# 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 POT 51 and POT 106; Poster P3)

### Invited Talks

| | | | | |
|---|---|---|---|---|
| KFM 1.1 | Mon | 9:00– 9:30 | POT 51 | **Investigations of multiferroic behavior within domains and domain walls of a multiferroic Aurivillius phase system** — •Lynette Keeney |
| KFM 1.5 | Mon | 10:45–11:15 | POT 51 | **Domains or no Domains in Wurtzite-Type Ferroelectrics** — •Simon Fichtner, Niklas Wolff, Tom-Niklas Kreutzer, Georg Schönweger, Adrian Petraru, Hermann Kohlstedt, Lorenz Kienle, Fabian Lofink |
| KFM 2.1 | Mon | 14:30–15:00 | POT 51 | **Formation of conducting channels along of dislocations in $SrTiO_3$** — •Christian Rodenbücher, Kristof Szot, Gustav Bihlmayer, Carsten Korte |
| KFM 2.4 | Mon | 15:55–16:25 | POT 51 | **Plastic properties of MgO : Insights from numerical modeling** — •Philippe Carrez |
| KFM 4.1 | Tue | 9:00– 9:30 | POT 51 | **Towards spatially resolved measurements of thermal transport and electrocaloric effects at the nanoscale in ferroelectric materials** — Rebecca Kelly, Olivia Baxter, Fran Kurnia, Amit Kumar, Marty Gregg, •Raymond McQuaid |
| KFM 7.1 | Wed | 9:00– 9:30 | POT 51 | **Novel device integration – combining bottom-up and topdown approaches** — •Artur Erbe |
| KFM 7.6 | Wed | 11:05–11:35 | POT 51 | **4D meso-scale electronics for next generation medical tools and electronic skins** — •Daniil Karnauschenko |

### Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

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| SYSD 1.1 | Mon | 9:30–10:00 | HSZ 04 | **Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli |
| SYSD 1.2 | Mon | 10:00–10:30 | HSZ 04 | **Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers |
| SYSD 1.3 | Mon | 10:30–11:00 | HSZ 04 | **Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann |
| SYSD 1.4 | Mon | 11:00–11:30 | HSZ 04 | **Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst |
| SYSD 1.5 | Mon | 11:30–12:00 | HSZ 04 | **The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala |

## Sessions

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| KFM 1.1–1.8 | Mon | 9:00–12:15 | POT 51 | **Focus: Domains and Domainwalls in (Multi)Ferroics I** |
| KFM 2.1–2.6 | Mon | 14:30–17:05 | POT 51 | **Focus: Dislocations in Ceramics: Mechanics, Structures and Functionality (joint session KFM/MA)** |
| KFM 3.1–3.3 | Mon | 14:30–15:30 | POT 106 | **Instrumentation and Methods for Micro- and Nanoanalysis (joint session KFM/CPP)** |
| KFM 4.1–4.10 | Tue | 9:00–13:10 | POT 51 | **Focus: Domains and Domainwalls in (Multi)Ferroic II** |
| KFM 5.1–5.4 | Tue | 10:00–11:00 | SCH A 315 | **Thin Film Properties (joint session DS/KFM)** |
| KFM 6.1–6.46 | Tue | 17:00–19:00 | P3 | **Poster** |
| KFM 7.1–7.9 | Wed | 9:00–12:35 | POT 51 | **Focus: High-resolution Lithography and 3D Patterning** |
| KFM 8.1–8.9 | Wed | 14:00–17:15 | POT 51 | **Diamond and related dielectric materials** |
| KFM 9.1–9.12 | Wed | 9:00–13:15 | POT 106 | **Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positron** |
| KFM 10.1–10.10 | Thu | 9:00–12:35 | POT 51 | **Battery Materials (joint session KFM/CPP)** |
| KFM 11.1–11.11 | Thu | 14:00–17:55 | POT 51 | **Crystal Structure Defects / Real Structure / Microstructure** |
| KFM 12 | Thu | 18:00–19:00 | POT 51 | **Members' Assembly** |
| KFM 13.1–13.7 | Thu | 10:00–12:35 | POT 106 | **Polar Oxide Crystals and Solid Solutions I** |
| KFM 14.1–14.7 | Thu | 14:00–16:35 | POT 106 | **Polar Oxide Crystals and Solid Solutions II** |

## Members' Assembly of the Crystalline Solids and their Microstructure Division

Thu 18:00–19:00 POT 51

# KFM 1: Focus: Domains and Domainwalls in (Multi)Ferroics I

The focus session is dedicated to advanced nanoscale characterization, property engineering, and modelling methods of (multi)ferroic materials. Typical examples may include ferroic domain walls, microstructural levers, or strain effects. Further, applications in novel nanoelectronic devices and nano-related engineering concepts for macroscopic properties of multiferroics are of interest.

Chair: Dr. Jan Schultheiß (University of Augsburg)

Time: Monday 9:00–12:15 Location: POT 51

**Invited Talk** KFM 1.1 Mon 9:00 POT 51

**Investigations of multiferroic behavior within domains and domain walls of a multiferroic Aurivillius phase system** — •Lynette Keeney — Tyndall National Institute, University College Cork, Lee Maltings Complex, Dyke Parade, Cork, Ireland, T12 R5CP

Single-phase multiferroics intertwine ferroelectric and ferromagnetic properties, providing novel ways to manipulate data and store information and provide opportunities for exploring new chemistry and physics. In recent years, my team reported the design of a room temperature multiferroic material with an Aurivillius phase structure demonstrating reversible magnetoelectric switching of ferroelectric domains under the influence of a cycled magnetic field. Our previous work used atomic structure determinations of preferred cation locations to advance comprehension of key mechanisms governing ferromagnetism within multiferroic domains. In this presentation, I will discuss fundamental electronic characteristics at differing bonding environments within this complex layered system. We reveal how crystal field splitting of the titanium cation is influenced by its position within the Aurivillius unit cell, correlating with the extent of tetragonal distortion, octahedral tilting and ferroelectric polarisation within the domains. I will discuss how electrostatic strain and elastic energy variations close to bismuth oxide interfaces and defect regions are not only influential in promoting magnetic cation partitioning and multiferroic behaviour, these also influence the formation of exotic charged domain walls and polar vortex domain walls, further initiating technology prospects for this intriguing multiferroic system.

KFM 1.2 Mon 9:30 POT 51

**Understanding sensitivity of ferroelectric domain walls to atmospheric parameters** — •Leonie Richarz[1], Jan Schultheiss[1,2], Edith Bourret[3], Zewu Yan[3,4], Antonius T.J. van Helvoort[1], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]University of Augsburg, Augsburg, Germany — [3]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [4]ETH Zurich, Zurich, Switzerland

Ferroelectric domain walls are natural interfaces, separating volumes with different orientation of the spontaneous polarization. The walls can develop completely different electronic properties than the surrounding domains. In ferroelectric oxides, oxygen off-stoichiometry is an additional versatile control parameter, reflected by neutral ferroelectric domain walls in hexagonal manganites: Depending on the oxygen content, their conductance varies from insulating to conducting.

In this work, we change the conductance state of neutral ferroelectric domain walls in high-quality $Er(Mn,Ti)O_3$ single crystals from insulating to conducting by annealing the samples in reducing conditions, e.g., nitrogen. The process can be reversed by annealing under oxidizing conditions, reflecting the outstanding chemical flexibility of the domain walls. The sensitivity to off-stoichiometry can be exploited to utilize the domain walls for sensing applications.

Our results provide new insight into the impact of environmental parameters on the electronic domain wall properties. This is of interest for the development of atmospheric sensors, adding a new direction to the field of domain wall nanotechnology.

KFM 1.3 Mon 9:50 POT 51

**Thermal and elastic stability of acceptor dopants in BaTiO3** — •Aris Dimou[1], Aldo Raeliarijaona[2], R. E. Cohen[2], and Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High-performance Materials (ZGH), Ruhr-University Bochum, Germany — [2]Extreme Materials Initiative, Earth and Planets Laboratory, Carnegie Institution for Science, Washington, DC 20015-1305, USA

The presence of defects, such as vacancies and aliovalent substitutions significantly impacts the functional properties of ferroelectric materials. Defect dipoles formed by acceptor dopants and oxygen vacancies have gained interest after the demonstration of superlative, reversible piezoelectric [1], and electrocaloric [2] responses. But so far a deep understanding of their stability is missing.

We compare the thermal stability of Fe, Cu, and Mn dopants, and explore the impact of biaxial strain on the defect stability by density functional theory and *ab-initio* molecular dynamics. We found the largest barrier for the $Cu_{Ti} - V_O$ defect complexes, and exhibit the enhanced barrier height under compressive biaxial strain.

References

[1] X. Ren, Nature Materials, 3(2):91-94, 2004
[2] A. Grünebohm et al., Phys. Rev. B, 93(13):134101, 2016

KFM 1.4 Mon 10:10 POT 51

**Probing hidden order in ferroelectric oxide thin films with single crystal diffuse X-ray scattering** — •Joohee Bang[1], Nives Strkalj[2], Martin Sarott[1], Morgan Trassin[1], and Thomas Weber[1] — [1]Department of Materials Science, ETH Zurich, Zurich, Switzerland — [2]Department of Materials Science and Metallurgy, Cambridge University, Cambridge, United Kingdom

Ferroelectric thin films have attracted great attention for its rich applications in energy-efficient electronic devices because of functional properties such as high dielectric constants and electrically switchable polarization. Recently, ferroelectric oxide superlattices with complex topologies such as long-range vortex-antivortex arrays of polarization have garnered much interest as they hold promise for alternative device configurations for microelectronics [1]. Here, we report on a newly discovered local order state in ferroelectric superlattices using a complete three-dimensional diffuse X-ray scattering data, which was collected by taking advantage of high-energy synchrotron X-rays in ultra-small grazing incidence geometry. The data was analyzed with the 3D-deltaPDF method [2], which not only gives a three-dimensional view of the disorder, but also the access to weak disorder that was previously not accessible. This work will contribute to understanding structure-property correlations of ferroelectric oxide superlattices and lay groundwork for developing a novel solid-state characterization technique.

[1] Yadav et al., Nature 530, 206; S. Das et al., Nature 568, 2019
[2]Weber and Simonov, Z. Kristallogr. 227, 2012

**15 min. break**

**Invited Talk** KFM 1.5 Mon 10:45 POT 51

**Domains or no Domains in Wurtzite-Type Ferroelectrics** — •Simon Fichtner[1,2], Niklas Wolff[1], Tom-Niklas Kreutzer[2], Georg Schönweger[1,2], Adrian Petraru[1], Hermann Kohlstedt[1], Lorenz Kienle[1], and Fabian Lofink[1,2] — [1]Faculty on Engineering, Christian Albrechts University, Kiel, Germany — [2]Fraunhofer ISIT, Itzehoe, Germany

For decades, the wurtzite structure served as a posterchild for pyroelectric, i.e. spontaneously polarized materials which are yet not ferroelectric. The resulting inability to control the dipole ordering after synthetization has largely limited research on wurtzite-type polarization domains and –walls to their suppression. Therefore, the growth of single domain materials of defined polarity has been one of the ultimate goals for the main applications of wurtzite-type semiconductors in the fields of MEMS, RF-, power- and optoelectronics.

Today though, the discovery of ferroelectricity in wurtzite-type solid solutions promises unprecedent possibilities in terms of reconfigurable polarization control in wurtzite-type materials, but also creates the necessity for renewed scientific attention to the domains and -walls of this structure. This contribution aims to provide a vantage point for this attention by giving a glimpse into the literature on this subject and by reporting on our preliminary experimental work on domains in

wurtzite-type ferroelectrics. Regarding the latter, transmission electron and piezoelectric force microscopy next to chemical anisotropy studies allow us to draw first conclusions regarding the nucleation, coalescence and distribution of domains in this particular material class.

KFM 1.6 Mon 11:15 POT 51

**The role of interfacial stress on the polarization stability of lead-free relaxor ceramics** — •Julia Glaum[1,2], Yooun Heo[2], Matias Acosta[3], Pankaj Sharma[2], Jan Seidel[2], and Manuel Hinterstein[2,4] — [1]NTNU, Trondheim, Norway — [2]UNSW Australia, Sydney, Australia — [3]TU Darmstadt, Darmstadt, Germany — [4]KIT, Karlsruhe, Germany

The unique structural, dielectric and electromechanical properties displayed by canonical relaxor systems, make these materials fascinating objects for fundamental studies as well as for industrial applications. Contributors to these unique properties are the multiple crystallographic phases present simultaneously even in individual grains, as well as the ferroelectric-relaxor phase transformation, which can become reversible in the vicinity of the transition temperature.

Here, we report on the thermal evolution of the crystallographic phases in a (Bi1/2Na1/2)TiO3-BaTiO3 relaxor ceramic. This system exhibits two polar phases, with the minority phase embedded into the majority phase. While the majority phase retains a stable poling state with increasing temperature up to the transition to the relaxor state, a gradual de-texturization of the poling state is observed for the minority phase over the whole temperature range. The surface domain structure decays already at significantly lower temperatures than expected from bulk observations. Development of interfacial stresses between majority and minority phases and differences in local stress state between surface and bulk are discussed as driving factors of the phase transition dynamics.

KFM 1.7 Mon 11:35 POT 51

**Effect of strain on the 3D domain structure of hexagonal manganites** — Nelly Natsch, •Aaron Merlin Müller, Amadé Bortis, Manfred Fiebig, and Thomas Lottermoser — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

We simulate and visualize the three-dimensional domain structure of strained hexagonal manganites. Due to the improper nature of their ferroelectric order, hexagonal manganites exhibit unconventional vortex domain patterns. In 3D, these vortex domain patterns are characterized by vortex lines, which are 1D topological defects that form arbitrarily oriented loops in bulk materials. We show that when strain is applied in the ab-plane, the domains exhibit an additional stripe-like order that is oriented perpendicular to the ab-plane. In addition, we show that the strain also acts on the vortex lines, forcing them to form closed loops aligned in the same plane as the domain walls. In our simulations, we observe two types of loops: one type that expands and another type that contracts and collapses. We relate both the formation of the stripe-like domains and the evolution of the vortex-line loops to a force acting directly on the vortex lines which is induced by the applied strain. Our numerical investigation is performed with a phase-field model to simulate the domain structure in three dimensions using a Landau-free-energy expansion.

KFM 1.8 Mon 11:55 POT 51

**Tracing property-determining structural alterations via scanning electron diffraction** — •Ursula Ludacka[1], Jiali He[1], Emil Frang Christiansen[1], Shuyu Qin[2], Manuel Zahn[1,6], Zewu Yan[3,4], Edith Bourret[4], Antonius van Helvoort[1], Joshua Agar[2,5], and Dennis Meier[1] — [1]NTNU, Trondheim, Norway — [2]Lehigh University, Bethlehem, USA — [3]ETH Zurich, Zurich, Switzerland — [4]Lawrence Berkeley National Laboratory, Berkeley, USA — [5]Drexel University, PA, USA — [6]Augsburg University, Germany

Ferroelectricity originates from polar displacements of lattice atoms, suggesting a one-to-one correlation between electronic and structural properties at the atomic level. Scanning electron diffraction (SED), a subcategory of 4D-STEM, in combination with direct electron detection (DED) is a powerful tool for probing functional properties on the atomic scale. We demonstrate the potential and opportunities of this innovative SED approach using improper ferroelectric ErMnO3, an ideal model system as its basic ferroelectric properties, such as local conductivity changes and atomic-scale structure are well understood. By utilizing a convolutional neural network on the SED dataset, we can deconvolve intrinsic scattering phenomena on the atomic level (ferroelectric domains and domain walls) from extrinsic scattering phenomena, such as thickness, bending, or scan distortions. Our results on this topic contain new insights into atomic scale property-structure relations for ferroelectrics. However, the gained knowledge is applicable to complex oxides in general.

## KFM 2: Focus: Dislocations in Ceramics: Mechanics, Structures and Functionality (joint session KFM/MA)

Contrasting the common (mis)belief that ceramics are brittle, a new horizon of dislocation engineering in ceramics is being revealed, where dislocations are used to harness the mechanical and electro-functional properties. This session will bring together researchers who are interested in dislocations in ceramics, covering experiments and simulations, to stimulate new ideas for dislocation-based mechanics, characterization, and functionality in ceramics.

Chair: Dr. Xufei Fang (TU Darmstadt), Dr. Till Frömling (TU Darmstadt)

Time: Monday 14:30–17:05 Location: POT 51

**Invited Talk** KFM 2.1 Mon 14:30 POT 51

**Formation of conducting channels along of dislocations in $SrTiO_3$** — •Christian Rodenbücher[1], Kristof Szot[2], Gustav Bihlmayer[3], and Carsten Korte[1] — [1]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research (IEK-14) — [2]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland — [3]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany

$SrTiO_3$ has become one of the most extensively studied metal oxides due to its exceptional electronic properties, which hold promising potential for applications in energy conversion and electronics. A key feature of $SrTiO_3$ is that its electronic transport properties are closely related to oxygen nonstoichiometry, which can be manipulated via redox reactions. Our nanoscale investigations on crystals and ceramics employing imaging techniques such as local-conductivity atomic force microscopy (LC-AFM) reveal that the reduction process is highly complex and heterogeneous on the nanoscale. Along extended defects such as dislocations there are easy reduction sites where oxygen vacancies are preferentially generated. In this way, filaments with high conductivity evolve around the dislocations in the originally insulating matrix and act as nanoscale short circuits. Upon application of mechanical stress, these filaments can even be moved through the crystal together with the dislocations. These findings not only can explain failure mechanisms in solid oxide electrolytes, but also raise fundamental questions regarding the mechanisms of electronic transport and superconductivity in self-doped transition metal oxides.

KFM 2.2 Mon 15:00 POT 51

**Dislocation engineering in oxides at room temperature: understanding the competition between plasticity and cracking** — •Xufei Fang — Technical University of Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany

Dislocations in ceramic oxides are drawing increasing attention owing to their promising physical properties, such as dislocation-tuned electrical conductivity, thermal conductivity, and electro-mechanical properties. However, due to the brittleness of most oxides at room temperature, it remains a great challenge to engineer dislocations without forming cracks, which is a prerequisite for harnessing the functionali-

ties. Here, we demonstrate dislocations can be effectively introduced into various ceramic oxides (SrTiO3, BaTiO3, KNbO3, TiO2) at room temperature by using nanoindentation pop-in stop tests. Interestingly, we find a size-dependent competition between purely dislocation-dominated plastic deformation under a critical tip radius and a concurrent appearance of cracks and dislocations when the tip radius is larger than a certain value. We further extend the deformation scale up to the millimeter regime and identify a reversal of the above size-dependent competition. We will address the underlying mechanisms by examining the dislocation nucleation, multiplication, and motion individually to shed new light on the dislocation mechanics in oxides, particularly at room temperature. Last but not least, the dislocation-tuned electrical and thermal conductivity will be briefly showcased using our developed methods for dislocation engineering.

KFM 2.3 Mon 15:20 POT 51

**Tuning dislocations in ferroelectric oxides by cyclic Indentation: dislocation toughening, domain fragmentation and phase stabilisation** — •Oliver Preuss, Fangping Zhuo, Enrico Bruder, Christian Minnert, Jürgen Rödel, and Xufei Fang — Department of Materials and Earth Sciences, Alarich-Weiss-Str. 2, 64287 Darmstadt, Technical University of Darmstadt

In light of the growing research interest in dislocation-tuned functionality in ceramics, promising proofs-of-concept have been most recently demonstrated enhanced ferroelectric properties, electrical conductivity, and superconductivity. Yet introducing dislocations into brittle ceramics remains a grand challenge, especially at room temperature. Here, we demonstrate a simple method using a large Brinell indenter to cyclically indent the sample surface to tune the dislocation densities over 4 orders of magnitude (from $10^{10}$ $m^{-2}$ up to $10^{14}$ $m^{-2}$) in single-crystal $KNbO_3$. A large, crack-free plastic zone ( 200 $\mu$m in diameter) is achieved on the sample surface at room temperature. More interestingly, both damage tolerance and fracture toughness have been improved. The interactions between dislocations and other microstructure features are examined in detail by optical microscopy, electron channelling contrast imaging, piezoresponse force microscopy methods and $\mu$-Raman spectroscopy to shed light on the impact of dislocations on the mechanical properties as well as microstructural evolution. Our findings open new questions that may raise interest for further studies in ductile ceramics such as dislocation-domain wall interaction, domain wall fragmentation and strain-induced phase stabilisation.

**15 min. break**

**Invited Talk** KFM 2.4 Mon 15:55 POT 51

**Plastic properties of MgO : Insights from numerical modeling** — •Philippe Carrez — Université de Lille, F-59000 Lille, France

Plastic properties of crystalline materials depend not only on the nature of the defects present in the crystal but also and more substantially on their mobilities and mutual interactions. This is typically the case for the creep properties of magnesium oxide (MgO), which has been the subject of numerous investigations over the years. Yet, the atomistic details of dislocation-point defects, dislocation-dislocation or dislocation-grain boundary interactions remain poorly described.

Nowadays, numerical modeling offers the possibility of modeling mechanical properties from the description of the elementary mechanisms of plasticity. As an example, we will discuss the interaction between 1/2<110>{110} dislocations and point defects in MgO. We will show how the edge dislocation core, within a region across the glide planes that expands over several Burgers vector, is a sink for vacancies, and thus enhances the pipe diffusion at moderate temperature. At higher temperature, point-defect absorption or emission along the dislocation lines allow the dislocation climb mechanism and can impact creep properties of MgO. We will thus show how atomic-scale simulations can elucidate the atomic configurations of the various jog configurations structure and give access to their formation energies.

KFM 2.5 Mon 16:25 POT 51

**Dislocation-tuned Schottky barrier in oxide ceramics** — •Mehrzad Soleimany[1,2], Till Frömling[1], Lukas Porz[1], Enrico Bruder[1], Marin Alexe[2], and Jürgen Rödel[1] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Department of Physics, University of Warwick, CV4 7AL Coventry, UK

For decades manipulation of interfaces and point defects in semiconductors have been the main focus of scientists for tuning the functional properties of materials. However, dislocations which are considered as one-dimensional defects, have not only been neglected but also tried to be avoided due to the assumption that they degrade desired properties of semiconductors. Nevertheless, it has recently been shown that this speculation can be challenged and dislocations can even be used to tune the thermal, electrical, and ferroelectric properties of materials, especially when they are introduced in high densities. In this work dislocation densities higher than $4\times$ $10^{13}$ $m^{-2}$ were introduced in a large volume of the n-type and p-type $SrTiO_3$ by mechanical deformation and cyclic loading. That has been confirmed via sample thinning and electron channeling contrast imaging. Utilizing electrochemical impedance spectroscopy and DC electrical measurements, we showed that based on doping, dislocations can reduce the Schottky barrier in the n-type $SrTiO_3$ by a factor of seven and can increase that by a factor of three in the p-type one.

