 16:00 P2/1OG

Laser-based inspection of technical dielectric thin films — •Simon Podendorf[1], Yannik Toschke[1], Jörg Rischmüller[1], Mirco Imlau[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

Fast, contactless and non-distructive inspection of technical dielectric thin films is of major importance for the quality and process control in light-alloy industry. Reflectometry, a widely available powerful tool, fails if applied to rough technical samples. It is because of the dominant role of diffuse scattering of the surfaces/interfaces, of inclusions and/or layer imperfections and, thus, a lack of an appropriate layer model.

We have adressed this problem by extending the principle approach of reflectometry considering the role of diffuse and specular scattering, as well. As an example, conversion coatings with a thickness of 20-70 nm on the aluminum alloy AA3003 and different process conditions serve for our systematic study. The layer architecture and its chemical constituents were analyzed in detail using REM and plasma spectroscopy and were used for modeling the reflection of an incident laser beam as a function of wavelength and angle of incidence. As a result, an optical configuration for the inline process control is proposed [M. Imlau et al., J. Oberfl. Techn. 59, 46 (2019)]. Financial support by the AiF in the framework of the program for "'industrielle Gemeinschaftsforschung"' (IGF, Vorhaben Nr. 19579 N) and the Bundesministerium für Wirtschaft und Energie (BMWi) is gratefully acknowledged.

KFM 15.22 Thu 16:00 P2/1OG

A supervised Machine Learning Approach for Shape sensitive Detector Pulse Discrimination in Positron Spectroscopy Applications — Danny Petschke and •Torsten Staab — Department of Chemistry and Pharmacy, University of Wuerzburg, Germany

The acquisition of high-quality positron spectra is crucial for a profound analysis, i.e. the correct decomposition to obtain the true parameters. Since the introduction of digital spectrometers for the techniques of PALS and CDBS, this is generally achieved by applying various physical filters on the digitized output-pulses from PMTs or HPGe-detectors prior to spectra generation. For instance, pile-up events can be easily rejected by applying pulse area or shape sensitive filters, which significantly increases the peak-to-background ratio.

Here, we present a novel approach for shape-sensitive discrimination of detector outputpulses using supervised machine learning (ML) based on a simple probabilistic classification model: the naive Gaussian Bayes classifier. In general, naive Bayes methods find wide application for many real-world problems such as famously applied for email spam filtering or document classification. Their algorithms are relatively simple to implement and, moreover, perform extremely fast compared to more sophisticated methods in training and predicting on high-dimensional datasets, e.g. detector-output pulses. We compared the quality and decomposability of lifetime spectra acquired on pure iron from a single measurement (pulse stream): (1) generated by applying the ML approach to lifetime spectra generated using exclusively physically filtering.

KFM 15.23 Thu 16:00 P2/1OG

Phase contrast imaging with sealed-tube sources — •Paul Meyer, Jasper Frohn, and Tim Salditt — Georg August Universität, Göttingen, Germany

Phase contrast x-ray tomography enables three-dimensional reconstruction of objects which cannot be probed by conventional tomography since their absorption-contrast is too weak. This is particularly important for soft biological tissues. However, phase contrast by free propagation relies largely on the availability of synchrotron radiation which provides the required degree of coherence. More recently, progress in laboratory sources and instrumentation has resulted in the implementation of phase contrast imaging with laboratory μCT sources, not only concerning Talbot interferometry but also propagation based phase contrast (Bartels et al., Appl. Phys. Lett. 2013). Apart from advanced liquid jet anode sources and sources with submicron spot size, phase contrast has also been realized based on a micro rotating anode with source size $s = 70\mu$m, given a sufficiently small detector point spread function σ_D and suitable geometry (Reichhard et al., Proc. SPIE 10391, 2017).

In this contribution, we investigate whether phase contrast effects can be exploited for radiography and tomography even with conventional sealed-tube sources, as used in diffraction experiments with typical anisotropic source sizes. As in the work above, small σ_D detectors are used to achieve small σ_{eff}. To this end, we present different combinations of source (anisotropic) sizes, anodes (Cu and Mo), geometry parameters, and detectors.

KFM 15.24 Thu 16:00 P2/1OG

Limitations of Quantitative Backscatter Electron Imaging at Low Voltages in the SEM — •Markus Löffler[1], Aránzazu Garitagoitia Cid[1,2,3], Rüdiger Rosenkranz[2,4], and Ehrenfried Zschech[2] — [1]Dresden Center for Nanoanalysis (DCN), Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Germany — [2]Fraunhofer-Institut für Keramische Technologien und Systeme (IKTS), Dresden, Germany — [3]Nebrija University, Department of Materials Science, Campus Dehesa de la Villa, Madrid, Spain — [4]Robert-Bosch GmbH

The design of the Zeiss Gemini SEM column with the energy selective backscatter (EsB) detector allows for surface-sensitive, low-voltage backscatter electron imaging.

Here we present results of the characteristic dependencies of the (filtered) low-voltage backscatter signal intensity on imaging parameters as well as on the atomic number (Z). Using proper calibration, contrasts between compounds can be predicted and the limitations of Z-sensitivity explored.

It was found that e.g. carbon on silicon can be detected with single-nm precision. Furthermore, the ability to distinguish even small differences in atomic number make this method an ideal tool for distinguishing similar compounds without strong edge or charging artifacts. It enables the operator to identify regions of compounds within the sample without the need for EDX (which typically requires much higher energies) and e.g. even allows for the identification of certain polymers in thin films that are sensitve to high energy electron irradiation.

KFM 15.25 Thu 16:00 P2/1OG

Nano-Characterization of Cu(In,Ga)(Se,S)$_2$ Solar Cells for Efficiency Improvement — •Sibylle Schwartmann, Oana Cojocaru-Mirédin, Jens Keutgen, Mohit Raghuwanshi, and Matthias Wuttig — RWTH-Aachen

The current record efficiency for Cu(In,Ga) (Se,S)$_2$ solar cells is at 22.6% [1]. This novel record was mainly due to a sodium post deposition treatment (Na-PDT). Besides Na-PDT, interdiffusion at the heterointerface of the p-n junction has a great influence on the efficiency as well by greatly influencing the band alignment between the layers involved. Therefore, understanding the effects of Na-PDT and interdiffusion on a nanometer level will help in understanding the mechanism responsible for the efficiency improvement of the Cu(In,Ga)(Se,S)$_2$ solar cell. In this work, atom probe tomography (APT) and cross-sectional electron beam induced current (EBIC) measurements are done on a solar cell with Cu(In,Ga) (Se,S)$_2$ absorber and Zn(S,O) buffer. The APT allows to determine the composition at nanoscale, while EBIC allows the determination of electrical properties of the p-n junction at sub-micrometer scale. Our recent APT results show that the grading of selenium and sulfur in the absorber were successfully realized. Moreover, noticeable interdiffusion of Se and S takes place. [1]Raghuwanshi et al. (2017) Influence of Na on grain boundary and properties of Cu(In,Ga)Se2 solar cells. Prog. Photovolt: Res. Appl., 25: 367– 375.

KFM 15.26 Thu 16:00 P2/1OG

KTP Z- and Y-cut surface structures calculated from first-principles — •Sergej Neufeld and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Potassium titanyl phosphate (KTiOPO4, KTP) is an important nonlinear optical material with a wide range of applications that profit from its large transparency range, large second harmonic generation (SHG) coefficient and excellent thermal stability [1]. Previous theoretical studies mainly focus on its electronic and optical bulk properties [2] as well as on the influence of point defects and non-stoichiometries on its properties [3]. Essentially nothing is known about the atomic structure of the KTP surfaces and their electronic structure. The present study aims to fill that gap. Ab initio thermodynamics based on density-functional theory is used to determine the most stable Z- and Y-cut surfaces. A strong tendency to form stoichiometric bulk-cut surfaces is found for both surface orientations. A detailed analysis on the spatial and energetic characteristics of the surface states is provided.

[1] M. Roth, Springer Handbook of Crystal Growth, pp. 691-723 (2010)

[2] S. Neufeld et al., J. Phys.: Matter. 2, 045003 (2019)

[3] A. Bocchini, J. Phys.: Condens. Matter 31, 385401 (2019)

KFM 15.27 Thu 16:00 P2/1OG

Point defects in KTP calculated from first principles — •Adriana Bocchini, Sergej Neufeld, Uwe Gerstmann, and Wolf Gero Schmidt — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The unique combination of optical and electric properties of potassium titanyl phosphate (KTiOPO4, KTP) combined with its excellent thermal stability enables a wide range of applications, e.g. for second harmonic generation (SHG) [1]. However, KTP is prone to photochromic damage, so-called gray tracking. Microscopically, the reduction of Ti atoms has been suggested to cause gray tracking: electron paramagnetic resonance (EPR) signatures assigned to Ti3+ in intrinsic defect centers were detected in crystals affected by gray tracks [2].