KFM 2.6 Mon 16:45 POT 51

**Tailoring ceramic functional properties of YSZ with dislocations** — •Till Frömling, Qaisar Muhammad, and Jürgen Rödel — 1Division of Nonmetallic-Inorganic Materials, Department of Materials and Earth Sciences, Technical University of Darmstadt, Alarich-Weiss-Str. 2, Darmstadt 64287, Germany

The defect chemistry of zirconia is usually modified by doping with high levels of yttrium. This induces a very high oxygen vacancy concentration which is responsible for the excellent ionic conductivity. There is a high demand for even better oxygen conductors because this would benefit applications like solid oxide fuel cells and solid state electrolyzers. Nevertheless, a limit has been reached concerning the doping strategy. Therefore, we suggestion to use dislocations as one-dimensional defects. These have so far been mostly disregarded as defects for modification of functional properties but are finding increasing attention recently. However, ceramics are generally brittle and thus not easily plastically deformable. Besides the difficulty of introducing dislocations into ceramics, their exact influence on functional properties is still unclear. Our investigations of yttria-stabilized zirconia show that mechanically introduced dislocations can enhance ionic conductivity significantly. This illustrates the opportunity to tune ceramics beyond what can be achieved by chemical doping.

## KFM 3: Instrumentation and Methods for Micro- and Nanoanalysis (joint session KFM/CPP)

Chair: Prof. Dr. Theo A. Scherer (KIT Karlsruhe)

Time: Monday 14:30–15:30 Location: POT 106

KFM 3.1 Mon 14:30 POT 106

**The Hitchhiker's Guide to BCARS on Solid-State Single Crystals** — •Franz Hempel[1], Lukas König[1], Federico Vernuccio[2], Dario Polli[2], Giulio Cerullo[2], Michael Rüsing[1], and Lukas Matthias Eng[1,3] — [1]Institut für Angewandte Physik, TU Dresden, 01187 Dresden, Germany — [2]Physics Department, Politecnico di Milano, 20133 Milano, Italy — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Broadband coherent anti-Stokes Raman scattering (BCARS) is an advanced Raman- spectroscopy technique that offers high-speed hyperspectral imaging and is so far widely applied in the biomedical field. For crystalline materials and their high-precision analysis, however, additional aspects of phase-matching, scattering direction, and background removal delicately need to be taken into account. To prove the reproducibility of BCARS results and pinpoint setup-related influences, we have performed a comparison study using (a) two different setups, and (b) comparing transmission with epi-detection BCARS experiments. A broad set of solid-state crystalline materials with increasing complexity was analyzed, achieving comparable, background-free spectra. Also, each machine allows the specification of optimum laser and setup parameters for inspecting the different samples.

KFM 3.2 Mon 14:50 POT 106

**Novel techniques for low-energy positron beam diagnostics.** — •Francesco Guatieri, Michael Berghold, and Michael Zimmermann — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

Modern surface analysis techniques based on low-energy positron annihilation require the use of a stable, focused and intense particle beam. Although several techniques are available to beam scientists to measure position, shape and intensity of a positron beam, each comes with its own limitations either in terms of precision, cost or measurement time. We will present two innovative techniques to detect low-energy positrons with the goal of performing beam optimization, each of which improves onto the previous state of the art.

KFM 3.3 Mon 15:10 POT 106

**Accessible electron microscopy: Adding an EELS workflow to the ChemiTEM project** — •Daniela Ramermann, Julia Menten, Elisabeth H. Wolf, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr

Transmission electron microscopy is a versatile tool for the investigation of micro- and nanostructures as well as chemical and electronic properties. However, TEM experts are needed to perform the majority of analytic measurements, which represents a bottleneck in the throughput of research. To broaden access to TEM investigations for every scientist, the ChemiTEM project[1] has developed workflows for the most used techniques (HRTEM, STEM, EDX). These are implemented in an app and guide the user through every step after only a basic training.

Now a workflow for EELS measurements has been added: For the three most used measurement scenarios, assessing sample thickness, elemental mapping and oxidation state determination, a decision-tree based workflow has been created. A prerequisite is the STEM alignment from the ChemiTEM app. A set of questions about the sample evaluates if EELS measurements using the workflow are possible or a TEM expert is needed. Step-by-step instructions guarantee a standardised measurement and data quality. The workflow can be easily adapted to other microscopes and makes EELS based techniques available to a broader community.

[1] Hetaba et al., Chemistry-Methods, 1, 401-407, https://doi.org/10.1002/cmtd.202100001

## KFM 4: Focus: Domains and Domainwalls in (Multi)Ferroic II

Chair: Prof. Dr. Lukas Eng (TU Dresden)

Time: Tuesday 9:00–13:10 Location: POT 51

**Invited Talk** KFM 4.1 Tue 9:00 POT 51

**Towards spatially resolved measurements of thermal transport and electrocaloric effects at the nanoscale in ferroelectric materials** — Rebecca Kelly, Olivia Baxter, Fran Kurnia, Amit Kumar, Marty Gregg, and •Raymond McQuaid — School of Mathematics and Physics, Queen's University Belfast, Belfast, U.K.

Scanning Thermal Microscopy (SThM) is a promising Atomic Force Microscopy technique for mapping the thermal properties of materials at the nanoscale. In this talk, I will discuss how SThM could be a powerful tool for studying the role of microstructure on heat flow in ferroelectric materials.

Interest in using ferroic domain boundaries to enable active control of heat flow has been steadily growing over the last decade. However, direct, spatially resolved measurements of domain wall thermal transport have yet to be reported. In the first part of the talk, I will describe our SThM based approach to map spatial variations in thermal conductivity associated with microstructural inhomogeneity. We map the contrast in thermal response of the electrode/dielectric layers of a multilayer ceramic capacitor (MLCC) to demonstrate proof of principle thermal imaging and then use this approach to investigate the thermal transport properties of conducting domain walls in LiNbO3.

In the second part of the talk, I will discuss how SThM can be adapted to measure electric field induced temperature changes in electrocaloric materials with sub-micron spatial resolution. Using our approach, 2D spatially resolved maps of electrocaloric heating and cooling can be generated, here demonstrated in a BaTiO3 based MLCC.

KFM 4.2 Tue 9:30 POT 51

**Real time polarization monitoring during growth for the design of artificial layered ferroelectrics** — •Ipek Efe[1], Elzbieta Gradauskaite[1], Alexander Vogel[2], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, Empa, Switzerland

Increasing the complexity of unit cells of ferroelectric oxides beyond the standard perovskite building block supports exotic functionalities such as superconductivity, magnetoresistance, and ferroelectricity. However, integrating complex crystal structures into epitaxial design is challenging, and routes to precisely monitor the non-perovskite systems have yet to be established. Here, we directly access the polarization dynamics of the layered ferroelectric model system Aurivillius $Bi_5FeTi_3O_{15}$ films during growth using in-situ optical second harmonic generation (ISHG). We identify the characteristic Aurivillius antipolar ordering of the dipoles along the growth direction, which leads to an oscillating intensity of the ISHG signal during the layer-by-layer deposition. In combination with reflection high-energy electron diffraction monitoring, we show how the polarization orientation of the films consistently changes from out-of-plane during the growth of perovskite blocks, to fully in-plane upon the completion of the unit-cell with the fluorite-like $(Bi_2O_2)^{2+}$ planes. We demonstrate how direct access to structure-dependent polarization dynamics during growth enables the development of novel layered systems incorporating various functional perovskite blocks into the Aurivillius structure.

KFM 4.3 Tue 9:50 POT 51

**3D mapping of grain boundary chemistry in ferroelectrics** — •Kasper Hunnestad, Jan Schultheiss, Anders Mathisen, Constantinos Hatzoglou, Antonius Helvoort, and Dennis Meier — Norwegian University of Science and Technology (NTNU), 7491

Trondheim, Norway

In this work, we study the impact of polar order on the local chemistry of charged grain boundaries, which naturally form in polycrystalline pyro- and ferroelectric materials during processing. Analogous to ferroelectric domain walls, these interfaces can develop new physical properties, representing intriguing functional 2D systems. Understanding the origin of the emergent interfacial phenomena, however, is a challenging task, requiring high-resolution imaging of the atomic-scale structure.

Here, we apply atom probe tomography (APT) to study the local chemistry at grain boundaries in ferroelectrics. APT combines high chemical sensitivity and accuracy with three-dimensional spatial resolution, allowing to map and quantify otherwise inaccessible changes in chemical composition. In our polycrystalline model system, $ErMnO_3$, we consistently find an enrichment of erbium and a depletion of oxygen at the grain boundaries. This trend occurs independently of the local charge state of each grain boundary and is unexpected as it implies a local violation of charge neutrality. Our results provide new insight into the defect chemistry at the grain boundaries in polar materials, suggesting pathways for local property engineering in ferroelectric oxides via grain-boundary-selective doping.

**15 min. break**

KFM 4.4 Tue 10:25 POT 51

**Impact of defect dipoles on ferroelectric domain-walls motion** — •Sheng-Han Teng and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Defect dipoles can alter the polarization switching and the dynamics of domain walls in ferroelectrics [1, 2], which may result in internal bias fields, domain-wall pinning [3] and bowing. In this work, we use *ab initio* based molecular dynamics simulations based on the effective Hamiltonian method [4, 5] to investigate the impact of defect dipoles on the domain-walls motion of tetragonal and orthorhombic phases in $BaTiO_3$. We find that the internal bias induced by defect dipoles may modify the potential energy landscape and leads to a completely different migration path for domain switching, which can pin and possibly even accelerate domain-wall motion.

[1] X. Ren, *Nat. Mater.* **3**, 91-94 (2004)
[2] A. Grünebohm, M. Marathe, R. Khachaturyan, R. Schiedung, D. C. Lupascu, and V. V. Shvartsman, *J. Phys.: Condens. Matter* **34**, 073002 (2021)
[3] A. Dimou, P. Hirel, and A. Grünebohm, *Phys. Rev. B* **106**, 094104 (2022)
[4] W. Zhong, D. Vanderbilt, and K. M. Rabe, *Phys. Rev. B* **52**, 6301-6312 (1995)
[5] T. Nishimatsu, M. Iwamoto, Y. Kawazoe, and U. V. Waghmare, *Phys. Rev. B* **82**, 134106 (2010)

KFM 4.5 Tue 10:45 POT 51

**Revealing hidden ferroelectric domain walls in sub-surface regions and their electronic properties via non-destructive conductance mapping** — •Jiali He[1], Manuel Zahn[1,2], Leonie Richarz[1], Ursula Ludacka[1], Erik D. Roede[1], Zewu Yan[3,4], Edith Bourret[4], István Kézsmárki[2], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Norway — [2]Universität Augsburg, Germany — [3]ETH Zurich, Switzerland — [4]Lawrence Berkeley National Laboratory, USA

Ferroelectric domain walls hold great promise for next-generation nanoelectronics. In particular, charged domain walls in improper ferroelectrics have triggered conceptually new application strategies. Although it is known that the electronic properties of domain walls are determined by their charge state, orientation, and curvature, non-destructive measurements of these parameters remain a major challenge. We investigate the correlation between electronic surface properties and hidden ferroelectric domain walls in $ErMnO_3$. By recording conductance maps using scanning electron microscopy (SEM) and conductive atomic force microscopy (cAFM) in combination with FIB-nanostructuring, we reveal that domain walls in surface-near regions give rise to distinct variations in surface contrast. The findings are rationalized in a simplified model, linking the contrast variations to the local charged state of the hidden domain walls, their orientation and distance from the surface. Our work introduces novel strategies to analyze the physical properties of ferroelectric domain walls in surface-near regions with nanoscale resolution in a non-destructive way.

KFM 4.6 Tue 11:05 POT 51

**Electronic transport at pristine neutral ferroelectric domain walls in lead titanate** — •Sabine Körbel[1] and Christophe Adessi[2] — [1]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany — [2]Institut Lumière Matière, Université Claude Bernard Lyon I, France

Ferroelectric domain walls are intrinsic interfaces that form spontaneously in ferroelectric materials, such as, for example, perovskite oxides. Whereas the ferroelectric perovskite oxide itself is an insulator, ferroelectric domain walls can be electrically conductive, as numerous experiments on different perovskite oxides have shown. This domain-wall conduction could serve, e.g., for charge-carrier transport in future photovoltaic absorbers. We investigated, using ab initio calculations based on Green's functions, the electronic transport along and through neutral ferroelectric domain walls in the prototype ferroelectric perovskite oxide $PbTiO_3$, and determined how the domain walls change the electronic transmission of bulk $PbTiO_3$ and the I-V curves of an ultrathin metal/perovskite/metal sandwich structure. We find that pristine neutral domain walls have a moderate effect on electronic transmission and I-V curve (within about one order of magnitude), much smaller than the experimentally measured conductivity increase at the walls by several orders of magnitude. We suggest that the measured conductivity increase does not directly originate in the electronic structure of the pristine neutral domain walls, but is caused by secondary effects, such as the accumulation of free charge carriers and/or the segregation of charged defects at the walls.

**15 min. break**

KFM 4.7 Tue 11:40 POT 51

**Ferrielectric phase boundaries in antiferroelectric lead zirconate** — •Gustau Catalan[1], Krystian Roleder[2], and Ying Liu[3] — [1]ICREA and ICN2, Barcelona, Catalonia — [2]Institute of Physics, University of Silesia in Katowice, Katowice, Poland — [3]ICN2-Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalonia

When antiferroelectric PbZrO3 is cooled down from the paraelectric phase, antiferroelectric domains nucleate and grow until they coalesce. Adjacent antiferroelectric domains can differ in the phase sequence of the antipolar arrangement, meaning that there is a polar discontinuity at the domain wall, also known as translational boundary or antiphase boundary. Using high resolution transmission electron microscopy, we have characterized such phase boundaries. We find that their internal structure is ferrielectric, with a basic unit cell that can be described as having two dipoles ion one direction and one in the antiparallel direction. We also find that such translational boundaries can cluster together, forming stripe domains of an incipient ferrielectric phase that can moreover be internally switched. We therefore propose that antiphase boundaries can act as the seed for a low-temperature ferrielectric phase that has been theoretically predicted and which might explain the remnant polarization sometimes observed as triple hysteresis loops in nominally antiferroelectric lead zirconate.

KFM 4.8 Tue 12:10 POT 51

**Field Effect Transistor employing the static negative capacitance of a ferroelectric nano-domain nucleus** — •Pavel Mokry[1], Vit Kosina[1], and Tomas Sluka[2] — [1]Faculty of Mechatronics, Informatics and Interdisciplinary Studies, Technical University of Liberec, Liberec, Czech Republic — [2]CREAL SA, Ecublens, Switzerland

Miniaturization of conventional field effect transistors (FETs) approaches the fundamental limits beyond which opening and closing the transistor channel require such a gate voltage swing, which causes an unacceptable increase in heat generation. This problem could be reduced by placing a ferroelectric layer between the FET gate electrode and the channel. In this ferroelectric-semiconductor sandwich structure, the gate voltage can be amplified due to the negative capacitance regime of ferroelectrics. However, the original idea of using a bulk ferroelectric for voltage amplification suffers several difficulties. In this work, we provide phase-field simulations of a system that provides static negative capacitance from a nano-domain nucleus. We model the nucleus of a ferroelectric domain with reversed polarization produced by applying the voltage on a small gate electrode. We show that such a nano-domain nucleus represents a reversible system, which follows a unique path during electrical cycling and inevitably crosses a higher energy state characterized by negative static differential capacitance. Phase-field simulations confirm the robustness of this concept offering

conveniently small effective negative capacitance and its compatibility with FET technology.

KFM 4.9 Tue 12:30 POT 51

**Novel functionalities at twin domain crossings** — •Kumara Cordero-Edwards[1,2], Philippe Tückmantel[2], Iaroslav Gaponenko[2], Sahar Saremi[3], Lane Martin[3,4], and Patrycja Paruch[2] — [1]Institut Català de Nanociencia i Nanotecnología, Barcelona, Catalonia. — [2]DQMP, University of Geneva, Geneva, Switzerland — [3]Department of Materials Science and Engineering, University of California, Berkeley, USA. — [4]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA.

In ferroelectrics, domain walls (DWs) are thin interfaces separating regions with different orientations of electric polarization. These interfaces can present physical properties quite different from the surrounding domains, allowing them to be used as active components in future device applications. Recent studies of DWs using scanning probe microscopy (SPM) have focused on mapping their response to different parameters in order to understand their structure-property relationships. In particular, the role of high strain gradients present at ferroelectric twins has been shown to enhance their electrical conduction and can lead to complex rotational polarization textures.

Here, I will present our investigation of ferroelastic twin domains in epitaxial PbTiO3 thin films grown on SrTiO3, explored with SPM. Our results suggest a complex polarization structure around the twin domains, which present an unusual and distinct lateral PFM signal, associated with a distinct current signature. Moreover, twin domain crossings show a unique mechanical response distinct from the surrounding ferroelectric phase, and enhanced electrical conduction.

KFM 4.10 Tue 12:50 POT 51

**Three-dimensional imaging of ferroelectric domains using digital holographic tomography** — •Pavel Mokry[1,2], Marek Mach[1,2], Pavel Psota[1], and Karel Zidek[1] — [1]Faculty of Mechatronics, Informatics and Interdisciplinary Studies, Technical University of Liberec, Liberec, Czech Republic — [2]Institute of Plasma Physics of the Czech Academy of Sciences, Prague, Czech Republic

The formation and evolution of domain patterns in ferroelectrics are fascinating physical phenomena, which determine to a large extent, the macroscopic properties of ferroelectric samples. Therefore, imaging of ferroelectric domains belongs to the essential characterization techniques of ferroelectric materials. This work demonstrates the three-dimensional (3D) imaging of ferroelectric domains using Digital Holographic Tomography (DHT). Our method is based on the construction of the Digital Holographic Microscope, which allows taking several images of the domain pattern projections from different directions. The 3D image of the ferroelectric domain pattern is then numerically reconstructed using our original method called Curvilinear Filtered Back-projection. Our experimental method has been demonstrated by imagining the domain structure in periodically poled lithium niobate single crystals. The developed method allows fast and accurate 3D observations of ferroelectric domain structures in the whole volume of the ferroelectric single crystals on the centimeter scale. The recent DHM and DHT systems, which allow high-resolution optical imaging and on-chip optical imaging of ferroelectric domain patterns, are demonstrated and discussed.

## KFM 5: Thin Film Properties (joint session DS/KFM)

Time: Tuesday 10:00–11:00 Location: SCH A 315

KFM 5.1 Tue 10:00 SCH A 315

**Defect nanostructure and its impact on magnetism of $\alpha$-$Cr_2O_3$ thin films** — •Ihor Veremchuk[1], Oskar Liedke[1], Pavlo Makushko[1], Tobias Kosub[1], Natascha Hedrich[2], Oleksandr Pylypovskyi[1], Fabian Ganss[1], Maik Butterling[1], René Hübner[1], Eric Hirschmann[1], Ahmed Attallah[1], Andreas Wagner[1], Kai Wagner[2], Brendan Shields[2], Patrick Maletinsky[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]Department of Physics University of Basel, Switzerland

Thin films of the magnetoelectric insulator $Cr_2O_3$ are technologically relevant for energy-efficient magnetic memory devices controlled by electric fields. We experimentally investigated the defect nanostructure of 250-nm-thick $Cr_2O_3$ thin films prepared under different conditions on single crystals of $Al_2O_3$ (0001) and correlate it with the integral and local magnetic properties of the samples. Positron annihilation spectroscopy reveals that the $Cr_2O_3$ thin films are characterized by the presence of complex defects at grain boundaries, formed by groups of monovacancies, coexisting with monovacancies and dislocations. The defect nanostructure strongly affects the magnitude of the electrical readout. Furthermore, the presence of larger defects like grain boundaries has a strong influence on the pinning of magnetic domain walls in thin films. We show that the Néel temperature is hardly affected by the formed defects in a broad range of deposition parameters.

KFM 5.2 Tue 10:15 SCH A 315

**Dynamics of phase transition in Lead-free Ferroelectric thin films** — •Mallika Khosla[1], Jutta Schwarzkopf[1], Daniel Schmidt[2], Daniel Hensel[1], and Peter Gaal[1,2] — [1]Leibniz-Institut für Kristallzüchtung, Berlin,Germany — [2]Tailored x-ray products, Hamburg,Germany

In this contribution, we monitor the dynamics of the phase transition in Potassium Sodium Niobate (KNaxNb1-xO3) by taking snapshots of the structure after optical excitation using pulsed synchrotron radiation in a pump-probe scheme. Our sample is a 50 nm KNaxNb1-x O3 film grown on 20 nm thin SrRuO3 on TbScO3 substrate. The low-temperature phase displays a hierarchical order of domains and superdomains on sub-100 nm and on few um length scales, respectively. First, we show that laser heating with 7 ns pulses has a similar effect locally in terms of structural rearrangement as static heating of the whole sample volume. However, in our localized excitation the transient phase transition required to transform a similar volume fraction of the sample in the high temperature phase is about 5 times higher compared to static heating. Comparison with finite-element simulations of heat-transport in our sample shows that the phase transition dynamics does not exactly follow the temperature evolution in the ferroelectric film. In addition, time-resolved diffraction imaging experiments reveal that the stability of a spatial domain morphology has a nonlinear dependence on the local laser-induced temperature. Our results indicate that it is essential to resolve both the temporal and spatial coordinate to monitor the equilibration path of such phase transition.

KFM 5.3 Tue 10:30 SCH A 315

**Ferroelectric thin films studied by X-ray standing waves** — •Le Phuong Hoang[1], Irena Spasojevic[2], David Pesquera[2], Gustau Catalan[2], Kai Rossnagel[3,5], Jörg Zegenhagen[4], Tien-Lin Lee[4], Ivan Vartanyants[5], Andreas Scherz[1], and Giuseppe Mercurio[1] — [1]European XFEL, Schenefeld, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain — [3]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [4]Diamond Light Source, Didcot, UK — [5]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

We investigated the structural properties of ferroelectric $BaTiO_3$ thin films by X-ray standing waves with the goal to determine the atomic positions within the tetragonal unit cell in samples with different strain. Our samples consist of $BaTiO_3$ thin films grown by pulsed laser deposition (with a $SrRuO_3$ bottom electrode) on three different substrates $SmScO_3$, $GdScO_3$, $DyScO_3$ providing increasing compressive strain. All the samples were characterized by X-ray reflectivity (XRR) and reciprocal space mapping (RSM). We present X-ray photoelectron spectroscopy, X-ray diffraction and X-ray standing waves data measured at the Diamond Light Source that provide Ba and Ti atomic positions within the unit cells of sample surface. In this study we show a relation between atomic positions and compressive strain of ferroelectric $BaTiO_3$ thin films.