In the present work we explore point defects in KTP, namely O and K vacancies and H interstitials, using density-functional theory. Particular attention is given to the charge redistribution inside the cell [3]. It is found that the impact of K vacancies on the properties of KTP is nearly neglectable, while O vacancies and H interstitials cause a charge reduction of the neighboring Ti atoms. In addition, both defects lead to similar P atom hyperfine splittings which qualitatively reproduce the experimental data [4]. These findings imply O and H defects to play a significant role in the formation of gray tracks.

[1] M. Roth, Springer Handbook of Crystal Growth (2010).

[2] M. G. Roelofs, J. Appl. Phys. 65, 4976 (1989).

[3] A. Bocchini et al., J. Phys.: Condens. Matter 31 385401 (2019).

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KFM 15.28 Thu 16:00 P2/1OG

Defect engineering in a single TiS3: A first-principles study — •Guy Moise Dongho-Nguimdo, Emmanuel l. Igumbor, Raji A. Tunde, Evans M. Benecha, and Enrico B. Lombardi — College of Science, Engineering and Technology, University of South Africa, P.O. Box 392, UNISA 0003 Pretoria, South Africa.

Contrary to other transition metal chalcogenides (TMC), TiS_3 has not received attention despite its relative easy exfoliation, and high carrier mobility. In this work, we used DFT investigate the stability, the structural and the electronic properties of vacancy and antisite defects in the transition metal trichalcogenides TiS3. It is found that the formation energy is strongly dependent on which of the symmetrically inequivalent sites the defect is located. In contrast to the dichalcogenide analogs, the energy required to create a sulfur divacancy under Ti-rich conditions are lower than that of the single vacancy independently of the location of the sulfur vacancy. The negative binding energy of the double vacancies is an indication that they will likely depose into the single sulfur defects. Based on both the binding and the formation energy, we also demonstrate that the Ti-rich is the ideal growth condition for the formation of the vacancy complexes. The presence of intermediate states in the bandgap of most of the defects considerably affects the electronic properties of the pristine, with the possibility of n-type and p-type conductivity. With the exception of V_{S^1}, $V_{Ti S^3}$, V_{Ti4S^1}, $V_{Ti4S^1 4S^3}$, S_{Ti} and $Ti_{S^3}S_{Ti}$, where there is no trace of magnetism as in the pristine system; all other defects acquired some magnetic moment.

KFM 15.29 Thu 16:00 P2/1OG

Machine Learning in VASP — •Ferenc Karsai[1], Ryosuke Jinnouchi[2], and Georg Kresse[2] — [1]VASP Software GmbH, Sensengasse 8, Vienna, Austria — [2]University of Vienna, Department of Physics, Sensengasse 8, Vienna, Austria

An efficient and robust on-the-fly machine learning force field method implemented into the Vienna Ab-initio Simulation Package (VASP) is presented. This method realizes automatic generation of machine learning force fields on the basis of Bayesian inference during molecular dynamics simulations, where the first-principles calculations are only executed, when new configurations out of already sampled data sets appear. The power of the method is demonstrated on several applications such as e.g. melting points of ionic and covalent compounds and solid-solid phase transitions in perovskites. The applications show that 99% of the ab-initio calculations are skipped. This way the calculations are accelerated by more than 3 orders of magnitude, while still being able to quantitatively reproduce the ab-initio results. The implementation of our on-the-fly learning scheme is fully automatized and is mainly controlled by a few parameters. This way the amount of human intervention for the usually laborious task of training is hugely reduced.