KFM 5.4 Tue 10:45 SCH A 315

**Exploring transition-metal substitution in $FeSe_2$ thin films formed by seleniation at various temperatures** — •Luqman Mustafa[1], Andreas Kreyssig[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Alfred Ludwig[2], and Anna E. Böhmer[1] — [1]Institute for Experimental Physics IV, Ruhr-Universität Bochum, Germany — [2]Materials Discovery and Interfaces, Institute

for Materials, Ruhr University Bochum, Germany

Transition-metal dichalcogenides with orthorhombic marcasite structure have been extensively studied for their applications in light energy conversion and photoelectrochemical devices. Lately this structure type has also gained interest for its magnetic properties as a candidate for the newly-predicted altermagnetic order.

Using combinatorial deposition and ex-situ selenization at 250°C, 350°C and 430°C, we have studied the substitution of iron with different TMs in (Fe,X)$Se_2$ thin films, (X= Co, Ni, Cr). This technique allowed to efficiently and quickly explore the possible ranges of substitution of TMs in this compound. We find that the marcasite structure of (Fe,Co)$Se_2$ forms with higher Co content when the selenization temperature is lower.

Our results represent an example for the agility of combinatorial deposition of thin films in exploring the phase diagrams of transition-metal dichalcogenides. It may be adapted for other systems, such as $FeSb_2$, and is therefore a unique tool to study a broad material family and its possible substitution ranges.

## KFM 6: Poster

Time: Tuesday 17:00–19:00 Location: P3

KFM 6.1 Tue 17:00 P3

**Electrochemical performance of $KTiOAsO_4$ (KTA) from density functional theory** — •Adriana Bocchini, Uwe Gerstmann, Tim Bartley, Hans-Georg Steinrück, Gerald Henkel, and Wolf Gero Schmidt — Universität Paderborn, 33095 Paderborn, Germany

The potassium titanyl phosphate ($KTiOPO_4$, KTP) family has been recently suggested as a promising electrode for alkali-ion batteries [1-3]. Here, we present a study [4] based on density functional theory (DFT) that investigates the electrochemical performance of potassium titanyl arsenate ($KTiOAsO_4$, KTA) as an electrode for potassium-ion batteries (KIBs). K-deficient $K_{1-x}TiOAsO_4$ ($x = 0.0 - 1.0$) and K-doped $KTiOAsO_4K_x$ ($x = 0.0 - 0.5$) is used to model cathode and anode materials, respectively. We show that KTA combines high average working voltages (up to 3.8 V) with a modest volume expansion (shrinkage) upon K (de)intercalation (both below 8%). Nudged elastic band (NEB) calculations are performed to investigate the (de)intercalation dynamics. It is shown that the most favorable K-ion (K-vacancy) diffusion path is located along the [001] direction and is characterized by activation energies lower 0.5 eV. Our results thus suggest a new application of the well-established KTA photonic crystal.

[1] Huang et al., J. Phys. Lett. 12, 2721 (2021)
[2] Huang et al., J. Chem. Phys. 156, 204702 (2022)
[3] Fedotov et al., Chem. Mater. 26, 411 (2016)
[4] Bocchini et al., Phys. Rev. Materials 6, 105401 (2022)

KFM 6.2 Tue 17:00 P3

**Lithium vacancies concentration in $LiNbO_3$ from first principles** — •Christa Fink, Felix Bernhardt, and Simone Sanna — Justus-Liebig-University, Giessen, Germany

Lithium niobate is known as a crystalline material with ferroelectric, piezoelectric, photorefractive, and electro-optical properties and therefore has multiple applications. One of the intrinsic point defects of $LiNbO_3$, the negatively charged Lithium vacancy $V'_{Li}$, is studied in this contribution from first principles. The isolated defect is investigated using density functional theory to calculate the temperature dependency of the defect concentration of Lithium vacancies in $LiNbO_3$ crystals. The defect concentration can be calculated assuming an Arrhenius behavior where the activation energy is given by the Gibbs energy of defect formation. The Gibbs energy itself is a sum of several terms which are all depending on temperature. Since *ab initio* calculations are always performed at $T = 0\,K$, a special formalism is used which allows adding a temperature dependency to the standard *ab initio* calculations. This formalism includes several approaches to take temperature into account. In addition, finite-size effects due to computational limitations need to be considered during the calculation of defect formation energies and formation entropies.

KFM 6.3 Tue 17:00 P3

**Modelling of CARS** — •Leonard M. Verhoff and Simone Sanna — Instutute for theoretical physics, Giessen, Germany

Coherent anti-stokes Raman spectroscopy (CARS) is a widely used method for material characterization which has been recently extended to crystalline solids. Even though it relies on the same vibrational modes as Raman spectroscopy, it yields a much stronger output signal. Being a third order, non-linear optical process, it depends on the material's $\chi^{(3)}$ tensor.

In this contribution, we report on our theoretical modelling of the CARS-signal. In particular, we model the generation of the signal beam by solving the underlying differential equations resulting from Maxwell's equations numerically for $LiNbO_3$, to extract a frequency-dependent amplitude that is also measured in experiments. The $\chi^{(3)}$ tensor is calculated from first principles using density functional theory before. Exploiting the symmetry of $LiNbO_3$ crystals, lower order non-linear optical effects can be neglected.

The partial differential equations defining the signal beam are further simplified by assuming plane waves for all involved lasers, including the pump, stokes and probe beam and explicitly using a specific scattering geometry.

KFM 6.4 Tue 17:00 P3

**Composition dependent optical properties of $LiNb_{1-x}Ta_xO_3$ solid solutions** — •Felix Bernhardt, Florian Pfeiffer, and Simone Sanna — Justus-Liebig-Universität, Gießen, Germany

Lithium niobate (LN) and lithium tantalate (LT) are ferroelectric crystals with a wide range of applications, extending from piezoelectric sensors [1] to integrated photonics [2]. Their structural similarities enable their combination to $LiNb_{1-x}Ta_xO_3$ (LNT) solid solutions. As the optical absorption edge of these alloys depend on their composition, one can determine the crystal composition non destructively, e.g. by optical spectroscopy.

Here, we use special quasi-random structures (SQS) to simulate LNT crystals with different compositions. These structures mimic an ideal random alloy, even when periodic boundary conditions are employed.

We calculate the first order dielectric tensor of LNT for different Ta concentrations by using density functional theory (DFT) and the indepent particle approximation (IPA). Furthermore, we employ the Bethe-Salpeter equation (BSE) on top of quasi-particle calculations in GW-approximation for pure LN and LT to model excitonic effects.

Our calculations show a clear dependence on the absorption edge with respect to the Nb/Ta ratio of the LNT crystals. The inclusion of quasi-particle effects significantly shifts the absorption edge to higher energies. Our results are in good agreement to experimental data.

[1] M. Xu et al., ACS Appl. Mater. Interfaces, 9, 40, (2017) [2] W. Sohler et al., Optics & Photonics News, 19, 1, (2008) [3] A. van de Walle et al., Calphad, 42, 13-18 (2013)

KFM 6.5 Tue 17:00 P3

**Hybrid Functionals for Periodic Systems in the Density Functional Tight-Binding Method** — •Tammo van der Heide[1], Bálint Aradi[1], Benjamin Hourahine[2], Thomas Frauenheim[1], and Thomas Niehaus[3] — [1]BCCMS, Univ. of Bremen, Bremen, Germany — [2]SUPA, Dep. of Physics, The Univ. of Strathclyde, Glasgow, G4 0NG, UK — [3]Institut Lumière Matière, Univ. Lyon, Univ. Claude Bernard Lyon 1, CNRS, Villeurbanne, France

Screened range-separated hybrid (SRSH) functionals within generalized Kohn-Sham density functional theory (GKS-DFT) have been shown to restore the correct $1/(r\epsilon)$ asymptotic decay of the screened Coulomb interaction in a dielectric environment ($\epsilon$). Major achievements of SRSH include an improved description of optical properties and correct prediction of polarization-induced fundamental gap renormalization in molecular crystals. The density functional tight-binding method (DFTB) is an approximate DFT that bridges the gap between first principles methods and empirical schemes. While RSH have already been accessible for molecular systems, effort has been made to generalize the theoretical foundation to extended systems beyond the Γ-point. For treating the periodic Fock exchange and its integrable singularity in reciprocal space, we resort to techniques successfully employed by DFT. Starting from the first principles Fock operator, we derive suitable expressions for the DFTB method, using standard inte-

gral approximations and their efficient implementation in the DFTB+ software package. Convergence behavior is investigated and demonstrated for the infinite acene series as well as 2D and 3D materials.

KFM 6.6 Tue 17:00 P3

**Vibrational and optical properties of $LiNbO_3$ and $LiTaO_3$ under uniaxial stress** — •Mike Pionteck[1], Ekta Singh[2], Sven Reitzig[2], Michael Lange[2], Michael Rüsing[2], Lukas Eng[2], and Simone Sanna[1] — [1]Justus-Liebig-Universität Gießen, Germany — [2]Technische Universität Dresden, Germany

In ferroelectrics, the bulk material and the domain walls differ strongly in their vibrational and optical properties. X-ray measurements have shown that the domain walls of $LiNbO_3$ and $LiTaO_3$ exhibit the structure of compressed bulk material [1]. Consequently, the knowledge of the Raman frequencies as well as the optical response of the bulk material as a function of stress can help to characterize the domain walls.

Our work provides, for the first time, a theoretical description of phonon frequencies under uniaxial stress along Cartesian axes using density functional theory (DFT). The calculations show a roughly linear dependence of the Raman frequencies on the applied stress, which is confirmed by corresponding Raman measurements. This behavior is very similar for $LiNbO_3$ and $LiTaO_3$ crystals. In particular, the E $TO_5$ and $TO_6$ modes show a strong dependence on uniaxial stress in the x and y direction. As the strain reduces the symmetry of the crystal, we predict degeneracy lifting for the E modes. In addition, we have calculated the linear and nonlinear optical behavior of $LiNbO_3$. In particular, this includes the second (SHG) and third harmonic generation (THG) coefficients as a function of the applied uniaxial strain. [1] M. Rüsing et al., Phys. Rev. Mat. 2, 103801 (2018).

KFM 6.7 Tue 17:00 P3

**Direct growth of iron-based compounds as anodes for potassium ion storage** — •Zidong Wang, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Potassium-ion electrochemical energy storage technologies have received much attention in recent years as an alternative to lithium-based energy storage technologies. Iron-based compounds, as a typical transition metal compound, have attracted much attention because of their low cost and high capacity as an anode of batteries. However, poor electrical conductivity and structural instability, which are common in transition metal compounds, hinder their further application in potassium-based energy storage technologies. In this work, the conductivity of electrodes was improved by a strategy of growing iron-based compounds directly on carbon papers, eliminating the binding agent in conventional preparation methods. Also, the directly grown active material can effectively reduce agglomeration during charging and discharging, thus enhancing the stability. The results show that this direct growth strategy can effectively improve the electrochemical potassium ion storage performance of iron-based compounds as a promising high-performance anode.

KFM 6.8 Tue 17:00 P3

**Fabrication of reproducible, conductive domain walls in lithium niobate** — •Julius Ratzenberger[1,2], Iuliia Kiseleva[1], Peter Hegarty[1], Zeeshan Amber[1], Michael Rüsing[1], and Lukas Eng[1,2] — [1]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence–EXC 2147, TU Dresden, 01062 Dresden, Germany

In recent years, extensive research on conductive domain walls (CDW) in lithium niobate as possible building blocks for nanoelectronic circuits has been carried out. However, a fundamental understanding of the relationship between poling, and the properties of highly-conductive domains has been missing so to date.

In this work, we systematically investigate the various poling parameters in order to come up with a recipe of how to reproducibly fabricate conductive, hexagonal domains into lithium niobate single crystals. Furthermore, by optimizing the relevant parameters, the CDW is reproducibly enhanced when following the work of Godau et al. [1]. To gain a deeper understanding into the formation of highly-conductive DWs, we apply 3D second-harmonic generation (SHG) microscopy [2] for direct real-space visualization. Our findings provide key insights into the formation of CDW in lithium niobate single crystals.

[1] Ch. Godau et al., ACS Nano 11, 5 (2017).
[2] T. Kämpfe et al., Phys. Rev. B, 89, 035314 (2014).

KFM 6.9 Tue 17:00 P3

**Photo-induced transport properties in ferroelectric lithium niobate single crystals and their domain walls** — •L. L. Ding[1], E. Beyreuther[1], K. Kempf[1], M. Rüsing[1], and L. M. Eng[1,2] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Ferroelectric materials exhibit a spontaneous and stable dielctric polarization, resulting in a variable assembly of domain and domain wall (DW) structures, that have received continuous attention[1]. Furthermore, the multifield-controlled electrical transport offers many prospects for the vivid application of ferroelectrics into electronic devices, such as ferroelectric sensors, memories, even synaptic circuits[2]. Notably, (external) control of the electronic transport through photons is very desirable since being non-invasive and ultrafast, but has been studied only sparsely. In particular, polarization switching of domains and DWs, bandgap modulation, or DW dynamics, all are susceptible to the photon-electron interaction, thus need fundamental clarifications and profound investigations. Here, we combine scanning probe techniques with analyzing the impact of light irradiation onto lithium niobate (domains and) DWs, and vary both intensity and wavelength to probe the local conductivity. This ansatz thus will improve our in-depth knowledge on the local band structure and energy level distribution within DWs, and will lay the foundation to design integrated electro-optical components thereof. [1] D. Meier, et al., Nat. Rev. Mater. 7, 157 (2022) [2] Z. D. Luo, et al., ACS Nano 14, 746 (2020)

KFM 6.10 Tue 17:00 P3

**Thermal Conductivity of CVT Grown FeS2 Crystals Measured by Optothermal Raman Method** — •Ayberk Özden[1], Esteban Zuñiga Puelles[2,3], Jens Kortus[1], Roman Gumeniuk[2], and Cameliu Himcinschi[1] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

In this study, natural mineral and needle-like pyrite crystals grown by chemical vapour transport were selected as model systems and their thermal conductivities were obtained by the optothermal Raman (OTR) method [1]. It is shown that the bulk model used accurately detects differences in the thermal conductivities of mineral and CVT crystals. This difference is attributed to point defects, such as sulphur vacancies or impurity doping. Balkanski-Klemens model analysis showed that three-phonon scattering of Ag and Eg modes and lattice thermal expansion are the dominant anharmonic contributions, while four-phonon scattering is negligible in pyrite-FeS2. Thus, OTR not only provides an easy access to the thermal conductivity of single crystals in their most native form but also sheds light on the underlying phonon scattering mechanisms.

[1]A. Özden, E. Zuñiga-Puelles, J. Kortus, R. Gumeniuk, C. Himcinschi, J. Raman Spectrosc. , DOI:10.1002/jrs.6456.

KFM 6.11 Tue 17:00 P3

**Dynamics of the electrocaloric effect in ferroelectric materials** — •Jan Fischer, Daniel Hägele, and Jörg Rudolph — Ruhr-Universität Bochum, Germany

Ferroelectric materials are promising candidates for sustainable and environmentally friendly cooling applications due to their electrocaloric effect (ECE). The reversible temperature change $\Delta T$ results from a change of polarization $P$ under adiabatic conditions. However, direct studies of the adiabatic temperature change are experimentally challenging. The vast majority of previous studies has used either indirect methods or slow temperature sensors. Systematic studies of dynamics of the ECE down to short timescales are completely missing.

Here, we present a direct and contactless method to study the dynamics $\Delta T(t)$ of the ECE with mK temperature resolution and $\mu$s temporal resolution via the infrared emission of the sample.[1,2] The simultaneous recording of applied electric field $E(t)$ and polarization $P(t)$ transients gives further the opportunity to correlate the caloric with the dielectric properties thus opening new perspectives for a fundamental understanding. The technique also allows for measurements faster than the heat exchange between sample and environment achieving adiabatic conditions. Our method is applicable to a wide range of materials and requires no sophisticated sample processing.

We present measurements on different materials ranging from bulk fer-

roelectrics over complex relaxor ferroelectrics to thin polymer films.
[1] J., Döntgen, *et al.*, Applied Physics Letters 106, 3 (2015)
[2] J., Döntgen, *et al.*, Energy Technology 6, 8 (2018)

KFM 6.12 Tue 17:00 P3

**Fabrication steps for realization of quantum tokens** — •Miriam Mendoza Delgado[1], Julia Heupel[1], Jan Thieme[2], Johann Peter Reithmaier[1], Kilian Singer[2], and Cyril Popov[1] — [1]Institute of Nanostructure Technologies and Analytics (INA), Center of Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany — [2]Institute of Physics, Center of Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany

Nitrogen-vacancy (NV) color centers in diamond are fluorescent defects which possess "atom-like" properties and can be implemented as single photon sources with high optical stability and quantum yield, even at room temperature. Furthermore, the coherent electron spin of NV can be used as a long lived qubit which can be applied in quantum information technology, e.g. in quantum repeaters or tokens. In order to enhance the photon emission from NV centers and the collection efficiency, they should be incorporated in photonic structures, like nanopillars. The aim of the current work is the fabrication of diamond nanopillars incorporated with NVs and integrated with microwave antennas and electrodes, for the realization of quantum tokens. The fabrication of arrays of monocrystalline diamond nanopillars with diameters between 150 nm and 250 nm, 1 $\mu$m height and center-to-center distance of 10 $\mu$m consisted of their definition by electron beam lithography and subsequent inductively coupled plasma reactive ion etching with oxygen. Different techniques are implemented for the creation of NVs, which can affect both their density and properties.

KFM 6.13 Tue 17:00 P3

**Engineering of Dendrite-Free and Activity-Enhanced Dual-Functional Electrodes for High-Energy Na-CO2 Batteries** — •Changfan Xu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Constructing suitable multifunctional electrodes for dendrite-free anodes and kinetics-enhanced CO2 cathodes is considered one of the most important ways to further advance the practical application of Na-CO2 batteries. Herein, Ru nanoparticles grown on carbon paper (RuCP) are rationally designed and employed as both Na anode and CO2 cathode in Na-CO2 batteries. The outstanding electrical conductivity, superior sodiophilicity, and high catalytic activity of RuCP electrodes can simultaneously contribute to homogenous Na+ distribution and dendrite-free sodium structure, and strengthen discharge and charging kinetics. The morphological evolution confirms uniform deposition of Na on RuCP anode with dense and flat interfaces, delivering enhanced Coulombic efficiency and cycling stability. Meanwhile, Na-CO2 batteries with RuCP cathode demonstrates low overpotentials and excellent cycling stability. Significantly, excellent electrochemical properties are obtained in the full battery (RuCP@Na || RuCP), laying the foundation for practical applications of Na-CO2 batteries.

KFM 6.14 Tue 17:00 P3

**Material dependent differences in spectroscopic changes of the transient reflectivity on ultrashort timescales** — Jonathan Frank, Julian Mertens, Felix Hoff, and •Matthias Wuttig — 1. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany

Optical spectroscopy is a well-established technique to characterize solids. It can be utilized to distinguish different types of chemical bonding, i.e. separate solids which employ metallic, ionic and covalent bonding. We have tried to understand if these differences in bonding are still visible if the materials are excited with femto-second laser pulses. Femtosecond pump-probe spectroscopy experiments at a fixed pump-pulse wavelength were carried out in an isotropic detection scheme, to investigate the wavelength dependent reflectivity changes of optically excited samples on sub-ps timescales for wavelengths ranging from the visible to the near infrared. The measurements were carried out on various pure metals, chiral topological semimetals and semiconductors. The reflectivity changes, for a given material, vary greatly in duration and magnitude, depending on the probe wavelength. Furthermore, while an initial decrease in the transient reflectivity may be observed at one probe wavelength, an increase may be measured with another. This behavior is intrinsically linked to the excitation of carriers, their subsequent relaxation and their interaction with the lattice. The results for different materials are presented and compared, and trends within a material group evaluated. A possible link to emergent properties, conductivity and dielectric function, is discussed.

KFM 6.15 Tue 17:00 P3

**Comparison of Infrared and Raman active phonon modes in Lithium Niobate** — •Soham Gharat[1], Susanne Kehr[1], Michael Rüsing[1], and Lukas M Eng[1,2] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

The isostructural crystal of Lithium niobate is among the most widely used single-crystalline ferroelectric crystal with applications ranging from nonlinear optics [1] and high-speed electro-optic modulators, to high-frequency electronic filters [2]. In this work, we investigate the Lithium niobate crystal using both Raman spectroscopy and Fourier transform infrared spectroscopy (FTIR) [3]. We focus on consistently assigning the phonons in this material system using the two techniques in order to characterize and compare all these vibrational modes and their associated optical response. This work hence serves as a basis for the future study of nanoscopic features in this material, i.e. especially domain walls, by means of nano-FTIR and micro-Raman spectroscopy [4].

[1] D. Zhu et al., Adv. Opt. Phot. 12, 242 (2021); https://doi.org/10.1364/AOP.411024. [2] C. Wang et al., Nature 562, 101 (2018); https://doi.org/10.1038/s41586-018-0551-y. [3] S. Margueron et al., J. Appl. Phys 111,104105 (2012). https://doi.org/10.1063/1.4716001. [4] M. Rüsing et al., Phys. Rev. Mater. 2, 103801 (2018); https://doi.org/10.1103/PhysRevMaterials.2.103801.

KFM 6.16 Tue 17:00 P3

**Control of structure and morphology of LiNi0.8Co0.1 Mn0.1 powder before and after calcination** — •slaheddine Jabri[1], Markus Rojer[2], Georg Garnweitner[2,3], Markus Etzkorn[1,3], and Uta Schlickum[1,3] — [1]Institute of Applied Physics, Technische Universität Braunschweig, 38106 Braunschweig, Germany — [2]Institute for Particle Technology, Technische Universität Braunschweig, 38104 Braunschweig, Germany — [3]Laboratory for Emerging Nanometrology (LENA), Technische Universität Braunschweig, 38106 Braunschweig, Germany

The demand of high energy density of lithium battery cells has strongly increased in the last years to enable long-range electric vehicle applications. Nowadays one focus lies on the optimization of the material composition of LiNi0.8Co0.1Mn0.1 (NMC811) as the promotor cathode material, which has the advantage of high specific capacity. However, the synthesis of high quality NMC811 material is still difficult due to its structure and thermal instability. Here, the NMC811 powder is prepared from acetate precursors in a cheaper and more environmentally synthesis procedure. The structure and the morphology of pre-calcinated und calcinated NMC811 were investigated using (cross section) Scanning Electron Microscopy (FIB-SEM) and Raman Spectroscopy. Beside the internal structure of single particles, this study provides information about the impurities present in the powder. In addition, the result shows that a compact and ordered layered rhombohedral phase structure of the NMC811 powder is obtained after annealing to 800 and 850 °C.

KFM 6.17 Tue 17:00 P3

**$RbTiPO_4F$: A novel electrode material?** — •Yingjie Xie, Uwe Gerstmann, Wolf Gero Schmidt, and Adriana Bocchini — Universität Paderborn, 33095 Paderborn, Germany

The development of renewable forms of energy goes hand in hand with the search for efficient energy storages. Battery technologies based on metal ions heavier than Li are discussed as a greener, more efficient, and less expensive energy storage alternative to lithium-ions in batteries. However, because of the larger ionic radii, new electrode materials are required to guarantee, e.g., high energy densities, a fast ion (de)intercalation, and a robust long-term operation. In this context, many recent studies indicate the potassium titanyl phosphate ($KTiOPO_4$, KTP) family as a promising electrode in alkali-ion batteries [1-4].

Here, we investigate the suitability of $RbTiPO_4F$ as a cathode for Rb-ion batteries using density functional theory (DFT). Particular attention is paid to the average voltages and the volume shrinkage caused by the deintercalation of Rb atoms from the crystal.

[1] Fedotov et al., Chem. Mater. 26, 411 (2016)

[2] Fedotov et al., J. Mater. Chem. 6, 14420 (2018)
[3] Huang et al., J. Phys. Lett. 12, 2721 (2021)
[4] Bocchini et al., Phys. Rev. Materials 6, 105401 (2022)

KFM 6.18 Tue 17:00 P3

**Nonlinear optical interactions in confined nanostructures** — •Zeeshan Hussain Amber[1], Kai Jürgen Spychala[2], Boris Koppitz[1], Lukas M Eng[1,3], and Michael Rüsing[1] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]Department of Physics, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Nonlinear optical (NLO) micro-spectroscopy is a very power tool for both investigating the material properties and noninvasively visualizing domains and domain walls in ferroelectric materials [1]. Thin film materials are usually supported on substrates leading to interference and reflection related phenomena during -spectroscopy, which make interpretation of experimental results particularly challenging. Here, we report on Second Harmonic (SH) and Third Harmonic (TH) generation experiments on wedge-shaped samples cut out from 5%Mg-doped congruent Lithium niobate single crystals, and compare these findings with numerical [2] and semi-analytical simulations. We find that thin-film interference, reflection and phase matching strongly affect the signal strength in SH/TH generation. The excellent agreement between the simulated and experimental data shows that rigorous theoretical analysis can help identifying genuine material properties through systematically varied sample and setup parameters during NLO analysis.

[1] M. Ruesing et al., J. Appl. Phys. 126,114105 (2019). [2] Z.H. Amber et al., J. Appl. Phys. 130,133102 (2021).

KFM 6.19 Tue 17:00 P3

**Quantitative electrical characterization of conductive ferroelectric domain walls in $LiNbO_3$** — •Manuel Zahn[1,2], Elke Beyreuther[1], Iuliia Kiseleva[1], Ahmed S. Lotfy[1], Michael Rüsing[1], and Lukas M. Eng[1,3] — [1]Institut für Angewandte Physik, Technische Universität Dresden, 01187 Dresden — [2]Experimentalphysik V, Zentrum für Elektronische Korrelation und Magnetismus, Universität Augsburg, 86135 Augsburg — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, 01187 Dresden

Ferroelectric domain wall (DW) conductance can be divided into two separate mechanisms, (a) the injection/ejection of charge carriers across the Schottky barrier formed at the (metal-)electrode-DW junction and (b) the transport of those charge carriers along the DW. Current-voltage (I-U) characteristics recorded at variable temperatures from $LiNbO_3$ DWs are clearly able to differentiate between these two contributions and, moreover, allow us to directly quantify the physical parameters relevant for the two mechanisms (a) and (b) mentioned above. These are, e.g., the resistance of the DW, as well as the saturation current, the ideality factor, and the Schottky barrier height of electrode/DW junction, moreover the activation energies needed to initiate the thermally activated hopping transport along DWs. We will show that this electronic transport along $LiNbO_3$ DWs can be elegantly viewed and interpreted in an adapted semiconductor picture based on a double-diode/double-resistor equivalent circuit model.

KFM 6.20 Tue 17:00 P3

**The impact of Schottky barriers when electrically contacting conductive domain-walls in lithium niobate single crystals** — •Iuliia Kiseleva[1], Uliana Yakhnevych[2], Julius Ratzenberger[1], Manuel Zahn[1,3], Elke Beyreuther[1], Michael Rüsing[1], Holger Fritze[2], and Lukas M. Eng[1,4] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Am Stollen 19 B, Goslar, 38640, Germany — [3]Experimentalphysik V, Universität Augsburg — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Conductive domain walls (DWs) in lithium niobate are promising constituents for applications in nanoelectronics, due to their high conductance and ability to be created quasi-on-will through high-voltage poling. However, electrically contacting the DWs leads to the formation of a Schottky barrier between the DW and the electrode material. In this work, we study a variety of different factors affecting the electronic transport across the barrier, e.g. the electrode material, the quality of the lithium niobate surface, and the influence of the applied voltages during the DW conductivity-enhancement procedure. It was found that all these factors have a significant influence on the Schottky barrier formation; moreover, the bulk structure of the DWs is also influenced by the interface's state. Our results demonstrate the importance of reproducible sample surface conditions and identifying promising directions for implementing improved DW conductivity.

KFM 6.21 Tue 17:00 P3

**Time-resolved reflectivity measurements of Sb2Se3:Bi2Se3 alloys and Sb2S3 as studied by an ultrafast Optical Tester** — •Ramon Pfeiffer, Maximilian Müller, Eric Lensker, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany

Laser-induced crystallization at a wavelength of 658 nm of alloys of Sb2Se3:Bi2Se3 has shown that the minimum crystallization time decreases with increasing Bi2Se3 content. This is, however, also accompanied by a reduction of the reflectance change upon crystallization. For higher Sb2Se3 contents, on the contrary, a slow and stochastic crystallization process was observed. Since Sb2Se3 has a much higher absorption coefficient at shorter wavelength, more efficient switching is expected with a blue laser diode. A similar consideration is made for Sb2S3 where hardly any light is absorbed below wavelength of about 600 nm. As a blue laser setup is much closer to the absorption maximum of Sb2S3, a better energy input is expected. For this reason, in our optical phase change tester, a blue laser diode (405 nm) has been implemented to investigate the materials mentioned above.

KFM 6.22 Tue 17:00 P3

**Simulation Study of the Multi-beam Ptychography Optics and Setup Optimization** — •Tang Li, Mikhail Lyubomirskiy, and Martin Seyrich — Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

Ptychography is a robust computational iterative phase retrieval imaging method using overlapping constraints to decouple the probe and object information. It has the ability to obtain nanometer resolution with a small probe size and efficient overlapping. However, for single beam ptychography, it is inefficient beam usage, where almost 99% of the photon flux is wasted, and time-consuming to collect a nanometer resolution dataset with a large field of view (FOV). Therefore, we propose using a developed multi-beam ptychography (MBP) to relax the sample size limitation and scan duration. The feasible FOV scales with the number of parallel beams.

Although, we demonstrate the feasibility of using six coded probes to reconstruct the sample successfully. It is still not clear what is the up limit for the probe number and the least requirements of the difference between the probes that we still can decouple the probe contribution from the diffraction pattern. Hence these boundaries are explored in this work. It focuses on the forward simulation framework using the MBP setup and investigates the influence of different physical parameters, such as probe distance, probe difference, probe number, noise level influence, etc. This work provides a feasible parametric design for MBP optical and experimental setup, and it also opens the way to further development.

KFM 6.23 Tue 17:00 P3

**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 6.24 Tue 17:00 P3

**Analysis of Structural Materials with Coincident Doppler Broadening Spectroscopy Using New Evaluation Software** — •Leon Chryssos, Vassily Burwitz, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

Coincident Doppler Broadening Spectroscopy (CDBS) of the 511 keV electron positron annihilation line not only provides defect sensitive studies of materials, but also elemental signatures at the positron annihilation site. This enables the analysis of foreign atoms in the host matrix, vacancy-solute complexes and precipitates in solids. Using a new data analysis software several structural materials were evaluated at the recently upgraded CDB spectrometer at the NEutron induced POsitron source MUniCh (NEPOMUC). The most important features of the software will be explained. The functionality of the experiment and analysis software will be evaluated using several structural materials including AlCu alloys and W single crystals.

KFM 6.25 Tue 17:00 P3

**Improved thermoelectric properties of SnSe through forming a phase employing metavalent bonding** — •Nan Lin, Yuan Yu, Tanmoy Ghosh, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University

SnSe only shows high ZT values above 750 K when the structure transforms from the asymmetrical Pnma phase to the higher symmetrical Cmcm phase. As a typical IV-VI compound bonded by p-state electrons, the Cmcm phase SnSe with an improved symmetry is expected to show the same chemical bonding with other rock-salt IV-VI compounds, which could be responsible for its excellent thermoelectric performance. Yet, it is challenging to stabilize the Cmcm phase at room temperature to characterize the bonding indicators. We successfully obtained the high-symmetry rock-salt SnSe phase by growing (SnSe)0.67(AgSbTe2)0.33 (SnSe)0.67(AgBiTe2)0.33, (SnSe)0.67(AgBiSe2)0.33, and (SnSe)0.5(AgSbSe2)0.5 alloys in a Bridgman oven. All cubic SnSe alloys show a unique portfolio of properties including a high optical dielectric constant, a large Born effective charge, and abnormal bond-breaking behavior in laser assisted atom probe tomography. All these characteristics are indicative of the metavalent bonding mechanism while are not found in the pristine SnSe. Concomitantly, zT increases from near 0.1 for the Pnma SnSe to about 1.0 for all the Fm -3m SnSe phases. Our work demonstrates that metavalent bonding could be the origin of many special properties of SnSe including the excellent thermoelectric performance.

KFM 6.26 Tue 17:00 P3

**Highly-ordered Ni nanoarrays as an effect current collector for dendrite-free sodium metal batteries** — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium metal batteries (SMBs) are attracting extensive attention for energy storage field due to its intrinsic high theoretical capacity and low redox potential, as well as its low cost and broad sources. Nevertheless, the inevitable side reactions and uncontrollable dendrite growth block its practical application. 3D confinement strategy demonstrates great potential for stabilizing the Na anode owing to its optimized ion/electron transportation, lower deposition overpotential, and structural stability. A technique via anodized alumina oxide (AAO) templates s is an advanced preparation technique to fabricate various 3D nanostructures. Here, a 3D Ni nano-arrays nanostructure was fabricated with highly-ordered structure, which provides a greater specific surface area, reduces local current density and inhibits of Na dendrite formation. Due to the unique 3D nanostructure, dendrite-free Na deposition and superior electrochemical performance improvements in SMBs have been realized.

KFM 6.27 Tue 17:00 P3

**Local control of ferromagnetic domain patterns via structural ordering** — •Ahmed Samir Lotfy, Lukas Kuerten, Yooun Heo, Elzbieta Gradauskaite, Morgan Trassin, and Manfred Fiebig — Department of materials, ETH Zürich, Zürich, Switzerland

Controlling domain patterns is closely linked to device functionalities in logic applications. However, the means to engineer domain locations are scarce so far, limiting this functionality. The recent utilization of substrate topography to predefine the ferroelectric domain patterns by engineering the substrate step spacing via different miscut angles motivates our investigation for a similar control mechanism over ferromagnetic domain patterns. Neodymium gallate (NGO) is our substrate of choice because it is the only oxide among the lanthanide gallates with no structural phase transitions in a very extended temperature range (12-1773K). Therefore, $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) films grown on NGO substrates exhibiting substrate steps were also investigated for such a correlation between the substrate topography and the ferromagnetic domain patterns in LSMO. Strikingly our results show an identical domain pattern to the substrate steps. This correlation might result from the ferroelastic nature of LSMO and could be utilized for ultrahigh-density memory devices.

KFM 6.28 Tue 17:00 P3

**How to employ advanced innovation tools to advance soft X-ray nanolithography** — •Andreas Späth — Institut für Nanotechnologie und korrelative Mikroskopie (INAM) gGmbH, 91301 Forchheim, Germany — Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The Theory of Inventive Problem Solving is becoming increasingly significant in technical engineering and design. The present work illustrates the potential of its most common tools to advance instrumentation in soft X-ray microscopy and nanolithography. The initial setup designed for Focused X-ray Beam Induced Deposition is analyzed in-depth by function modelling to identify harmful or defective interactions between components. These problematic interactions are tracked back to root causes by cause-effect chain analysis. Root causes are often disguised technical or physical contradictions. TRIZ employs abstract innovation principles to solve such contradictions after they are categorized based on the nature of conflicting parameters. Another approach is to transfer harmful/defective interactions into a substance-field model of the problem that can be addressed by suitable substance-field models of potential solutions. The analysis yielded ideas for a significantly improved FXBID setup. The project benefited from funding by DFG (grant SP 1775/1-1).

KFM 6.29 Tue 17:00 P3

**X-ray near-edge absorption spectroscopy and X-ray diffraction on thin AlCrVYN films** — •Eric Schneider[1], Nicola Thiering[1], Michael Paulus[1], Finn Ontrup[2], Nelson Filipe Lopes Dias[2], and David Kokalj[2] — [1]Fakultät Physik/DELTA TU Dortmund, 44221 Dortmund, Deutschland — [2]Fakultät Maschinenbau TU Dortmund, Dortmund, Deutschland

In materials science tool coatings are optimized for use at elevated process temperatures. AlCrVYN thin films are promising candidates in this area, as vanadium can form so called Magnéli phases, which reduce the coefficient of friction. The aim of this project is to gain a fundamental understanding of the dependence between deposition parameters, layer structure and oxidation behavior of AlCrVYN coatings. For this purpose, the coating systems were deposited on a WC-Co composite substrate by a hybrid procedure of DC sputtering and high-energy pulse magnetron sputtering (HiPIMS). In addition, different cathode-target combinations will be tested to determine their influence on the structure of the thin films. For the investigation of the samples we used synchrotron radiation at beamline BL9 and BL10 of the synchrotron radiation source DELTA (Dortmund, Germany) to perform XRD and XANES measurements. The samples were annealed ex situ in an oven to temperatures up to 1000°C to study their oxidation behavior. Depending on the process parameters, different oxidation behaviour and residual stresses present in the samples were observed. We thank DELTA for providing synchrotron radiation. This work was supported by the DFG via TO 169/21-1.

KFM 6.30 Tue 17:00 P3

**Combine circular economy with analytical facilities, instruments and know-how** — •Eric Hirschmann, Maik Butterling, Maciej Oskar Liedke, Ahmed Gamal Attallah, and Andreas Wagner — Zentrum Dresden-Rossendorf, Dresden, Germany

As part of the ReMade@ARI (REcyclable MAterials DEvelopment at Analytical Reserach Infrastructures) project of the Horizon Europe program, we present the Positron Research Infrastructure (pELBE) at the ELBE linear accelerator of the HZDR. PELBE is a collection of methods and instruments that can characterize defects, determine open volumes and investigate open or closed microporous systems using positron annihilation spectroscopy. The ReMade@ARI project is committed to foster the development of innovative, sustainable materials for key components in a wide range of sectors including electronics, batteries, vehicles, construction, packaging, plastics, textiles and food.

The project aims to simplify the use of large-scale research facilities at HZDR or other European sites for both academic and industrial players in the circular economy. The poster will provide a closer look at the outline of the project as well as the positron research infrastructure (pELBE) at HZDR.

KFM 6.31 Tue 17:00 P3

**Growth and characterization of $Ni_{37}Co_{13}Mn_{33}Ti_{17}$ single crystals** — •David Koch[1], Benedikt Beckmann[1], Gavin Vaughan[2], Oliver Gutfleisch[1], and Wolfgang Donner[1] — [1]Intitute of Material Science, Darmstadt, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France

Since 2015 the „all-d-Heusler"material Ni(Co)MnTi is object of interest due to its magneto-functional applications linked to a martensitic phase transition, like solid state cooling and magnetic shape memory effect. Nevertheless, for many characterization methods single crystals are necessary but not reported in literature so far. Here we report on the growth and preparation of $Ni_{37}Co_{13}Mn_{33}Ti_{17}$ single crystals based on anomalous grain growth. The resulting single crystals are several mm in size, can be used for various experiments and show a reversible martensitic phase transition around 200 K. Here, the samples are characterized using magnetometry and various laboratory single crystal diffraction experiments. In addition, we use high energy synchrotron experiments to improve the dynamic intensity range and to reconstruct the whole reciprocal space.

KFM 6.32 Tue 17:00 P3

**Metavalent Bonding empowers the High Thermoelectric Performance in Bi2Te3-based Alloys** — •Yinghao Tao — I.Physikalisches Institut of RWTH Aachen

Bi-Te-based alloys show outstanding thermoelectric performance near room temperature due to the large Seebeck coefficient, high electrical conductivity, and low thermal conductivity. Even though the excellent properties of these alloys have been recognised for decades, the origin of these favorable characteristics has not been fully revealed. Very recently, a special combination of properties has been found in group IV-VI and V2-VI3 compounds due to an unconventional bonding mechanism, coined metavalent bonding (MVB). Bi2Te3-based alloys also utilize MVB. This raises the question of whether the excellent thermoelectric performance stems from the MVB. In this work, we have prepared single-crystal BixSb1-xTe3 (x=0.5, 0.6, 0.7) samples by Bridgman oven and then measured the transport properties by thermal transport option (TTO) in PPMS. We have also measured the optical properties and the bond-breaking behavior of these compounds using Fourier-transform infrared spectroscopy (FTIR) and atom probe tomography, respectively. These methods prove the metavalent bonding nature in these compounds. Finally, we relate the favorable transport properties to the close relationship between chemical bonding and the electronic band structure. Metavalent compounds are characterized by a large valley degeneracy, a small band effective mass, and strong phonon anharmonicity. All of these attributes lead to high thermoelectric performance.

KFM 6.33 Tue 17:00 P3

**First X-ray diffraction measurement from high pressure hydrostatic cells for X-ray scattering applications** — •Kevin Lehninger, Eric Schneider, Jaqueline Savelkouls, Michael Paulus, and Christian Sternemann — Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

Small-angle and wide-angle X-ray scattering (SAXS/WAXS) at moderate pressures are of increasing importance for the investigation of e.g. protein denaturation or stimulus-responsive materials. One of the experimental challenges is the precise pressure control in the pressure range up to 10 kbar while separating the sample volume from the pressure-transmitting medium. To this end, we present two dedicated hydrostatic high pressure cells designed for use at the beamlines BL2 and BL9 of the synchrotron radiation source DELTA, which use water for pressure transmission, and show first measured diffratograms of gold and potassium bromide. The WAXS cell with an opening angle of 60 degrees allows a sample volume with a cross-sectional area of one square millimetre to be exposed to a maximum pressure of 5000 bar. The sample volume is enclosed in a flexible capillary tube capillary tube, which is located between two diamond windows and can have a maximum diameter of 1.5 mm. The SAXS cell can be operated up to a pressure of 10kbar and an opening angle of 20 degrees. Here, the sample volume is contained in a cylinder sealed with polyimide film which is screwed into the high-pressure cell via a sliding system.

KFM 6.34 Tue 17:00 P3

**Optical and Spin Properties of NV Center Ensembles in Diamond Nano-Pillars** — •Kseniia Volkova[1], Julia Heupel[2], Sergei Trofimov[1], Fridtjof Betz[3], Rémi Colom[3], Rowan W. MacQueen[1], Sapida Akhundzada[4], Meike Reginka[4], Arno Ehresmann[4], Johann Peter Reithmaier[2], Sven Burger[3], Cyril Popov[2], and Boris Naydenov[1] — [1]ASPIN, Helmholtz-Zentrum Berlin, Germany — [2]INA, CINSaT, University of Kassel, Kassel, Germany — [3]Zuse Institute Berlin, Berlin, Germany — [4]IP, CINSaT, University of Kassel, Kassel, Germany

Nitrogen-vacancy (NV) centers in diamond integrated in nano-pillars could be used as tips for scanning probe for magnetic field imaging with high sensitivity and nano-scale spatial resolution. We present the fabrication of diamond nano-pillars with diameters up to 1000 nm in type Ib diamonds with two crystal orientations [100] and [111] using electron beam lithography and inductively coupled plasma reactive ion etching. The NV centers ensembles were created by 6 keV-He ion bombardment and subsequent annealing. Estimated numbers of NVs per pillar to be 4300 ± 300 and 520 ± 120 for the [100] and [111] samples, respectively. Lifetime measurements of the NV's excited state showed two time constants with average values of $\tau_1 \approx 2$ ns and $\tau_2 \approx 8$ ns, which are shorter than a single NV center in a bulk crystal. This is probably due to interaction with defects created by the helium ion bombardment and substitutional nitrogen. Optically detected magnetic resonance contrast was about 5% and average coherence times are $T_2$ [100] = 420 ± 40 ns, $T_2$ [111] = 560 ± 50 ns.

KFM 6.35 Tue 17:00 P3

**High-speed domain wall imaging using broadband coherent anti-Stokes Raman scattering** — •Robin Buschbeck[1], Franz Hempel[1], Sven Reitzig[1], Julius Ratzenberger[1], Lukas König[1], Peter Andrew Hegarty[1], Zeeshan Hussain Amber[1], Michael Rüsing[1], and Lukas Eng[1,2] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Spontaneous Raman spectroscopy (SR) is a broadly used and versatile method for the analysis of structures in crystalline materials, such as strain distributions or ferroelectric domain walls. A large disadvantage of this technique are the high acquisition times of up to several seconds per data point to visualize these structures. In this work, we demonstrate the use of a promising alternative, broadband coherent anti-Stokes Raman scattering (B-CARS) and compare this technique with SR at the example of poled Lithium niobate. We demonstrate a more than resulting in a 100 times higher signal-to noise ratio, while maintaining similar intensities. These results promise the use of B-CARS for high-speed spectral imaging in the context of solid-state materials, such as ferroelectrics and their domain walls.