KFM 15.30 Thu 16:00 P2/1OG

Structural Investigations and Stacking Faults in the Quasi

2D van der Waals Layered Compound $Ni_2P_2S_6$ — •Sebastian Selter[1,2], Adam P. Dioguardi[1], Hans-Joachim Grafe[1], Mihai-Ionut Sturza[1], Saicharan Aswartham[1], and Bernd Buechner[1,2] — [1]Institute for Solid State Research, Leibniz IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Institute of Solid State and Materials Physics, Technische Universität Dresden, 01062 Dresden, Germany

Van der Waals layered compounds, such as the structural family of $T_2P_2S_6$ (T = 3d transition metal) or CrX_3 (X = Cl, Br, I), recently moved in the focus of research due to the interplay between magnetism and a quasi two dimensional structural lattice. However, such van der Waals layered compounds are prone to exhibit crystallographic defects along the stacking direction, because of weak structural interactions between layers. Understanding the stacking behavior in these compounds is key to disentangle intrinsic and defect driven physical phenomena.

Here, we present a comprehensive investigation on $Ni_2P_2S_6$ by X-ray diffraction methods. Strong evidence is found for a high concentration of stacking faults along the c*-direction. As the magnetic easy axis of $Ni_2P_2S_6$ is found parallel to the a-direction in the monoclinic unit cell, in-plane rotation studies in the magnetically ordered state by magnetometry and ^{31}P-NMR allow further insight in the nature of these defects. Resulting from these studies, stacking faults are found to be well defined by a 60° rotational twinning in this compound.

KFM 16: Annual General Meeting of the KFM division

Time: Thursday 18:30–19:30 Location: TOE 317

KFM 17: Microstructure, Real Structure and Crystal Defects

Time: Friday 9:30–12:30 Location: TOE 317

KFM 17.1 Fri 9:30 TOE 317

Emitter-Site Specificity of Hard X-ray Photoelectron Kikuchi-Diffraction — •Olena Fedchenko[1], Aimo Winkelmann[2], Sergey Chernov[1], Katerina Medjanik[1], Sergey Babenkov[1], Steinn Agustsson[1], Dmitry Vasilyev[1], Moritz Hoesch[3], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]JGU, Institut für Physik, Mainz, Germany — [2]ACMiN, AGH University of Science and Technology, Krakow, Poland — [3]DESY Photon Science, Hamburg, Germany

High-resolution full-field imaging of (k_x, k_y) photoelectron distributions (angular resolution 0.03°) in a large field of view (up to 20 Å^{-1} dia.) gives access to subtle details in Kikuchi-type diffractograms [1]. This method opens a new avenue to structural analysis via hard X-ray Photoelectron Diffraction (hXPD). We present a theoretical study of the emitter-site specificity by simulating hXPD patterns for arbitrary positions of emitter atoms in the unit cell. Using the Bloch wave approach to photoelectron diffraction from lattice planes [2], the diffraction patterns from an arbitrary number of positions in the unit cell can be obtained simultaneously making use of the reciprocity theorem. Simulations for emitter atoms at various positions in the unit cell of silicon reveal surprisingly strong changes (despite the fact that the entire lattice is kept fixed). The results are compared with measurements for Si doped with Te using ion-implantation [3].

[1] O. Fedchenko et al., New J. of Phys, 21,113031 (2019); [2] A. Winkelmann et al., New J. of Phys. 10, 113002 (2008); [3] M. Hoesch et al., this conference.

KFM 17.2 Fri 9:50 TOE 317

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

Aluminium-copper alloys receive their strength during hardening by the formation of copper-rich precipitates. Their size, distribution and crystal structure are responsible for their mechanical properties. Adding small amounts of cadmium, indium or tin influences the precipitation behavior as well as the final strength of Al-Cu alloys. Quenched-in vacancies are bound to trace element atoms in the aluminium matrix. Thus, the diffusion behavior of the copper atoms is influenced. For high-purity ternary alloys we investigate the interaction of copper atoms and trace elements (In, Sn, and Pb) with quenched-in vacancies. Annealing the quenched alloys at elevated temperatures leads to finely distributed θ'- precipitates on the nanoscale.

KFM 17.3 Fri 10:10 TOE 317

Using atomic force microscopy to tune functionality at the nanoscale — •Donald M. Evans[1], Theodor S. Holstad[1], Aleksander B. Mosberg[1], Didrik R. Småbråten[1], Per E. Vullum[2], Anup L. Dadlani[1], Zewu Yan[3,4], Edith Bourret-Courchesne[4], Jan Torgersen[1], Antonius T. J. van Helvoort[1], Sverre M. Selbach[1], and Dennis Meier[1] — [1]NTNU, Trondheim, Norway — [2]SINTEF Industry, Trondheim, Norway — [3]ETH Zurich, Zürich, Switzerland — [4]Lawrence Berkeley National Laboratory, Berkeley, USA

The control of conductivity is critical to any electronic device. In this context, oxide materials are particularly interesting as their conductivity can be continuously tuned via an electric field. In addition, they have a plethora of inherent functionalities arising from the electronic degrees of freedom, such as, superconductivity, magnetism, and ferroelectricity. However, utilizing both these changes in conductivity and electronic degrees of freedom simultaneously requires the ability to change one without affecting the other. Usually this is a problem, as the net redox reaction that gives the change in conductivity also affects the electronic degrees of freedom. In this talk, I demonstrate how stable, nanoscale, enhancement of conductivity can be achieved in ferroelectrics without net mass transfer, net change in stoichiometry, or the build-up of spurious electric and chemical gradients. This approach permits both the multiple orders of magnitude change in conductivity and the inherent functionality of oxides to be utilized independently and in parallel to each other.

KFM 17.4 Fri 10:30 TOE 317

Exploring electronic properties of topological insulators using nuclear magnetic resonance — •Robin Guehne and Jürgen Haase — Felix Bloch Institute, Leipzig University, Leipzig, Germany

The investigations of 3-dimensional topological insulators such as Bi_2Se_3 focus chiefly on the gapless surface states that emerge as a consequence of the special energy band inversion near the Fermi level induced by spin-orbit coupling. Not as much studied are the real-space properties of the bulk, although, the band inversion, for example, changes the wave function of the free carriers in the bulk, compared to the topologically trivial counterpart without band inversion.

Recently we have shown that nuclear magnetic resonance (NMR) as a local, bulk probe can detect this band inversion through the electric quadrupole interaction that, in addition, measures the concentration of free carriers, e.g. originating from self-doping effects [1]. Furthermore, our orientation dependent ^{209}Bi NMR experiments in single crystalline Bi_2Se_3 reveal a so far unknown effect in condensed matter – a magnetic field induced charge symmetry that leaves the electric field gradient at the Bi site to rotate rather freely with the external magnetic field B_0 due to spin-orbit coupling as experienced by conduction electrons.

NMR data in external fields up to 17 T, i.e., shifts, linewidths and quadrupole splittings, in three-dimensional topological insulators will be discussed.

[1] R. Guehne, V. Chlan, G. V.M. Williams, S. V. Chong, K. Kadowaki, A. Pöppl, and J. Haase. J. Magn. Res. 302, 34 - 42 (2019)

20 min. break

KFM 17.5 Fri 11:10 TOE 317

Hidden Diversity of Vacancy Orderings in Prussian Blue Analogues — •Arkadiy Simonov[1,2], Hanna B. Boström[2], and Andrew L. Goodwin[2] — [1]Multifunctional Ferroic Materials, Materials Department, ETH Zürich — [2]Inorganic chemistry laboratory, University of Oxford

Prussian blue analogues (PBAs) are a broad and important family of microporous inorganic solids, famous for their gas storage, metal-ion immobilisation, proton conduction, and stimuli-dependent magnetic, electronic and optical properties, The family also includes widely investigated hexacyanoferrate/hexacyanomanganate (HCF/HCM) battery materials. Central to the various physical properties of PBAs is the ability to transport mass reversibly, a process made possible by structural vacancies. In the absence of a better model the distribution of such vacancies was assumed random.

In this talk I would like to present the latest results of analysis of the diffuse scattering from PBA single crystals which show that vacancy show surprisingly strong local ordering. Moreover, the distribution of these vacancies is influenced by crystallisation conditions. Our results establish a clear foundation for correlated defect engineering in PBAs as a means of controlling storage capacity, anisotropy, and transport efficiency.