KFM 6.36 Tue 17:00 P3

**Low Temperature combined Confocal/AFM microscope for photo-luminescence and magnetic resonance experiments** — •Elizaveta Starykh, Michael Dotan, and Boris Naydenov — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Measuring small magnetic fields emanating from spins or magnetic nanoparticles, both with high spectral resolution and under diverse conditions has always been an ambitious task. Nanoscale magnetic imaging using nitrogen-vacancy (NV) colour centres in diamond has been proven to be a reliable method due to their unique properties and ability to be effectively manipulated by external magnetic fields. With laser light, it is possible to both initialize and read out the NV spin state, thereby non-destructively determining the magnetic profile of the sample.

With recent developments in technology, it is now possible to fabricate single NVs on the tip of an AFM cantilever and measure a magnetic field map from a sample. Due to the NVs' high sensitivity and susceptibility to the external environment, precise control of many parameters must be observed.

To combine different techniques to perform such complex experiments, we built a confocal setup on top of a attoCUBE closed-cycle cryogenic system. With optical access at the top, microwave and radio frequency control, AFM cantilever and separate temperature control for magnets and sample volume, we can now access a wide range of physical properties of solid-state materials.

KFM 6.37 Tue 17:00 P3

**Interatomic Potential for Laser-Excited NV-Centers in Diamond** — •Malwin Xibraku, Bernd Bauerhenne, and Martin E. Garcia — Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Nitrogen-vacancy-centers (NV-centers) are of interest for quantum computing, sensing and encryption. However, the fabrication of NV-centers is quite challenging. Recently, we have proposed a new fabrication method in which N atoms and vacancies far from each other find each other after femtosecond laser excitation. We simulated this method in a diamond bulk cell, consisting of 288 atoms, using density-functional-theory (DFT) and observed, that it works at very high laser excitations. To include surface effects and consider the electron-phonon coupling it is necessary to perform large-scale moleculardynamics-simulations, with millions of atoms. This is only possible using an interatomic potential, which respects the excitation of the electrons by considering the electronic temperature Te. Here, we present a Te-dependent interatomic potential for laser-excited NV-centers in diamond, which was developed from a large DFT-data set, widely covering the phase space of the system.

KFM 6.38 Tue 17:00 P3

**Combined Confocal-AFM setup** — •Sergei Trofimov, Klaus Lips, and Boris Naydenov — BerlinJoint EPR Laboratory and Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Single nitrogen-vacancy (NV) centers in diamond can be utilized for magnetic field sensing with high spatial resolution and high sensitivity. It is even possible to detect spin ensembles or magnetic nanoparticles if they are placed in the vicinity of an NV center. However, precise positioning of such structures is challenging. To tackle this problem AFM cantilevers can be utilized. One can move nanoparticles with a cantilever or attach them to it in order to bring them close to an NV center.

To conduct these experiments a Confocal-AFM setup based on a Park Systems NX12 AFM was built. This setup allows to place a cantilever in the vicinity of an NV center in a diamond sample using a moving sample stage and obtain luminescence maps with laser scanning technique using a set of galvo-mirrors.

To test the setup a diamond plate with NV centers was used to visualize magnetic field lines of a ferromagnetic cantilever. It was shown that the technique can be also applied to image and separately address NV centers that are as close as 10 nm apart. The maximum measured magnetic field strength was 146 ± 2 G when an NV center was 180 ± 10 nm away from the cantilever. A magnetic field gradient at this distance was estimated to be 0.3 G/nm.

KFM 6.39 Tue 17:00 P3

**Investigation of ferroelectricity in $BaTiO_3$-relaxors by PFM** — •Philipp Münzer[1], Markus Kratzer[1], Christian Maier[3], Klaus Reichmann[3], Marco Deluca[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria — [2]Materials Center Leoben, Leoben, Austria — [3]Institute for Chemistry and Technology of Materials, Graz, Austria

$BaTiO_3$ relaxor systems are promising materials for energy storage applications in microelectronic devices. These lead-free dielectrics are thermally stable and suitable for high-temperature operation due to their broad and high permittivity response and low electric coercivity. The relaxor behaviour can be achieved by homo- or heterovalent substitution of $Ti^{4+}$ ions in the perovskite cell, which disrupts the long-range ferroelectric order. We investigated the presence of ferroelectricity in homovalent ($Zr^{4+}$) and heterovalent ($Nb^{5+}$) substituted polycrystalline $BaTiO_3$ systems utilizing Piezoresponse Force Microscopy (PFM). We used Single-Frequency-PFM to image the domain structure of the relaxors and conducted polarization switching with a biased tip. Furthermore, local hysteresis loops were recorded utilizing Switching-Spectroscopy-PFM. The results indicate that the grade of ferroelectric disruption is strongly dependent on the amount and type of substitutes.

KFM 6.40 Tue 17:00 P3

**Synthesis of depth confined nitrogen vacancy centers in diamond** — •Karolina Schüle[1], Christoph Findler[1,2], Johannes Lang[1,2], and Fedor Jelezko[1,3] — [1]Institute for Quantum Optics, Ulm University, Ulm, Germany — [2]Diatope GmbH, Ummendorf, Germany — [3]Center for Integrated Quantum Science and Technology (IQST), Ulm

The negatively charged nitrogen-vacancy center (NV) is a paramagnetic defect (S=1) in diamond which shows coherence times T2 up to milliseconds even at room temperature. The NV is a promising candidate for quantum applications as its spin state can be initialized, read out optically, and manipulated by a microwave field. One way to fabricate NV centers is ion implantation where nitrogen is added into a single crystal diamond layer followed by an annealing process. The depth of the implanted nitrogen can be adjusted by the implantation energy. Larger kinetic energies are leading to deeper NV centers. At the same time, however, the depth distribution gets also broader limiting the degree of depth confinement. This contradicts the goal of homogeneous properties of the NVs beneficial for e.g. NMR applications. Using the method of indirect overgrowth, where implanted nitrogen is buried below a nanometer-thin capping layer of diamond. The resulting depth of the NV centers is decoupled from the implantation ion energy. Here, we show outstanding depth confinement resulting in single NVs which are located at a depth of around 20 nm confined in a range of approx. 1.4 nm. These NV centers are exhibiting a T2 up to ~100 $\mu$s.

KFM 6.41 Tue 17:00 P3

**Multiphoton imaging of ferroelectric domain structures by means of tunable, high energy fs-pulses** — •Fiete Breer[1], Felix Kodde[1], Laura Vittadello[1], Jan Klenen[1], Michael Ruesing[2], and Mirco Imlau[1] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ. — [2]Inst. Applied Physics, Nöthnitzer Str. 61, Techn. Univ. Dresden

Multiphoton imaging is a powerful tool for the analysis of polar oxide crystals and has been recently used to reveal previously not expected topologies present in ferroelectric domain walls [https://arxiv.org/abs/2207.01307]. In addition to non-linear optical effects, the system-specific parameters of the optical measuring arrangement in the microscope also determines the detected measurement signals. This includes, for example, the collimation of the infrared excitation light, the direction between excitation and detection, but also the apertures in the beam path of the confocal beam geometry and, therefore, require careful consideration when interpreting experimental results. In this work a Tunable hIGh EneRgy (TIGER) multiphoton microscope [Vittadello et al., Nanomaterials 11, 3193 (2021)] pumped by high energy fs-laser pulses from an optical parametric amplifier allowing for widefield SHG is used to study ferroelectric domain structures. The results are comparatively evaluated for different measurement setups, discussed and possible consequences for the interpretation of the origin of the SHG signal from widefield and scanning modes are presented. Funded by the DFG (project IM 37/12-1, FOR 5044 and RU 2474/1-1).

KFM 6.42 Tue 17:00 P3

**Small-polaron dynamics in lithium niobate tantalate solid solutions studied by means of fs-pump, cw-probe spectroscopy** — •Niklas Dömer[1], Anton Pfannstiel[1], Mirco Imlau[1], and Steffen Ganschow[2] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ. — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin

The inspection of transport and recombination dynamics of optically generated small polarons with strong coupling enables far-reaching insight into the electronic and microscopic (defect) structure of polar oxide crystals using macroscopic measures. Here, we use the absorption cross-section of small polarons to relate fs-pulse induced transient absorption with the temporal evolution of small polaron number densities, i.e. with the 3D hopping transport of small polarons within a lattice with intrinsic defect structure. For the first time, fs-pump continuous-wave probe spectroscopy is applied to lithium niobate tantalate (LNT, $LiNb_xTa_{1-x}O_3$ with $0 \leq x \leq 1$) solid solutions. Remarkably, a two-step decay with lifetimes in the order of microseconds and minutes is uncovered, which has not been observed in the widely studied edge compositions lithium niobate (LN, x=1) and lithium tantalate (LT, x=0). This finding is studied over the entire composition range ($0 \leq x \leq 1$) at distinct wavelengths according to the maxima of small polaron absorption features. A microscopic model based on the simultaneous presence of two types of intrinsic antisite defect centers, $Nb_{Li}$ and $Ta_{Li}$, is deduced to explain two different polaron decay channels. Financial support by the DFG (project IM 37/12-1 and GA 2403/7-1, FOR 5044).

KFM 6.43 Tue 17:00 P3

**UV-triggered polymerisation of photosensitive resins via harmonic emission of Bariumtitanate nanocrystals** — •Eugen

Wolf and Mirco Imlau — Institute of Physics, Barbarastr. 7, Osnabrueck University

Ultraviolet-photosensitive resins are important in various industrial applications like laser-based 3D printing or fibre-reinforced polymers. Spatially localized polymerization becomes possible using laser light at photon energies that are adjusted to the absorption features of the corresponding photoinitiator. A drawback of this approach, however, is the transmission loss of the incident UV light, so that it can be applied only for polymerization of surfaces or thin volumes. To overcome this limitation, the use of infrared light in combination with nanoscaled photocatalytic containers in the resin has been proposed. In this contribution, we present an alternative approach based on the use of harmonic nanocrystals, i.e. to convert the incident infrared to the UV region deep inside the resin. For this purpose, commercially available Bariumtitanate nanocrystals and a regneratively amplified fs-laser system are used. Remarkably, a high reproducibility of the polymerization process as a function of the light propagation coordinate is uncovered. Furthermore, our setup allows for the inspection of the dynamics and shape of the liquid-solid phase front for different laser parameters. We discuss our results taking a simplified model for nonlinear optical emission of nanoparticles stochastically distributed in the resin into account.

KFM 6.44 Tue 17:00 P3

**Optical damage and hologram recording in as-grown Lithium-Niobate-Tantalate solid solutions** — •Sören Domke[1], Bjoern Bourdon[1], Steffen Ganschow[2], and Mirco Imlau[1] — [1]Institute of Physics, Barbarastr. 7, Osnabrück Univ. — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin

Lithium niobate tantalate (LNT, $LiNb_xTa_{1-x}O_3$ with $0 \leq x \leq 1$) solid solutions provide a promising material platform for nonlinear-photonics due to the ability for tuning the optical and electrical properties via composition. However, so far, very little is known about the (nonlinear) optical characteristics and intrinsic defect structure of LNT compared to its edge compositions lithium niobate (LN, x=1) and lithium tantalate (LT, x=0). In this respect, the presence of optical damage, i.e. the transient change of the index of refraction by the action of an incident light beam, is of particular importance as it drastically degrades the components' usability, but can also be used for wave-mixing applications. Originally discovered in LN, we report of our observations of a comparable nonlinear optical phenomenon in nominally undoped LNT samples and present the results of our systematic studies using the recording and reconstruction of elementary holographic gratings. As a particular feature of our finding, the phenomenon shows a transient behavior with a lifetime in the order of tens of hours that can only be erased using white light illumination and/or thermal treatment. The results are discussed in the framework of the photorefractive effect and an intrinsic defect model. Financial support by the DFG (projects IM37/12-1, GA 2403/7-1, FOR 5044).

KFM 6.45 Tue 17:00 P3

**Laser induced damage threshold (LIDT) of additively manufactured components in photonics** — •Moritz Huesmann, Yannic Toschke, and Mirco Imlau — Institute of Physics, Osnabrück University, Germany

Nowadays, desktop additive manufacturing technologies, e.g., 3D-printing based on thermoplastics (filaments), are widely available. They are increasingly finding their way into research laboratories in photonics due to the possibility to manufacture optomechanical components, such as versitale optical adapters, optomechanical mounts and sample holders. While the mechanical properties of the thermoplastics have been studied intensively in literature, nearly nothing is known about the laser damage threshold (LIDT) of these materials. Without this knowledge, the use in optical setups is limited to laser beams with moderate to low average power for safety reasons. In the second step, the damage threshold for PLA and PETG of different color was systematically determined under the exposure with intense femtosecond and nanosecond laser pulses. We discuss the determined LIDT values in the framework of applications in photonics, but also analyze the photophysical processes of the laser-induced damages based on a detailed topographic inspection. Financial support by the BMBF within Open Photonik Pro (project 13N15230, optocubes).

KFM 6.46 Tue 17:00 P3

**Temperature dependence of the optical band gap of LNT solid solutions (20–330 K)** — •T. Hehemann[1], A. Pfannstiel[1], S. Sanna[2], N. Syvorotka[3], K.-D. Becker[4], S. Ganschow[5], and M. Imlau[1] — [1]Inst. Phys., Osnabrück Univ. — [2]Inst. Phys., Univ. Giessen — [3]Inst. Energy Res., TU Clausthal — [4]Inst. Phys. Theo. Chem., TU Braunschweig — [5]Leibniz-Inst. f. Kristallzüchtung, Berlin

Lithium niobate tantalate solid solutions (LNT, $LiNb_xTa_{1-x}O_3$ with $0 \leq x \leq 1$) represent a promising class of polar oxide materials for photonics due to their favourable linear & nonlinear optical, but also photoelectrical properties. A mandatory basic requirement for customised optical applications is the (precise) knowledge of the optical band edge energy $E_{\mathrm{gap}}^{\mathrm{opt}}$. While $E_{\mathrm{gap}}^{\mathrm{opt}}$ and its relation to the intrinsic defect structure has been well investigated for the edge compositions $LiNbO_3$ (LN, x=1) and $LiTaO_3$ (LT, x=0), nearly nothing is reported for LNT in literature, so far. In particular, there are no data available for the important low temperature region 20–330 K. We here present temperature dependent absorption spectra of LNT in the vicinity of the optical band edge covering the entire composition range ($0 \leq x \leq 1$). The analysis of the data set follows the established fitting routines and reveals, both the composition and temperature dependent shifts of $E_{\mathrm{gap}}^{\mathrm{opt}}(x, T)$. The former is discussed in the framework of the intrinsic defect structure, while the latter is related with the properties of the electronic structure. All findings are compared with respective shifts widely reported for LN and LT. Financial support by the DFG (projects IM 37/12-1, SA 1948/3-1, FR 1301/40-1, GA 2403/7-1 of the FOR 5044)

## KFM 7: Focus: High-resolution Lithography and 3D Patterning

While high-resolution 2D lithography and structuring is relatively matured and also widely applied in industrial processes, work on its 3D variant is mostly focusing on fundamental aspects and process development. At the lower edge of possible 3D feature dimensions, certainly methods such as focused electron beam induced deposition (FEBID), non-linear multi-photon-laser lithography and thermal scanning probe lithography techniques are required. This session will discuss most of these dedicated 3D methods in detail. For the fabrication of complex 2D and 2.5D patterns, advanced electron beam and X-ray methods are continuously developed further. In addition, new methods such as high resolution Talbot lithography for relatively large areas are already entering industrial maturity. This session will also discuss some of the latest developments in this field of binary lithography.

Chair: Dr. Frank Heyroth (Martin-Luther-Universität Halle)

Time: Wednesday 9:00–12:35 Location: POT 51

**Invited Talk** KFM 7.1 Wed 9:00 POT 51

**Novel device integration – combining bottom-up and top-down approaches** — •Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — TU 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 that has not been solved so far. We have therefore developed techniques that use self-assembly to create conducting nanostructures to create small, self-assembled circuits that can then be contacted reliably using standard lithographic methods. In this talk, we will show how DNA Origamis can be used

for the self-assembly of metallic nanowires, which are contacted using electron beam lithography and electrically characterized. Self-assembly can be used to integrate semiconducting nanoparticles or single molecules for building nanodevices. Further integration of such nanostructures into standard silicon electronics may for example be achieved by connecting these nanodevices to silicon nanowires or transistors based on 2-dimensional materials. We have therefore developed reconfigurable transistors based on these materials using electron beam lithography and further processing (i.e. using a classical top-down approach), which are reconfigurable. With the combination of these transistors with self-assembled nanostructures, a large variety of electronic nanocircuits can be constructed in future applications.

KFM 7.2 Wed 9:30 POT 51

**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 IP-n162. We use a modified and automized Pulfrich refractometer setup, utilizing critical angles of total internal reflection with an accuracy of 5*10^-4 in the visible and near-infrared spectral range. We compare Cauchy and Sellmeier fits to the dispersion curves and 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 7.3 Wed 9:50 POT 51

**3D direct laser writing of miniature optical apertures with highly absorptive photoresist** — •Michael Schmid[1,2], Andrea Toulouse[2,3], Simon Thiele[2,3,4], Simon Mangold[1,2], Alois Herkommer[2,3], and Harald Giessen[1,2] — [1]4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [3]Institute of Applied Optics (ITO), University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany — [4]Printoptix GmbH, Johannesstraße 11, 70176 Stuttgart

In recent years, 3D direct laser writing and its possible application developed rapidly. Different complex micro-optical systems have been demonstrated, such as multi-lens objectives. However, it is still challenging to integrate microscopic apertures to these systems. We present a novel approach to create 3D direct laser written apertures using an opaque material suitable for 2-photon lithography. This way, it is possible to integrate microscopic apertures into 3D printed micro-optical systems improving the imaging quality. We demonstrate this potential by combining 3D printed black apertures with singlet lenses made of the commonly used photoresist IP-S. A significant contrast improvement of the imaging is achieved. Furthermore, due to the absorption coefficient, it is possible to create thin lenses with the black material enabling the fabrication of optical lens and aperture in one step.

KFM 7.4 Wed 10:10 POT 51

**Self-Folding micro cubes of laser-cut templates** — •Pierre Lorenz[1], Ye Yu[2], Ronald Franz[3], Joachim Zajadacz[1], Martin Ehrhardt[1], Robert Kirchner[2], Gregory Lecrivain[3], and Klaus Zimmer[1] — [1]Leibniz Institute of Surface Engineering, Permoserstr. 15, Leipzig, 04318, Germany — [2]Institute of Semiconductor and Microsystems, TU Dresden, Nöthnitzer Straße 64, Dresden, 01187, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Fluiddynamik, Bautzner Landstraße 400, Dresden, 01328, Germany

3D microstructures exhibit manifold applications with compact system integration in mind. Especially self-folding processes of laser-cut 2D templates allow for fast, flexible, and cost-effective fabrication of 3D structures. A UV ps laser was used for the laser cut of polyimide foil-based 2D templates. Two different folding concepts were tested: water-droplet self-folding and vacuum micro forming (VMF). The VMF concept is based on an array of cavities in a Teflon plate, which work similarly to deep drawing as a guide for the VMF of the 2D templates. In the water-droplet concept, a water droplet was added by a tweezer with a defined volume resulting in self-folding due to the surface tension. Both concepts allow the well-defined folding of sub-mm cubes after optimization of the 2D template geometry. Especially the VMF allows a parallelization and miniaturization of the folding process, which was monitored and analyzed by high-speed imaging.

KFM 7.5 Wed 10:30 POT 51

**High resolution and process stability tests on new HSQ based resists** — •Nicolas Kunzfeld and Axel Rudzinski — Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany

Many new resist providers for hydrogen silsesquioxane (HSQ) based high resolution e-Beam-resist emerged on the market in the last few years.

Until now, the experience with these new resists regarding resolution capabilities, process stability and long term behaviour is very limited.

To expand the experience with these resist, further testing based on statistical methods like a process capability evaluation based on the CpK-Value is required.

This work presents the latest high resolution, process capability and long term stability tests of these HSQ-based resists provided by different resist suppliers.

We achieved isolated single pixel lines with sub 6 nm line width with a CpK-Value of 1 and were also able to get a first impression about the resist behaviour over a time frame of almost 30 days.

**15 min. break**

**Invited Talk** KFM 7.6 Wed 11:05 POT 51

**4D meso-scale electronics for next generation medical tools and electronic skins** — •Daniil Karnauschenko — Research Center MAIN, Technical University Chemnitz, Rosenbergstr. 6, 09126 Chemnitz, Germany

State-of-art mesoscale systems for IoT, e-skins or smart-dust applications, medical or commercial products are essentially 3D architectures, whose geometry plays vital role when providing communication, sensing, actuation and power management functions. Conventional components carrying electronic functions are static, functionally heterogeneous and spatially separated requiring nontrivial sequential assembly and packaging procedures, which hinder further miniaturization and development of next generation mesoscale systems. 3D self-assembled architectures are envisioned to become a driving force for 3D electronic devices designed, microfabricated and self-assembled from planar thin-film structures and self-organized electronic components. Dynamic (4D) parallel assembly operating at mesoscale (1 um - 1 mm) allows offers improved performance while reducing overall manufacturing complexity of devices and components by harnessing the relative ease in which it can produce mesoscopic 3D geometries i.e. origami folded structures and "Swiss-roll" architectures. These architectures and benefits will lead to tighter a system integration e.g. electronic skins and medical tools made out of electronic components including active matrix, capacitors, power sources, coils, sensors, actuators and antennas with reduced costs fabricated from a single wafer.

KFM 7.7 Wed 11:35 POT 51

**Two-Photon Polymerization Lithography Structures Characterized via Raman Spectroscopy and Nanoindentation** — •Severin Schweiger[1,2], Tim Schulze[1,2], Peter Reinig[1], Simon Schlipf[3], and Harald Schenk[1,2] — [1]Fraunhofer Institute for Photonic Microsystems, Maria-Reiche-Str. 2, Dresden, Germany, 01109 — [2]Brandenburg University of Technology, Platz der Deutschen Einheit 1, Cottbus, Germany, 03046 — [3]Fraunhofer Institute for Ceramic Technologies and Systems, Maria-Reiche-Str. 2, Dresden, Germany, 01109

Additive manufacturing using two-photon polymerization (TPP) lithography has gathered interest in industry and research. Parameter sweeps of cuboid structures fabricated using TPP lithography were investigated to find dependent mechanical material properties across the parameters of the laser power and scan speed. Raman spectroscopy and micro- or nanoindentation were used on the cuboids to find the degree of conversion (DC) of monomer to polymer and the Youngs modulus (E), respectively. The DC and E found for the photoresist IP-Dip was 20 % to 45 % and 1 to 2.1 GPa, respectively. These results were compared to reports found in the literature. The DC and E found for the photoresist IP-Q, was 53 % to 80 % and 0.5 to 1.3 GPa,

respectively. The properties found for IP-Q are the current state of knowledge for this photoresist. Many structures fabricated via TPP and based on IP-Q can benefit from this knowledge and the customizability of the material. Examples are evaluated and discussed in the presentation.