KFM 17.6 Fri 11:30 TOE 317

Structural defects in silicon observed in situ by X-ray diffraction imaging during heating and solidification — •Maike Becker, Gabrielle Regula, Serge W. Neves Dias, Hadjer Ouaddah, Guillaume Reinhart, and Nathalie Mangelinck-Noël — Marseille Univ, Université de Toulon, CNRS, IM2NP, Marseille, France

Dislocations affect decisively the crystal quality and thus, the minority carrier lifetime, which is problematic for the efficiency of silicon in photovoltaic applications. The understanding of the formation of the dislocation arrangement is of particular importance whenever seeds are part of the Si ingot manufacturing process. To explore the role of seed crystals, this work focuses on dislocation nucleation and mobility in a seed during heating up to the melting point and during the start of solidification. Synchrotron in situ X-ray diffraction imaging (topography) is used to observe extended crystallographic defects in a silicon wafer. During heating, dislocations are generated at the sample edges and propagate in the sample. We measure their motion which intensifies with increasing temperature and observe their interactions. When solidification is triggered, some dislocations initially present in the seed propagate in the regrown crystal with the solid-liquid interface. The density of these growth dislocations decreases in the up-grown crystal when interacting with $\Sigma 3$ grain boundaries. Besides, the formation of new dislocation sources can be observed during the experiment nearby higher-order grain boundaries.

KFM 17.7 Fri 11:50 TOE 317

Examination of defects and lattice vibrations in rare and common polytypes of Silicon Carbide — •Maximilian von Roeder, Jurek Lange, Detlev Hofmann, Sangam Chatterjee, and Peter Klar — I. Physikalisches Institut and Zentrum für Materialforschung, Justus-Liebig-Universität, 35392 Gießen, Deutschland

Silicon Carbide is a wide band gap semiconductor existing in multiple polytypes. The most common polytypes are 4H- and 6H-SiC, rare ones are 8H- and 21R-SiC. The polytypism has significant effects on various properties of the material, especially the electronic band gap and thermal stability. The polytypism originates from different stacking of the layers composed of SiC_4-tetrahedra. This results in quasi-cubic and quasi-hexagonal lattice sites in the crystal of a polytype. We used Raman-spectroscopy to show the dependence of the A_1 acoustic phonon branch on the stacking type. It can be used as a fast and non-destructive way to classify the polytype at room temperature. Point defects (vacancies and impurities) were studied by electron paramagnetic resonance (EPR) spectroscopy. Furthermore, lattice vacancies are created by high-energy ($E_P = 190$ MeV) proton radiation vacancies in 4H-SiC-samples with fluxes of 10^{11} cm^{-2}, 10^{13} cm^{-2} and 10^{14} cm^{-2}. The EPR-spectra were analyzed in terms of the g-tensor, the exchange splitting (D), and the hyperfine interactions. The results of our investigation will be used to discuss the effects on the electrical properties of the silicon carbide polytypes.

KFM 17.8 Fri 12:10 TOE 317

Investigation of the real structure by means of unconventional methods of the analytical electron microscopy — •Enrico Langer — Technische Universität Dresden, Institut für Halbleiter- und Mikrosysteme, 01062 Dresden, Germany

The primary beam of a scanning electron microscope generates a local X-ray source in the investigated sample, which besides the standard application for the energy dispersive X-ray spectroscopy leads in crystalline volumes directly to lattice source X-ray interferences (Kossel technique). A further possibility consists in a focus of electrons on thin metallic foils (e.g. Fe, Ti) close to the sample surface, which is suited for the generation of a X-ray source in transmission, whereby a tube shields from the bremsstrahlung. Pseudo-Kossel interferences emerge from the diffraction of these divergent X-rays at mono- and polycrystalline material. Beside the X-ray topography this is another method for the mapping and characterization of crystal defects. However, the influence of crystal lattice defects on pseudo-Kossel X-ray interferences was only partly investigated. This work should contribute to a better understanding. The basic investigations range from the real structure characterization of intermetallic alloys to semiconductor materials, such as silicon and GaAs. The deviations from the ideal pseudo-Kossel reflection show the fault of the crystal lattice. These will be assigned to a local section of the original curve on the crystal surface by simulation of complex curves of the 4^{th} order using the further developed program KOPSKO[1]. Especially reflections ruptures can be assigned to the mosaic structure and sub-grains resp., small angle tilt or twist grain boundaries and can be measured with high accuracy. Curve sections with reflection broadening correspond to a local increase of the dislocation density, which were for example found near to grain boundaries in a Fe-Al alloy. Smallest local variations of the lattice constants lead to changes in the position perpendicular to the pseudo-Kossel curve. Even at single-crystals much more complicated regular line structures can be observed, but the formation of models is still not finished.

[1] E. Langer, R. Kurt, S. Däbritz, Cryst. Res. Technol. 34 (1999) 801.