KFM 7.8 Wed 11:55 POT 51

**Dry film resists: A promising material class for micro-/acoustofluidic chip fabrication** — •Andreas Winkler — Group "Acoustic Microsystems", IFW Dresden, Helmholtz str. 20, 01069 Dresden, Germany

Dry film resists (DFRs) promise low-cost and greener microfabrication, and can partly replace conventional technologies for microstructure fabrication being associated with high-energy demands and intense use of toxic and climate-active chemicals. Due to their mechanical stability and superior film thickness homogeneity, DFRs also outperform spin-on resists, such as SU-8, as structural materials, especially when high-resoluted two- and three-dimensional architectures are required such as the case in acoustofluidic chip devices. We investigated various dry film resists in the recent years for their suitability in micro-/acoustofluidic applications. While in general their performance was found to be highly promising and also allowed completely new solutions, properties of commercially available DFRs can vary strongly between individual products and even product charges, and literature on - as well as description of - these materials is still scarce. Here, we introduce this relatively young material class and present selected results regarding technically important effects and limitations, optical properties and performance in acoustofluidic cell separation and aerosol generation.

KFM 7.9 Wed 12:15 POT 51

**Artificial Intelligence for high resolution multi-photon lithography** — •Julian Hering-Stratemeier[1], Sven Enns[1,2], Nicolas Lang[1], and Georg von Freymann[1,2,3] — [1]Physics Department and State Research Centre OPTIMAS, TUK, 67663 Kaiserslautern, Germany — [2]Opti-Cal GmbH, 67663 Kaiserslautern, Germany — [3]Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany

Multi-photon lithography, a.k.a. direct laser writing (DLW), is one of today's most flexible high resolution 3D additive manufacturing technologies. Nevertheless, there are fundamental restrictions, limiting its resolution and structure-conformity: First, the shape of the polymerization-triggering laser focus limits the minimal volume that gets solidified (voxel). Hence, laser focus shape distorting optical aberrations within the beam path worsen the quality of the 3D printed outcome. Second, the physico-chemical properties of the photo resins influence the sharpness and extensions of single voxels, and, therefore, the 3D printed structure quality and resolution as well. Here, we show very first steps (i) towards a fast algorithm for predicting those error-loaded structures. Moreover, we use artificial intelligence (ii) to correct for optical aberrations within the beam path and (iii) to pre-compensate for the photo resin's outcome-worsening properties. Especially correcting aberrations is crucial for, e.g., extending DLW to high resolution STED-inspired DLW which is analogue to the well-known and Nobel price warded STED-microscopy.

## KFM 8: Diamond and related dielectric materials

In this session the basics of NV-centers and other defects in diamond were presented. The influence to applications in different fields are obvious. So, there is an influence on dielectric properties of diamond, used e.g. in high power microwave components for fusion applications in the GHz to THz frequency range. Biological diamond applications and applications in quantum photonics are also considered in this field of diamond and related materials.

Chair: Prof. Dr. Theo A. Scherer (KIT Karlsruhe)

Time: Wednesday 14:00–17:15 Location: POT 51

KFM 8.1 Wed 14:00 POT 51

**Optimal Control for Quantum Sensing with NV Centers in Diamond** — •Matthias Müller — Forschungszentrum Jülich GmbH

Diamond based quantum technology is a fast emerging field with both scientific and technological importance. The performance relies on unique features like superposition and entanglement and depends on sophisticated mechanisms of control to perform the desired tasks. Quantum Optimal Control (QOC) has proven to be a powerful tool to accomplish this task. I will give a brief overview on the use of QOC for quantum sensing with NV centers in diamond and report on recent applications.

[1] P. Rembold et al., AVS Quantum Sci. 2, 024701 (2020) [2] M.M. Müller et al., Sci. Rep. 8, 14278 (2018) [3] N. Oshnik et al., Phys. Rev. A 106, 013107 (2022) [4] A. Marshall et al., arXiv:2112.15021 (2022)

KFM 8.2 Wed 14:20 POT 51

**Influence of N defects on dielectric properties of diamond** — •Theo Scherer — KIT Karlsruhe

Atomistic structures and elastic and dielectric properties including first simulations of loss tangent, tan $\delta$ of diamond with small nitrogen impurities can be calculated using the first principles methods. The effect of a single nitrogen substitutional atom on the Raman and IR absorbance spectra is analyzed and compared with other calculations. It is shown that nitrogen defects do not affect tan $\delta$ at far IR region used in diamond windows in fusion reactors for plasma heating and stabilization.

KFM 8.3 Wed 14:40 POT 51

**Technical application of CVD Diamond windows in fusion reactor heating systems.** — •Peter Späh — KIT, Institute for applied materials, Karlsruhe

The application of CVD diamond windows in fusion experiments often comes along with challenging design requirements. Diamond windows and associated components must be protected properly from harsh environmental conditions. This is particularly the case for the future demonstration power plant reactor (EU DEMO), where sensitive applications shall operate under severe conditions in terms of heat, mechanical loads and radiation.

For the EU DEMO, an EC Heating and Current Drive System (ECH&CD) is under development, where CVD diamond windows together with microwave reflectors (mitre-bends and mirrors), corrugated waveguides, waveguide switches, shutter valves and confinement barrier feed-throughs, will be precisely integrated into a millimetre wave power transmission system. The entire system is installed into massive launching components and reactor building structures. The design takes into account mechanical integrity, dissipation of heat by powerful cooling systems, radiation shielding and the capability to be serviced and maintained by remote handling procedures.

This talk presents the conceptual design and integration of the ECH&CD launching system into the EU DEMO fusion power plant.

KFM 8.4 Wed 15:00 POT 51

**Fabrication and Characterization of Thin Single-Crystal Diamond Membranes for Quantum Photonics** — •Julia Heupel[1], Maximillian Pallmann[2], Johann P. Reithmaier[1], David Hunger[2], and Cyril Popov[1] — [1]Institute of Nanostructure Technologies and Analytics (INA), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Physikalisches Institut, Karlsruher Institute für Technologie (KIT), Wolfgang-Gaede-Str.1, 76131 Karlsruhe, Germany

Due to its exceptional physical and chemical characteristics, single-crystal diamond (SCD) in a form of thin membranes is a promising material for the fabrication of high-quality photonic devices and for envisioned applications in quantum information technologies (QIT). In

order to structure SCD membranes with a good quality and thickness of few micrometer or below, it is important to minimize defects originating from polishing (e.g., grooves and pits) or etching procedures (e.g., micro-masking effect). Here we report on the fabrication of thin SCD membranes, exhibiting a low surface roughness down to 0.2 nm by means of inductively coupled plasma reactive ion etching (ICP-RIE). A significant roughness reduction was achieved by using distinct Ar/Cl2 etching recipes as a planarization step before the actual structuring process. These planarized SCD membranes are successfully bonded via van der Waals forces on plane cavity mirrors and optically characterized in a fiber-based Fabry*Pérot microcavity regarding their mode structure and finesse.

KFM 8.5 Wed 15:20 POT 51

**Enhanced protein immobilization by nanostructuring of UNCD surface** — •Daniel Merker[1], Daniela Bertinetti[2], Rolf Merz[3], Michael Kopnarski[3], Friedrich W. Herberg[2], Johann P. Reithmaier[1], and Cyril Popov[1] — [1]Institute of Nanostructure Technologies and Analytics (INA), Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany — [2]Department of Biochemistry, CINSaT, University of Kassel, Germany — [3]Institut für Oberflächen- und Schichtanalytik GmbH, Kaiserslautern, Germany

Investigations of molecular mechanisms related to the formation of the inner clock require detection of coupling factors, e.g. secreted neuropeptides, that mediate synchronization. In this work we study the application of ultrananocrystalline diamond (UNCD) as biosensor for detection of such coupling factors. The crucial part is the feasibility of protein immobilization on UNCD surfaces. From all investigated coupling routs only photochemical attachment of alkenes gave acceptable results when the green fluorescent protein (GFP) was immobilized. A process to create nanostructures was developed to increase the effective surface for protein immobilization. Both functionalization and structuring have beneficial effects on immobilization performance, but especially in combination the immobilization efficacy increases significantly. Lastly, the immobilization of different binding proteins against GFP - antibodies, nanobodies, DARPins - was investigated, with the last two showing promising results for high specificity and affinity capture of target molecules in a future UNCD biosensor.

**15 min. break**

KFM 8.6 Wed 15:55 POT 51

**Numerical analyses of CVD diamond windows in high power microwave applications** — •Gaetano Aiello[1], Andreas Meier[1], Heinrich Peter Laqua[2], Theo Scherer[1], Sabine Schreck[1], and Dirk Strauss[1] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany — [2]Max Planck Institute for Plasma Physics (IPP), 17491 Greifswald, Germany

Nuclear fusion reactors require electron cyclotron heating and current drive (EC H&CD) systems for plasma heating and stabilization. Chemical vapor deposition (CVD) polycrystalline diamond windows on both the torus and gyrotron sides of the reactors act as confinement and/or vacuum boundaries allowing the transmission of high-power microwave beams. For example, the beam power scenarios of 1.5 MW and 2 MW are the current targets considered respectively in Wendelstein 7-X and European DEMO fusion machines. In this work, with reference to both reactors, the numerical analyses required to verify the thermal and structural performance of the windows are discussed. Experimental measurements of loss tangent in diamond provided inputs for the numerical analyses. Sensitivity studies of the windows with respect to loss tangent and other parameters were also carried out to check the temperature reserve margins of the design.

KFM 8.7 Wed 16:15 POT 51

**Simulation study of LC superconducting microresonators for diamond characterization** — •Francesco Mazzocchi, Dirk Strauss, and Theo Scherer — Karlsruhe Institute of Technology KIT IAM-AWP, Eggenstein-Leopoldshafen, Germany

The development of high optical quality, ultra-low losses single crystal diamond windows is paramount for the realization of future nuclear fusion facilities like DEMO, given the foresaw increase in power of microwave ECRH systems. Precise determination of the dielectric characteristics ($\epsilon r$ and $\tan\delta$) of these innovative materials have so far relied on techniques involving Fabry-Perot microwave open resonators in various configurations. High Q, superconducting thin film resonators can be effectively used to determine dielectric characteristics of extremely low losses materials like single- and poly-crystalline diamond. Their extremely high-quality factors allow for a substantial increase in resolution in the determination of these parameters when compared to state-of-the-art Fabry Perot open resonators. We hereby report a detailed simulation study of the chosen resonators configurations (Lumped Elements and Circular) that lead to the final design of the devices.

KFM 8.8 Wed 16:35 POT 51

**CVD Diamond Disks for ITER ECH windows - dielectric loss characterization and optical inspection** — •Sabine Schreck[1], Gaetano Aiello[1], Pablo Estebnez[2], Andreas Meier[1], Theo Scherer[1], Dirk Strauss[1], Christoph Wild[3], and Eckhard Woerner[3] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany — [2]Fusion for Energy, 08019 Barcelona, Spain — [3]Diamond Materials, 79108 Freiburg, Germany

Diamond disks with a diameter of 70 mm and a thickness of 1.11 mm will be installed into windows of the Electron Cyclotron Heating and Current Drive System (EC-HCD) of the fusion reactor ITER. The bare disks, manufactured by a microwave plasma assisted chemical vapor deposition process, need to ensure high mechanical stability, thermal conductivity and transmission of MW-class microwave beams. Factory acceptance tests of the disks produced by Diamond Materials include a check of dimensional properties and a determination of its dielectric loss. The loss characterization and the comparison with the respective specifications is performed at KIT using dedicated Fabry-Perot resonators, that allow the measurement of the loss tangent at the disk centre and a mapping of it over the disk area. An optical inspection with a digital microscope completes the examination. More than 60 diamond disks need to be qualified prior to their integration into the window assemblies and the application in the ITER EC-system. The disk qualification activities are performed within a contract between F4E and KIT and the talk will present the current status.

KFM 8.9 Wed 16:55 POT 51

**CVD Diamond Windows for Electron Cyclotron Resonant Heating in Fusion** — •Dirk Strauss, Gaetano Aiello, Andreas Meier, Theo Scherer, and Sabine Schreck — aKarlsruhe Institute of Technology, Institute for Applied Materials, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Electron cyclotron resonant heating (ECRH) in nuclear fusion combines the injection of multi megawatt power with the possibility to focus the millimeter wave beam to small spot sizes of few centimeters. The ECRH allows efficient plasma heating as well as localized current drive for magneto-hydrodynamic stabilization of e.g. neoclassical tearing modes that create local magnetic islands with a fast loss of plasma confinement. One of the key challenges for high power ECRH systems is the provision of suitable confinement windows.

The low loss tangent, high thermal conductivity and outstanding mechanical properties qualify diamond as the state of the art material for high power millimeter wave heating systems in nuclear fusion devices. Artificial diamond disks are grown by CVD in diameters up to 180mm, sufficient for the usual waveguide diameters.

The principles of ECRH systems will be presented with a focus on the permittivity of diamond, which determines the loss tangent and suitable disk thicknesses. Further concepts and status for small and broadband windows for frequencies of 100-240GHz and beam powers up to 2MW will be discussed.

# KFM 9: Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positron

Chair: Prof. Dr. Theo A. Scherer (KIT Karlsruhe)

Time: Wednesday 9:00–13:15 Location: POT 106

KFM 9.1 Wed 9:00 POT 106

**$FePX_3$ (X: S, Se): A stable new 2D material for water splitting** — •Hafiz Muhammad Zeeshan[1], Sandhya Sharma[1], Elena Voloshina[1,2], and Yuriy Dedkov[1,2] — [1]Centre of Excellence ENSEMBLE3 Sp. z o.o., Wolczynska Str. 133, 01-919 Warsaw, Poland. — [2]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, P. R. China.

The interaction of high-quality transition metal trichalcogenides (TMTs) single crystals $FePX_3$ (X: S, Se) with water molecules is studied using NEXAFS and XPS in a wide range of temperature and partial pressure of $H_2O$. The physisorption nature of interaction between $H_2O$ and $FePX_3$ is found at low temperatures and relatively small concentrations of water molecules, that is supported by the DFT results. When temperature of the $FePX_3$ samples and partial pressure of $H_2O$ are increased, the interaction at the interface is defined by two competing processes - adsorption of molecules at high partial pressure of $H_2O$ and desorption of molecules due to the increased surface mobility and physisorption nature of interaction. Our intensive XPS/NEXAFS experiments accompanied by DFT calculations bring new understanding on the interaction of $H_2O$ with surface of a new class of 2D materials, TMTs, pointing to their stability and reactivity, that is important for further applications in different areas, like sensing and catalysis.

KFM 9.2 Wed 9:20 POT 106

**Solving complex nanostructures with ptychographic atomic electron tomography** — •Philipp Pelz — Institute for Micro- and Nanostructure Research, Friedrich-Alexander Universitaet Erlangen, Cauerstr. 3, 91058 Erlangen

Knowledge of the three-dimensional atomic structure of natural and manufactured materials allows us to calculate their physical properties and deduce their function from first principles. Phase-contrast electron microscopy methods like ptychography are ideally suited to solve the 3D atomic structure of nanomaterials containing light and heavy elements. We perform mixed-state electron ptychography from 34.5 million diffraction patterns to reconstruct a high-resolution tilt series of a double wall-carbon nanotube (DW-CNT), encapsulating a complex ZrTe sandwich structure. Class averaging of the resulting reconstructions and subpixel localization of the atomic peaks in the reconstructed volume reveals the complex three-dimensional atomic structure of the core-shell heterostructure with 17 picometer precision.

KFM 9.3 Wed 9:40 POT 106

**Status and Upgrades of the Beam Facility at the High-Intensity Positron Source NEPOMUC** — •Christoph Hugenschmidt — Forschungs-Neutronenquelle Heinz Maier-Leibnitz (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The bright low-energy positron beam provided by the neutron induced positron source in Munich (NEPOMUC) at FRM II is used in a large variety of experiments in materials science, condensed matter and surface physics as well as in fundamental research, e.g., for the creation of a positron-electron pair plasma. Within this contribution, an overview of the current status and developments of the positron beam facility with its instrumentation is given. Plans for the installation of a buffer gas trap for the creation of high-density positron pulses as well as ideas for increasing the performance of the remoderated positron bam are elucidated. The upgrades of the positron beam instruments (i) Coincident Doppler-Broadening Spectrometer (CDBS) using a scanning positron micro beam, (ii) instrument for the 2D measurement of the Angular Correlation of Annihilation Radiation (2D-ACAR), and (iii) the surface spectrometer are highlighted. Finally, the planned extension of the positron beam facility and the future operation of positron beam experiments in the experimental hall East are presented.

KFM 9.4 Wed 10:00 POT 106

**Optimising the scintillator geometry for positron annihilation spectroscopy - A GEANT4 Simulation** — •Dominik Boras — Chair of chemical technology and material synthesis, Würzburg, Germany

To better understand the efficiency and the role of backscattering events of a Positron annihilation lifetime spectrometer, a GEANT4 simulation of the atomic processes is conducted. The gamma quanta from the radioactive decay of 22-Na and from the annihilation positron are detected by a scintillator-photomultiplier combination. In the basic setup of the simulation, as scintillation material plastic BC422Q-0.5wt.% was used due to its good energy resolution. Different geometries of the scintillator (box, cone, pyramid and tube) were simulated and their influence on the detection efficiency and the instrument resolution function was investigated. Furthermore, the influence of the measured sample material (density, atomic number) on the scattering of gamma quanta was considered.

KFM 9.5 Wed 10:20 POT 106

**Formation and time dynamics of hydrogen-induced vacancies in nickel** — •Maik Butterling[1], Luca Chiari[2], Masanori Fujinami[2], Maciej Oskar Liedke[1], Eric Hirschmann[1], Ahmed Gamal Attallah[1], and Andreas Wagner[1] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Chemistry and Biotechnology, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan

The formation of hydrogen-induced defects in nickel was investigated by positron annihilation lifetime spectroscopy and the time dynamics of those defects during room temperature aging was tracked with an unprecedented time resolution of the order of minutes using an ultrahigh-flux slow positron beam. Those measurements showed the formation of a large number of atomic vacancies simply by hydrogen addition at room temperature. It could be proved that they were monovacancy-level defects and that hydrogen was trapped and bound to those vacancies during the hydrogen charge. Room temperature aging, i.e. below the stage III temperature in Ni, and the concomitant hydrogen desorption induced the agglomeration of those monovacancies into large vacancy clusters which remained even after all the hydrogen had desorbed and hydrides had disappeared.

These results [1] constitute the first empirical evidence that vacancy-hydrogen complexes are induced in Ni only by hydrogen charging and demonstrate that hydrogen has a primary role in the formation and stabilization of vacancies even at room temperature.

[1] L. Chiari, et al., Acta Materialia 219(2021), 117264

KFM 9.6 Wed 10:40 POT 106

**Electron tomography analysis of Ge/SiGe asymmetrically coupled quantum wells** — •Ekaterina Paysen[1], Giovanni Capellini[2,3], and Achim Trampert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [3]Dipartimento di Scienze, Università degli Studi Roma Tre, Roma, Italy

We present a method for the three-dimensional (3D) characterisation of the morphology and chemical intermixing of buried interfaces in a Ge/SiGe asymmetrically coupled quantum well structure applying electron tomography method based on high-angle annular dark-field (HAADF) scanning transmission electron microscopy. For this purpose, a needle-shaped specimen with a diameter of a few 100 nanometres is prepared with a focused ion beam, from which a tilt series of HAADF projections is recorded. Subsequently, the series is used to calculate a complete 3D image or tomogram of the specimen with the simultaneous iterative reconstruction technique. The analysis of iso-concentration surfaces enables a quantitative determination of morphological quantities such as the root mean square roughness and lateral correlation length individually for each interface. Subnanometre-thin cross-sections from the tomogram are used to measure the chemical interface width with the highest spatial resolution. An advantage of this method is thus the investigation of the interfaces as 3D entities in their buried state on a length scale of a few 100 nanometres without the projection problem.

**15 min. break**

KFM 9.7 Wed 11:15 POT 106

**Weak-signal extraction enabled by deep-neural-network de-**

**noising of diffraction data** — •Jens Oppliger[1], Michael Marco Denner[1], Julia Küspert[1], Qisi Wang[1], Oleh Ivashko[2], Ann-Christin Dippel[2], Martin von Zimmermann[2], Fabian Donat Natterer[1], Mark Hannes Fischer[1], Titus Neupert[1], and Johan Chang[1] — [1]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Deutsches Elektronen-Synchrotron DESY, Notkerstrasse 85, 22607 Hamburg, Germany

Removal or cancellation of noise has wide-spread applications for imaging and acoustics. In every-day-life applications, denoising may even include generative aspects which are unfaithful to the ground truth. For scientific applications, however, denoising must reproduce the ground truth accurately. We show how data can be denoised via a deep convolutional neural network such that weak signals appear with quantitative accuracy. In particular, we study X-ray diffraction on crystalline materials. We demonstrate that weak signals stemming from charge ordering, insignificant in the noisy data, become visible and accurate in the denoised data. This success is enabled by supervised training of a deep neural network with pairs of measured low- and high-noise data. This way, the neural network learns about the statistical properties of the noise. We demonstrate that using artificial noise (such as Poisson and Gaussian) does not yield such quantitatively accurate results. Our approach thus illustrates a practical strategy for noise filtering that can be applied to challenging acquisition problems.

KFM 9.8 Wed 11:35 POT 106

**Positron beams for materials research** — •Andreas Wagner[1], Maik Butterling[1], Ahmed Gamal Elsherif[1], Eric Hirschmann[1], Maciej Oskar Liedke[1], and Reinhard Krause-Rehberg[2] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Dept.of Physics, 06099 Halle/Saale, Germany

The Helmholtz-Center Dresden - Rossendorf operates several user beamlines for materials research using positron-annihilation energy and lifetime spectroscopy. The superconducting electron linear accelerator ELBE drives several secondary beams including hard X-ray production from electron-bremsstrahlung, which serves as an intense source of positrons by means of pair production. The Mono-energetic Positron Source MePS [1] utilizes positrons with variable kinetic energies ranging from 0.5 to 18 keV for depth profiling of atomic defects and porosities on nm-scales in thin films. High timing resolutions ($\sigma$t *100 ps) at high average rates (105 s-1) and adjustable beam repetition rates allow performing high-throughput experiments. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). AIDA was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox) and by the Helmholtz Energy Materials Characterization Platform. [1] A. Wagner, et al., AIP Conference Proceedings, 1970, 040003 (2018).

KFM 9.9 Wed 11:55 POT 106

**Strain Distribution in Au/ZnO Microstructures for bio-magnetic sensing utilizing Scanning X-Ray Nano Diffraction and Coherent X-Ray Diffraction Imaging** — •Philipp Jordt[1], Niklas Wolff[1], Stjepan Hrkac[2], Jorit Gröttrup[1], Sindu Shree[1], Di Wang[3], Anton Davydok[4], Christina Krywka[4,1], Ross Harder[5], Christian Kübel[3], Oleg Shpyrko[2], Rainer Adelung[1], Olaf Magnussen[1], Lorenz Kienle[1], and Bridget Murphy[1] — [1]Kiel University, Germany — [2]UCSD, USA — [3]KNMF, KIT, Germany — [4]Hereon, Germany — [5]XSD, ANL, USA

Magnetic field sensors based on piezoelectric and magnetostrictive materials are a possible path to a new generation of sensors, capable of detecting bio-magnetic fields from human physiology at room temperature in an unshielded environment. A huge hurdle are the very low field strengths of these signals. One approach to further enhance the sensitivity is employing the piezotronic effect, which arises from the combination of a piezoelectric material and a Schottky contact. Here, a study on the strain distribution in ZnO nano and microrods coated with gold is presented. Scanning X-ray nano diffraction mapped the 2 dimensional strain distribution across 30-50 $\mu$m rods together with insitu current-voltage curves. It is demonstrated that the gold coating and the resulting Schottky contact has a direct impact on the lattice parameters in vicinity of the Au/ZnO interface and further, that the crystal quality of the ZnO is immensely influential on the properties of the Schottky contact. The full 3D strain distribution inside a 1 $\mu$m rod was characterized by coherent X-ray diffraction imaging.

KFM 9.10 Wed 12:15 POT 106

**Correlation of Mechanical Stress and the Positron Lifetime in Aluminum Alloys** — •Lucian Mathes[1], Vassily Vadimovitch Burwitz[1], Adrian Langrehr[1], Maik Butterling[2], Maciej Oskar Liedke[2], Eric Hirschmann[2], Andreas Wagner[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

Positron annihilation lifetime spectroscopy (PALS) is a sensitive technique to analyze the type and concentration of lattice defects on an atomic level. We applied ex-situ and in-situ PALS to plastically deformed technical Al and Al alloys. Thereby we are able to observe the creation and evolution of stress-induced defects in the region beyond the elastic Hook regime of the specimen. The in-situ bulk measurements were performed using a $\beta^+$ emitter in a new experimental setup combining tensile tests and PALS at TUM that also allows for investigation of the reversible elastic deformation of samples. The depth-dependent positron lifetime was measured ex-situ at the accelerator-based positron source MEPS at ELBE. For each sample we recorded the tensile stress, and the corresponding stress-strain curves. This allows us to determine the relation between applied stress, strain and mean positron lifetime. Within this contribution, we also discuss the evolution of the defect population with increasing deformation by examining the intensity change of the different positron lifetime components found in the PALS spectra.

KFM 9.11 Wed 12:35 POT 106

**Start-to-end simulations of partially coherent X-ray imaging experiments at synchrotron beamlines** — •Martin Seyrich — Deutsches Elektronen-Synchrotron DESY, Centre for X-ray and Nano Sciece CXNS, Hamburg, Germany

In the last decade, coherent X-ray imaging techniques, such as ptychography and holography, have grown a large user base at third and fourth generation X-ray light sources. In contrast to conventional microscopy techniques, coherent imaging techniques do not directly project an image on a detector. Instead, the image of the object is retrieved algorithmically from interference patterns, usually under the assumption of a fully coherent illumination.

Real X-ray sources are not perfectly coherent, they can be simulated as stochastic sources emitting an ensemble of waves. These waves can be propagated from the source through the entire beamline ending at the detector. The simulated interference patterns can then be treated with the same phase retrieval algorithms as experimental data.

Here, we present our extensions to existing established simulation software (OASYS / SRW) that permit the user to perform such start-to-end simulations with relative ease. We will present simulated data sets of ptychographic and holographic experiments, and discuss the computational demands of such simulations.

KFM 9.12 Wed 12:55 POT 106

**Illumination corrected X-ray near-field microscopy** — •Thea Engler[1,2], Johannes Hagemann[1], Christian G. Schroer[1,2], and Mathias Trabs[3] — [1]Deutsches Elektronen-Synchrotron, DESY, Germany — [2]Universität Hamburg, Germany — [3]Karlsruhe Institut of Technology, KIT, Germany

At synchrotron facilities, such as Petra III at DESY, small objects ($\mu$m) can be imaged with X-ray propagation-based phase-contrast imaging, i.e. near-field holography (NFH).

Reaching high resolution involves the use of nano-focusing optics. The imperfections of these optics cause aberrations in the illumination of the object and also upon further propagation in the measured hologram of the object. To correct the hologram for these artifacts, a flat-field correction must be applied. Considering a temporally stable beam, the hologram is divided by an empty-beam image, i.e. an image of the illumination without the object. With the common flat-field correction, the hologram is not fully corrected for the illumination function since the division is performed only in intensities in the detector plane.

Instead, the division of illumination and object should be performed in terms of complex wavefields in the sample plane, where the object transmission function physically interacts with the illumination function. Using a simulated dataset, we develop an algorithmic scheme using the recently proposed refractive formulation to take the illumination during the phase retrieval process properly into account.

# KFM 10: Battery Materials (joint session KFM/CPP)

Chair: Prof. Dr. Anna Grünebohm (Ruhr-University Bochum)

Time: Thursday 9:00–12:35 Location: POT 51

KFM 10.1 Thu 9:00 POT 51

**Materialanalyse von NMC111 Kathodenmaterial aus recycelten Lithium-Ionen-Batterien mittels XRD, AFM und EDX/REM** — •Claudia Schöberl, Hanno Käss und Stephan Appel — Hochschule Esslingen, Kanalstraße 33, 73728 Esslingen, Deutschland

In einem industriellen Recyclingverfahren für Lithium-Ionen-Batterien wird Kathodenmaterial von der Trägerfolie mit Wasser abgestrahlt und getrocknet. In einem an der Hochschule Esslingen laufenden Forschungsprojekt wird die so gewonnene Schwarzmasse, die hauptsächlich aus NMC111 besteht, mittels Röntgendiffraktometrie (XRD), Rasterelektronenmikroskopie (REM) und elementanalytischen Methoden untersucht, um Hinweise auf die chemische Zusammensetzung und auf strukturelle Veränderungen zu erhalten. Ziel ist es unter anderem, passende Auswahlkriterien für die Qualität des Recyclingmaterials zu definieren, das nach Verarbeitung erneut in Lithium-Ionen-Batterien eingesetzt werden soll. Dazu zählen, neben dem Rest-Bindemittelgehalt, der Kohlenstoffanteil sowie der Anteil an Fremdelementen wie Kupfer und Aluminium. Das wiedergewonnene, recycelte Aktivmaterial wird bei einem Projektpartner zur Herstellung neuer Kathodenfolien verwendet, die in einer Messzelle elektrisch charakterisiert werden. Mittels Rasterkraftmikroskopie (AFM) werden diese neu präparierten Kathodenfolien an der Hochschule Esslingen untersucht. Mit Hilfe eines speziellen Messmodus, der quantitativen nanoskaligen mechanischen Charakterisierung, wird insbesondere die Korrelation von Strukturmerkmalen und mechanischen Eigenschaften überprüft.

KFM 10.2 Thu 9:20 POT 51

**Structural response in NCA-type battery cathodes** — •Tobias Hölderle[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

Battery-powered electric drivetrains in electric vehicles (EVs) are heavily limited and constrained to the performance of the energy storage device, i.e. battery. Batteries with higher power/energy densities, capacities, and cycling life are needed to increase EVs' performance and reduce greenhouse gas emissions. Mixed high nickel content $Li_xNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) cathode material is one of a few today that simultaneously possess high energy and power densities at lower costs. However, NCA materials suffer from poor thermal stability and limited power density. They display capacity fading/efficiency loss due to antisite defects (cation mixing) in their structure, actively discussed in literature. In order to address the issue of cation mixing, a systematic ex-situ neutron powder diffraction study was done for a series of electrochemically delithiated NCA cathodes. The collected set of structural data was modeled using full-profile Rietveld method and results were discussed in line with observed electrochemical behavior. It is observed that lithium occupancies showed a decreasing character upon charging, independent from transition metal occupancies and indicating an absence of antisite defects (cation mixing) in the commercial NCA material during cell operation.

KFM 10.3 Thu 9:40 POT 51

**Dynamic structure evolution of extensively de-lithiated high voltage spinel LNMO** — Nicola Jobst[1], •Neelima Paul[2], Premysl Beran[3,4], Marilena Mancini[1], Ralph Gilles[2], Margret Wohlfahrt-Mehrens[1], and Peter Axmann[1] — [1]Accumulators Materials Research (ECM), ZSW Cen-tre for Solar Energy and Hydrogen Research Baden-Württemberg, DE-89081 Ulm, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, DE-85747 Garching, Germany — [3]Nuclear Physics Institute CAS, CZ-25068 Rez, Czech Republic — [4]European Spallation Source ERIC, Box 176, SE-221 00 Lund, Sweden

High voltage spinel is one of the most promising next-generation cobalt-free cathode materials for Li-ion batteries. Besides the typical compositional range of LixNi0.5Mn1.5O4 0<x<1 in the voltage window 4.90 to 3.00 V, additional 1.5 mol of Li per formula unit can be introduced into the structure, in an extended voltage range to 1.50 V. Theoretically, this leads to significant increase of the specific energy from 690 to 1190 Wh/kg. However, utilization of the extended potential window leads to rapid capacity fading, voltage polarization that lack a comprehensive explanation. In this work, we conducted potentiostatic entropymetry, operando XRD and neutron diffraction on the ordered stoichiometric spinel LixNi0.5Mn1.5O4 within 0 < x < 2.5 in order to understand the dynamic structure evolution and correlate it with the voltage profile. We were able to provide a conclusive explanation for the additional voltage step at 2.10 V, the sloping voltage profile below 1.80 V, and the additional voltage step at ~3.80 V.

KFM 10.4 Thu 10:00 POT 51

**Computational Screening of Oxide Perovskites as Insertion-Type Cathode Material** — •Johannes Döhn[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Helmholtz Institute Ulm, Germany

The intermittency of wind and solar power - the solely sustainable energy sources which are considered to be abundantly available - leaves only one consequence: For the transition towards renewable energy systems, efficient and reliable storage technologies are needed. Batteries are one of the most widely used storage devices but current technology based on the transfer of Li-ions faces several challenges including their dependence on critical materials with respect to both, scarcity and toxicity.

In our contribution we will discuss atomic-scale investigations of potential future battery materials carried out using density functional theory (DFT). We employed a high-throughput approach in order to screen the well known material class of oxide perovskites as insertion-type cathode materials and we derived several crucial battery properties including voltage and theoretical energy density for in total 280 compounds. For those candidate materials with promising properties, we evaluated additional features such as the voltage profile and diffusion barriers for ionic transport.

Such in silico investigations significantly narrow down the potential materials space for experimental coworkers and thereby contribute to finding green, cheap and reliable devices for energy storage.

KFM 10.5 Thu 10:20 POT 51

**Construction of cobalt oxyhydroxide nanosheets with rich oxygen vacancies as high-performance Lithium-ion Battery anodes** — •Yonghuan Fu[1,2], Huaping Zhao[1], Jianhong Liu[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Graphene Composite Research Center, College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, P. R. China

Cobalt oxyhydroxide (CoOOH) is a promising anode material for lithium-ion batteries (LIBs) due to its high electronic conductivity and theoretical specific capacity. Herein, CoOOH nanosheets are successfully obtained using a facile one-pot method, and a hierarchical nanoporous structure is formed by oxidizing cobalt hydroxide (Co(OH)2) in NaOH and (NH4)2S2O8 solution. The CoOOH anode shows better electrochemical performance compared to Co(OH)2 and Co3O4 electrodes when applied to LIBs. The hierarchical nanoporous structure and high electronic conductivity of the CoOOH anode contribute to its outstanding initial discharge capacity, high initial coulombic efficiency, and excellent cyclability. Experiments and density functional theory (DFT) calculations confirmed that the high ICE and prominent rate capability of the nanosheets could be ascribed to the rapid and complete conversion reaction of CoOOH upon lithiation/delithiation facilitated by hydroxyl groups and oxygen vacancies. This study provides new insights into the structure-property relationship of transition-metal oxyhydroxide anode materials for LIBs.

KFM 10.6 Thu 10:40 POT 51

**The dielectric behaviour of lithium intercalated graphite anodes - as a function of the state of charge** — •Simon Annies, Chiara Panosetti, and Christoph Scheurer — Fritz Haber Institut Berlin

The dielectric behaviour of battery materials is a crucial piece of information for understanding atomistic mechanics and modelling diffusion-

and charging processes. However, for the most common anode material in today's lithium ion batteries (lithium intercalated graphite), literature results regarding this property are sparse, conflicting and only available for graphite, i.e. the empty state of charge (SOC).

Utilizing our recently developed DFTB parametrization [1] which is based on a machine-learned repulsive potential, we are – for the first time – able to compute the dielectric behaviour of lithium intercalated graphite for the entire range of charge from 0% to 100% - finding a linear dependency from around $\epsilon_r$=7 at 0% SOC to around 25 at 100% SOC. We achieve this by sampling the Coulomb interactions between pairs of Li-ions and vacancies in large cells with varying intercalant concentrations in the adjacent layers.

Our results agree with experiments in the limit of "empty" graphite, as well as for (bilayer-) graphene, which we consider a validation of our approach. With this, we lay an important piece of foundation for the understanding and multi-scale modelling of entire charging and discharging cycles of graphite anodes in Li-ion batteries.

[1] Anniés, Simon, et al., Materials 14.21 (2021): 6633.

KFM 10.7 Thu 11:00 POT 51

**Hypothetical t-LGPO as a good ionic conductor, and the influence of Li core electrons on diffusion** — Giuliana Materzanini[1], •Nicola Marzari[2,3], and Gian-Marco Rignanese[1] — [1]Modelling Division, Universite catholique de Louvain, 1348 Louvain-la-Neuve, Belgium — [2]Theory and Simulations of Materials (THEOS), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [3]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Following the computationally found high Li-ion conductivity in tetragonal Li10GeP2O12 (t-LGPO), we study here the role of Li core electrons on Li diffusion in this hypothetical superionic material. We calculate Li diffusivity from two sets of Car-Parrinello canonical molecular dynamics simulations, one using Li pseudopotential with all electrons (1s22s1), and one with just one electron (2s1). The Arrhenius plots show a marked influence of the Li 1s electrons on the Li-ion diffusivity in t-LGPO, being the diffusion coefficient at 600 K one order of magnitude larger, and the activation barrier between 600 and 1200 K 1.5 times smaller, for the Li all-electrons with respect to the Li one-electron calculations. Similar sets of simulations performed for the analogue sulfide material, tetragonal Li10GeP2S12 (LGPS), show, oppositely, that for LGPS the influence of Li 1s electrons on Li diffusivity is minimal. The different response of Li mobility to the explicit treatment of 1s electrons reveals fundamental differences in the ionic conductivity mechanism in these two classes of materials.

**15 min. break**

KFM 10.8 Thu 11:35 POT 51

**Sodiation-induced reactivation of micro-nano flower for ultra-long cycling life sodium-ion batteries** — •Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

A rational micro-nano hierarchical structure is demonstrated to prolong the cycle life of sodium-ion batteries (SIBs) by relieving the volume expansion and preventing active material agglomeration. In this work, micro-nano flower 3D-VSx was fabricated as an anode electrode for SIBs. The advanced features of micro-nano flower and the unique crystal structures of NiAs-type vanadium sulfides synergistically contribute to enhancing the electrochemical kinetics of 3D-VSx, and finally achieved remarking electrochemical performances with an ultra-high capacity (961.4 mAh/g at 2 A/g) and an ultra-long cyclability (more than 1500 cycles). Furthermore, ex situ X-ray diffraction, Raman, and SEM bring to light a gradual reactivation process of 3D-VSx for sodium storage. Fortunately, upon reactivation, the electrochemical impedance of the 3D-VSx anode gradually weakens, and the diffusion-controlled charge storage mode further dominates compared to the capacitively-controlled mode, all of which facilitate the 3D-VSx to maintain a stable sodium storage capability. This work presents a general approach for preparing super-high specific capacity and rate capacity electrode materials for further improving the SIBs performance.

KFM 10.9 Thu 11:55 POT 51

**Sodium diffusion mechanism in NASICON solid electrolyte materials studied via quasi-elastic neutron scattering** — •Ivana Pivarníková[1,2], Stefan Seidlmayer[1], Martin Finsterbusch[3], Gerald Dück[3], Niina Jalarvo[4], Peter Müller-Buschbaum[1,2], and Ralph Gilles[1] — [1]TUM, MLZ, Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]FZJ, IEK-1, Jülich, Germany — [4]ORNL, Oak Ridge, TN, USA

The sodium superionic conductor materials, also known as NASICON, have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries. The aim of this work is to clarify the reason for extremely high conductivity exhibited by Na1+xZr2SixP3-xO12 (0-x-3) and to explain the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which supposedly occurs at around 170°C. We also investigate the overall temperature dependence of the ionic conductivity in the temperature range of 297-640K. The quasi-elastic neutron scattering (QENS) is used to measure the spatial and temporal dynamic properties of diffusion of Na-ions in the crystal structure. The Na-ion diffusion mechanism can be described by the right choice of the diffusion model. Important parameters, such as diffusion coefficients, activation energies, jump distances between the occupation sites and residence times are extracted from the measured and modelled QENS data. Temperature dependent X-ray diffraction data have been obtained and analysed in order to confirm the results obtained from the QENS data.

KFM 10.10 Thu 12:15 POT 51

**3D flower-like MnV12O31 center dot 10H2O as a high-capacity and long-lifespan cathode material for aqueous zinc-ion batteries** — •Yan Ran[1], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

In this work, MnV12O31 center dot 10H2O (MnVO) synthesized via one-step hydrothermal method is proposed as a promising cathode material for AZIBs. Because its stable layered structure and hieratical morphology provide a large layer space for rapid ion transports, this material exhibits a high specific capacity (433 mAh g-1 at 0.1 A g-1), outstanding long-term cyclability (5000 cycles at current density of 3 A g-1), and sufficient energy density (454.65 Wh kg-1). To illustrate the intercalation mechanism, ex-situ X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS) are adopted, uncovering a H+/Zn2+ dual-cation co-intercalation processes. Besides, density functional theory (DFT) calculation analysis shows that MnVO has a delocalized electron cloud and the diffusion energy barrier of Zn2+ in MnVO is low, which promotes the Zn2+ transport and, consequently, improves the reversibility of the battery upon deep cycling. The results provide key and enlightening insights for the design of high-performance vanadium-oxide-based cathode materials for AZIBs.

# KFM 11: Crystal Structure Defects / Real Structure / Microstructure

Chair: Prof. Dr. Theo A. Scherer (KIT Karlsruhe)

Time: Thursday 14:00–17:55 Location: POT 51

KFM 11.1 Thu 14:00 POT 51

**eutectic: a game changer** — •Sandhya Sharma[1], Hafiz Muhammad Zeeshan[1], Elena Voloshina[1,2], and Yuriy Dedkov[1,2] — [1]Centre of Excellence ENSEMBLE3 Sp. z o. o., Wolczynska Str. 133, 01-919 Warsaw, Poland — [2]Department of Pysics, Shanghai University, 99 Shangda Road, 200444 Shanghai, P.R. China

The world of semiconductors has drastically improved the lifestyle due to its versatile applications. The demand for new efficient semiconductors is increasing day by day, giving birth to the idea of new synthesis methods. Many synthesis techniques have been utilized to engineer band gap of semiconductors to achieve higher efficiency. Here, a perspective on the importance of semiconductor eutectic materials has been presented as one of the future potential candidates, along with the micro ($\mu$) pulling method (as a synthesis method for semiconductor eutectic materials) that not only control factors effecting the devices but also provides variety of options for band gap modification. The efficiency of the present devices in comparison with the eutectic composites has been made, showing the semiconductor eutectic materials as a better candidate for future devices.

KFM 11.2 Thu 14:20 POT 51

**Determining the Crystallization Mechanism in Optical Switching Experiments with Electron Backscatter Diffraction** — •Maximilian Müller and Matthias Wuttig — I. Institute of Physics (IA), Aachen, Germany

To tailor phase-change materials for computing and data storage applications unraveling the contribution of nucleation and crystal growth to crystallization is essential. Usually, these processes are studied at low temperatures. Subsequently, from the temperature dependence of both processes at low temperature, the role of these processes at high temperatures is extrapolated. This is inherently dangerous if the underlying processes do not follow Boltzmann kinetics.

In this study, crystallization was achieved by short laser pulses with pulse lengths between a few ns to several *s. Afterwards, the resulting grain structure was analyzed by different techniques, including atomic force microscopy and Electron BackScatter Diffraction (EBSD). The grain size distribution is determined by these experiments which helps disentangling the processes of nucleation and growth. Significant differences are observed concerning the nucleation of different compounds. Trends for the nucleation and growth rate as a function of stoichiometry are analyzed and explained based upon systematic changes in bonding.

KFM 11.3 Thu 14:40 POT 51

**Vacancies in Prussian White Cathode Materials employing Positron Annihilation Spectroscopy** — •Dominik Boras[1], Ida Nielsen[2], Alexander Buckel[3], Tore Ericsson[2], Lennart Häggström[2], Torsten E.M. Staab[1], and William R. Brant[2] — [1]Institute for Functional Materials and Biofabrication, Julius-Maximilians Universität Würzburg, 97070 Würzburg, Röntgenring 11 — [2]Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, SE-751 21 Uppsala, Sweden — [3]Altris AB, Kungsgatan 70b, SE-753 18 Uppsala, Sweden

We are presenting a novel attempt to characterise Prussian blue analogues. Prussian White samples have been synthesized with different sodium content and, then, characterized by common methods (ICP-OES, TG, SEM) but also by Mösbauer spectroscopy. We prepared there different sample states: fully and half-sodiated as well as desodiated. As a new method positron annihilation lifetime spectroscopy (PALS) has been applied to characterize the different samples states. We can state that the methods of PALS gives reasonable results for Prussian White with varying sodium and water content. The relative intensity of the longer positron lifetime component (405ps) is increasing with deceasing sodium content, which is an indication that the positron "sees" less of the open crystal channels filled by movable ions, since those become more and more occupied by intercalated Na-atoms. This first attempt aims to present the potential of PALS to characterise Prussian Blue analogue materials with respect to defects and occupation of of its crystal channels by movable ions.

KFM 11.4 Thu 15:00 POT 51

**Disorder engineering for symmetry lowering in Prussian Blue analogues (PBAs)** — •Yevheniia Kholina, Thomas Weber, and Arkadiy Simonov — ETH Zürich, Switzerland, Department of Materials, Laboratory for Multifunctional Ferroic Materials

A simple consequence of Neumann's principle is that certain properties can exist in crystals with a certain symmetry. As a result, a lot of materials engineering is focused on designing particular symmetries, which allow the properties of interest. In oxide perovskites as well as their molecular analogues, control of crystal symmetry is achieved by octahedral tilts and cation ordering. In this work we show an alternative way of symmetry lowering, using disorder. We focus on Mn[Co] PBA with the chemical composition $Mn[Co(CN)_6]_{2/3}$. These crystals have 1/3 of $Co(CN)_6$ sites vacant. The structure of such PBAs is believed to be cubic with space group $Fm\bar{3}m$. However, the optical measurements indicate that the crystal is twinned and an actual structure has tetragonal symmetry or lower. We collect single-crystal x-ray diffuse scattering from untwined crystal to probe the local structure and quantitatively characterise defect distribution, using 3D-$\Delta$PDF analysis. The symmetry of the local structure is reduced to tetragonal by local vacancies ordering. The vacancies have stronger correlation along c direction. Such asymmetry is formed because the crystal is growing in this direction. This means the symmetry can be lowered by choosing a specific direction of the crystal growth. We believe this result can be applied to other disordered crystalline materials and be an effective way to lower the symmetry for properties design.

KFM 11.5 Thu 15:20 POT 51

**Single crystal growth of the Mott insulator BaCoS2: structure and hole doping** — •Haneen Abushammala, Teslin Thomas, Andreas Kryssig, and Anna Boehmer — Experimentalphysik IV, Ruhr-Universitaet Bochum, Universitaetsstrasse 150, 44801 Bochum, Germany

The quasi-2D $BaCoS_2$ is a Mott insulator with a stripe-like antiferromagnetic ordering at $T_N$=290 K. Both chemical doping or hydrostatic pressure drive the system into a paramagnetic metallic phase. Interestingly, there is no structural transition at the metal-insulator transition of this phase, which offers ideal conditions to investigate the Mott transition in a model multiband system [1].

Nevertheless, $BaCoS_2$ remains little studied, and the interplay of electronic and structural features is still unclear. High-quality single crystals are needed to elucidate this issue. The synthesis of single-crystalline $BaCoS_2$ is challenging owing to its metastability, with a decomposition into $Ba_2CoS_3$, CoS and S below 850°C. The $BaCoS_2$ phase can only be obtained via quenching from high temperature. Moreover, $BaCoS_2$ melts incongruently, which calls for a flux growth method necessitating separation of the crystals from the flux by the end of the growth. We have successfully grown single crystals of pure and the hole-doped $BaCoS_2$ using a self-flux method with high-temperature flux separation and quench. The structural and anisotropic electrical transport properties are determined and discussed.

[1] Abushammala, Lenz, Baptiste, Casula, Klein and Gauzzi, in preparation (2022).

KFM 11.6 Thu 15:40 POT 51

**Monitoring the S-phase formation in an high-purity Al-Cu-Mg alloy by truncation during heating-up** — •Torsten E.M. Staab, Dominik Boras, Sebastian Breitfelder, and Timo Strobl — IFB, Julius-Maximilians Universität Würzburg, 97070 Würzburg, Röntgenring 11

We are presenting a novel attempt to combine in-situ and ex-situ measurements for aluminum alloys. As a model alloy we have chosen an Al-1.7Cu-1.3Mg (at.%) alloy, which has been cast from high purity elements (5N5 Al, 4N Cu and 4N Mg). As basic method DSC (heating ramp: 5 K/min) has been employed to determine different states during S-phase formation: onset, maximum of the exothermal peak, end of exothermal reaction. Sample states were frozen-in by an abrupt truncation of the heating ramp (5 K/min), i.e. cooling quickly to room temperature. So, the current sample state is frozen-in. After truncation all samples have been measured without further preparation by X-

ray diffraction (XRD) and positron annihilation lifetime spectroscopy (PALS). Thus we could correlate exactly different sample states, which is impossible by conventional experiments, i.e. heating to a certain temperature and then holding a certain time. This paves the way to investigate defined and comparable sample states by methods, which require an extensive sample preparation, like TEM or 3DAP, and in-situ methods like DSC or XRD at synchrotron beamlines.

**15 min. break**

KFM 11.7 Thu 16:15 POT 51

**Local structure of titanite $CaTiSiO_5$** — •Arkadiy Simonov — ETH Zürich, Zürich, Switzerland

Titanite, $CaTiSiO_5$, is a multifunctional nesosilicate mineral which recently received attention as a material for building tunable capacitors and oscillators. Near 500K titanite shows a nonlinear dielectric response with positive dielectric tunability and thus its dielectric susceptibility can be efficiently controlled using a voltage bias, moreover capacitors made of this material have unusually low dielectric losses and thus high quality factor [1]. The origin of such a good performance is not currently understood, but one hypothesis is that it is related to an unusual locally antipolar disordered structure which is observed in titanite above 500K in the paraelectric $A2/a$ phase.

In this work we present the analysis of the local structure of titanite in the $A2/a$ phase. We use single crystal diffuse scattering as our probe and analyze it using a non-parametric method based on three dimensional difference pair distribution function (3D-ΔPDF) refinement. We show that despite the $A2/a$ structure is on average paraelectric, locally it is antipolar. It shows $Ti^{4+}$ displacements which have strong ferro correlations along the b direction and weak locally anti-ferro correlations in a and c directions. Such locally antipolar structure can provide a crossover path for the low temperature $P2_1/a$ structure under applied electric field and thus explain the low dielectric losses observed in this material.

[1] Murata, T., Asaka, T., Hirose, S. (2021). J. Am. Cer. Soc. 104(11), 5794-5802.

KFM 11.8 Thu 16:35 POT 51

**Pfaffian invariant identifies magnetic obstructed atomic insulators** — •Daniel Varjas[1,2,3,4], Isidora Araya Day[3,4], Anastasiia Varentcova[3], and Anton R. Akhmerov[3] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm, Sweden — [3]QuTech, Delft University of Technology, Delft 2600 GA, The Netherlands — [4]Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 4056, 2600 GA Delft, The Netherlands

We derive a $Z_4$ topological invariant that extends beyond symmetry eigenvalues and Wilson loops and classifies two-dimensional insulators with a $C_4T$ symmetry. To formulate this invariant, we consider an irreducible Brillouin zone and constrain the spectrum of the open Wilson lines that compose its boundary. We fix the gauge ambiguity of the Wilson lines by using the Pfaffian at high symmetry momenta. As a result, we distinguish the four $C_4T$-protected atomic insulators, each of which is adiabatically connected to a different atomic limit. We establish the correspondence between the invariant and the obstructed phases by constructing both the atomic limit Hamiltonians and a $C_4T$-symmetric model that interpolates between them. The phase diagram shows that $C_4T$ insulators allow $\pm 1$ and 2 changes of the invariant, where the latter is overlooked by symmetry indicators.

KFM 11.9 Thu 16:55 POT 51

**Probing Centrosymmetricity of Emergent Materials by Convergent Beam Electron Diffraction** — •S. Subakti[1,2], Y. Wang[3], A. Chakraborty[4], A.K. Srivastava[4], D. Wolf[1], T. Doert[3], M. Ruck[3], S.S.P. Parkin[4], B. Büchner[1,2], and A. Lubk[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [3]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany — [4]Department for Nano-Systems from Ions, Spins, and Electrons (NISE), Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle(Saale), Germany

Many exotic physics present in materials, such as chiral magnetic textures, hinges on the (non)existence of centrosymmetry. Consequently unambigous structural determination beyond x-ray diffraction (XRD), which is to a certain extend blind to centrosymmetry, is indispensable. Here, we present structural investigation of two emergent quantum materials, namely $Fe_3GeTe_2$ and $Rh_2NiSb$, by means of convergent beam electron diffraction (CBED). Analyzing the diffraction group symmetries of the CBED patterns in combination with extinction rules and results from XRD analysis, we conclude the space group of these materials. Importantly, both phases are non-centrosymmetric, suggesting possible presence of chiral magnetic textures and multiferroicity.

KFM 11.10 Thu 17:15 POT 51

**Nonsymmorphic chiral symmetry and solitons in the Rice-Mele model** — •Edward McCann — Lancaster University, Lancaster, United Kingdom

The charge-density-wave (CDW) phase of the Rice-Mele model in one dimension has alternating onsite energies and constant nearest-neighbor hopping parameters. The chiral symmetry of the CDW wave phase is nonsymmorphic, resulting in a breaking of the bulk topology by an end or a texture in the alternating energies. We consider the presence of solitons (textures in position space separating two degenerate ground states) in finite systems with open boundary conditions. We identify the parameter range under which an atomically-sharp soliton in the CDW phase supports a localized state which lies within the band gap, and we calculate the expectation value of the nonsymmorphic chiral operator for this state, and the soliton electric charge [1]. Finally, we discuss other models with similar, nonsymmorphic nonspatial symmetries.

[1] R. E. J. Allen et al, Phys. Rev. B 106, 165409 (2022).

KFM 11.11 Thu 17:35 POT 51

**The Initial Molecular Interactions in the Course of Enthalpy Relaxation and Nucleation in Polyethylene terephthalate (PET) as Monitored by Combined Nanocalorimetry and FTIR Spectroscopy** — •Wycliffe Kipnusu[1], Evgeny Zhuravlev[2], Christoph Schick[2,3], and Friedrich Kremer[1] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University, Linnestr. 5, 04103, Leipzig, Germany — [2]Universitat Rostock Institute of Physics, Albert-Einstein_str. 23-24, Rostock, DE 18051, Germany — [3]Kazan, Russia

Fast scanning calorimetry (FSC) and Fourier transform infrared (FTIR) spectroscopy are combined to trace for the same sample the evolution of the calorimetric properties and of the intra- and intermolecular interactions in polyethylene terephthalate (PET). FSC enables to rapidly quench the sample to amorphous state and to monitor nucleation and crystal growth at isothermal conditions. By Determining the difference IR spectra between a quenched and an annealed sample unravels the the intra- and inter-molecular interactions in detail; (i) as first response already during enthalpy relaxation, the far reaching Coulomb interactions between the polar C=O moieties are active; (ii) in contrast, the ethylene unit and the aromatic ring show a response only, if homogeneous nucleation sets in, while the COC moiety remains uninfluenced; (iii) a hierarchy is observed in the sequence of the response of the different molecular moieties.

## KFM 12: Members' Assembly

Time: Thursday 18:00–19:00 Location: POT 51

**All members of the Crystalline Solids and their Microstructure Division are invited to participate.**

# KFM 13: Polar Oxide Crystals and Solid Solutions I

Chair: Prof. Dr. Holger Fritze (TU Clausthal)

Time: Thursday 10:00–12:35 Location: POT 106

KFM 13.1 Thu 10:00 POT 106

**Polaronic structures in $LiNbO_3$ and $LiTaO_3$ modelled from first principles** — •Nils Andre Schäfer and Simone Sanna — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

Polaronic defects impact among other properties the optical response of $LiNbO_3$ (LN). Changes in their optical properties are of interest for the applications of LN in optoelectronics. These are relatively well known in LN but in $LiTaO_3$ (LT) less so. In order to improve our knowledge of polaronic structures in LT, we modeled polarons in LN and LT from first principles using the DFT+U method as implemented in VASP.

We explore different microscopic polaronic structures in both polar oxides with respect to changes in their electronic band structures and optical properties, especially with respect to Jahn-Teller distortions. Similarities and differences between different polaronic defects and both compounds are discussed as well.

KFM 13.2 Thu 10:20 POT 106

**Crystal growth and thermal analysis of Li(Nb,Ta)O3 solid solutions** — •Umar Bashir Ganie — IKZ, Berlin

This work presents the growth and thermal analysis of Lithium Niobate Tantalate (Li(Nb,Ta)O3, LNT) single crystals for different LiTaO3 (LT) mole fractions (xLT), (xLT = nLT/(nLT+nLN)). Our crystal growth experiments show that growth of LNT single crystal over the entire LT mole fraction is not only possible but can be achieved with weaker constituent segregation and therefore higher degree of homogeneity than considered previously. Our differential thermal analysis (DTA) measurements show that the melting temperature increases with increasing fraction of LT and follow the behavior of a (pseudo)binary phase diagram as published previously [1]. Thorough evaluation of the DTA results allows to propose an improved version of the LN-LT phase diagram that is not only thermodynamically stringent but also allows to explain the component distribution observed in LNT single crystals and to design growth experiments yielding crystals of higher homogeneity. We also performed specific heat capacity measurements of single crystals of LNT solid solutions. The aim was to investigate the variation of ferroelectric Curie temperature with composition. We observed that the ferroelectric Curie temperature decreases linearly with growing Ta composition in the LNT solid solution crystals.

KFM 13.3 Thu 10:40 POT 106

**Hydrogen Diffusion in LiNbO3 and LiTaO3** — •Kofahl Claudia[1], Dörrer Lars[1], Suhak Yuriy[2], Yakhnevych Uliana[2], Fritze Holger[2], and Schmidt Harald[1,3] — [1]Institut für Metallurgie, AG Festkörperkinetik, TU Clausthal, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Germany — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Germany

LiNbO3 and LiTaO3 crystals are technologically important polar metal oxides with exceptional combinations of ferroelectric, piezoelectric, acoustic, optical and ion conductivity properties. The presence and diffusion of H in these materials has an important influence on the materials properties, reducing optical damage, increasing optical birefringence and changing ionic conductivity. The diffusion mechanism is unclear up to now. Therefore, it is of particular interest to study the diffusion of hydrogen. For this purpose, we use two different analytical methods, SIMS (Secondary Ion Mass Spectroscopy) and IRS (Infrared Spectroscopy). For the SIMS measurements, the crystals are loaded with high amounts of H by means of proton-exchange and the redistribution of H is monitored after post-annealing. In contrast, for the IRS experiments, only hydrogen of about 300 ppm, which is introduced by crystal growth in air, is replaced by deuterium during exchange anneals in D2O. The measured diffusion coefficients of the two methods differ from each other, but are higher than Li diffusivities as given in literature. The activation energies are similar. Possible reasons for the differences are discussed.

KFM 13.4 Thu 11:00 POT 106

**Acoustic loss in Lithium Niobate-Lithium Tantalate solid solutions with different Nb/Ta ratios at temperatures up to 900°C** — •Uliana Yakhnevych[1], Claudia Kofahl[2], Stepan Hurskyy[1], Steffen Ganschow[3], Yuriy Suhak[1], Harald Schmidt[2], and Holger Fritze[1] — [1]Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Germany — [2]Institute of Metallurgy, Clausthal University of Technology, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Lithium niobate-lithium tantalate solid solutions (LNT) are poorly studied materials in modern materials science, which must be seen in the light that they can combine the advantages of the edge compounds lithium niobate (LN) and lithium tantalate (LT). These crystals are expected to exhibit high piezoelectric coefficients and thermal stability. This work focuses on comparing the Q-factor of LN, LT, and LNT as well as on the analysis of loss contributions in samples. Electromechanical losses of the samples were determined using two different approaches, namely noncontacting resonant ringdown spectroscopy and resonant piezoelectric spectroscopy using Pt electrodes. LNT thickness-shear mode (TSM) acoustic resonators exhibit significantly lower loss than LN. The study of the acoustic loss in LNT resonators operated in the TSM showed strong frequency dependent loss increases at temperatures above 450°C. The loss was modelled using independent materials data. Based on the modelling, the abovementioned loss above 450°C is associated with a conductivity-induced piezoelectric/carrier relaxation mechanism governed by Li migration.

**15 min. break**

KFM 13.5 Thu 11:35 POT 106

**High-temperature stability of electrical and acoustic properties of congruent and near stoichiometric single crystalline LiNbO3, LiTaO3 and LiNb0.94Ta0.06O3** — •Yuriy Suhak[1], Stepan Hurskyy[1], Uliana Yakhnevych[1], Fatima El Azzouzi[1], Claudia Kofahl[2], Harald Schmidt[2], Steffen Ganschow[3], Klaus-Dieter Becker[4], and Holger Fritze[1] — [1]Institute for Energy Research and Physical Technologies, Clausthal University of Technology, Goslar, Germany — [2]Institute of Metallurgy, Clausthal University of Technology, Clausthal-Zellerfeld, Germany — [3]Leibniz Institut für Kristallzüchtung, Berlin, Germany. — [4]Braunschweig University of Technology, Braunschweig, Germany

It is known that the intrinsic properties of LiNbO3, LiTaO3 and, consequently, of Li(Nb,Ta)O3 solid solutions are strongly dependent on lithium stoichiometry. In current work the electrical and acoustic properties of congruent and near-stoichiometric single crystalline Li(Nb,Ta)O3 are studied as a function of temperature by means of impedance spectroscopy and resonant piezoelectric spectroscopy, respectively. The preparation of near-stoichiometric samples was performed by vapor transport equilibration technique (VTE). It is shown, that VTE-treated samples generally exhibit lower conductivity and lower acoustic loss, which implies better thermal stability. The latter was examined by a long-term measurement of electrical conductivity at 500 °C in air. After about 330 hours of uninterrupted thermal treatment the conductivity of a congruent LiNb0.94Ta0.06O3 specimen was found to decrease only for about 3 %.

KFM 13.6 Thu 11:55 POT 106

**A high-temperature optical spectroscopy study of lithium niobate, LiNbO3** — •Klaus-Dieter Becker[1], Jianmin Shi[1], Piotr Gaczynski[1], Misha Sinder[2], Uliana Yakhnevych[3], Natalia Syvorotka[3], Yuriy Suhak[3], Steffen Ganschow[4], and Holger Fritze[3] — [1]Institute of Physical and Theoretical Chemistry, TU Braunschweig, Braunschweig, Germany — [2]Materials Engineering Department, Ben Gurion University of the Negev, Beer-Sheva, Israel — [3]Institute for Energy Research and Physical Technologies, TU Clausthal, Goslar, Germany — [4]Leibniz Institut für Kristallzüchtung, Berlin, Germany

Optical absorption spectra of chemically reduced LiNbO3 (LN) show broad bands in the vis and NIR region which have been attributed to various types of electron small polarons. At 1000°C, spectra are dominated by an absorption band at 0.9 eV due to free small polarons,

i.e. to electrons localized on niobium ions on regular sites. Band intensity has been found to follow a power-law dependence on oxygen partial pressure PO2 of the form (PO2)^m with m= -0.23(+-)0.02. This m-value is in excellent agreement with the value of -1/4 predicted from point defect thermodynamics of the chemical redox model of LN. The experimental kinetics of reduction and oxidation following a rapid change in oxygen partial pressure have been found to provide a novel route to diffusion of lithium vacancies at high temperatures as well as to that of lithium ions in LN.

KFM 13.7 Thu 12:15 POT 106

**Looking undercover - Probing subsurface properties by Piezoresponse force microscopy (PFM)** — •Matthias Roeper[1], Samuel D. Seddon[1], Lili Ding[1], Michael Rüsing[1], and Lukas M. Eng[1,2] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Piezoresponse force microscopy (PFM) is one of the most widespread methods for investigating and visualizing ferroelectric domain structures at the nanometer length scale, even along all 3 dimensions (3D) [1]. PFM couples to the local dielectric displacement that is present near the sample surface, and hence is also sensitively probing into the bulk of the sample under investigation, i.e. into a subsurface volume with penetration d [2]. In this work, we systematically analyze in both theory and experiment, the contrast and depth resolution capabilities of PFM as a function of the various relevant experimental parameters. PFM tool properties such as the tip radius, ac driving voltage, and ac frequency were optimized, while equally dedicated sample structures incorporating (known) buried features, i.e. ferroelectric domain walls, fabricated into the bulk host at a distance d below the surface, were analyzed Our finding allow to accurately adjust the image contrast to a certain penetration depth d, and thus quantify those local features with high precision.

[1] L. M. Eng et al., Appl. Phys. Lett. 74, 233 (1999) [2] F. Johann et al., Appl. Phys. Lett. 94, 172904 (2009)

## KFM 14: Polar Oxide Crystals and Solid Solutions II

Chair: Prof. Dr. Holger Fritze (TU Clausthal)

Time: Thursday 14:00–16:35 Location: POT 106

KFM 14.1 Thu 14:00 POT 106

**Domain wall current in lithium niobate single crystals at temperatures up to 370°C** — •U. Yakhnevych[1], M. Kunzmer[1], I. Kiseleva[2], J. Gössel[2], J. Ratzenberger[2], M. Rüsing[2], L.M. Eng[2,3], and H. Fritze[1] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Am Stollen 19 B, Goslar, 38640, Germany — [2]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [3]Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Lithium niobate (LN) ferroelectric crystals with an artificially formed domain structure are widely used in novel electronic devices. So far, a complete picture of the electrical transport mechanism at domain walls is still missing, including its high temperature behavior. This work focuses on the determination of the domain wall conductivity from room temperature up to 370 °C. Using 5%MgO:LN, conductive DWs are prepared and enhanced following the procedure by Godau et al. [1]. Direct current measurements using an electrometer amplifier and impedance spectroscopy are applied to locally map the temperature-dependent DW current. A strong dependence of the electrical conductivity on temperature is observed. The activation energy shows distinct values for low-to-medium and high temperatures, respectively, reaching values of ~0.1 eV and ~0.15*eV. For further analysis, the obtained samples should be measured at even higher temperatures. [1] C. Godau, T. Kämpfe, A. Thiessen at al. ACS Nano 11, 5, 4816-4824 (2017). https://doi.org/10.1021/acsnano.7b01199

KFM 14.2 Thu 14:20 POT 106

**Ferroelectric domains and domain walls under uniaxial stress * A case study in lithium niobate** — Ekta Singh[1], Henrik Beccard[1], Michael Lange[1], Sven Reitzig[1], Zeeshan H. Amber[1], Clifford W. Hicks[3], Julius Ratzenberger[1,2], •Michael Rüsing[1], and Lukas M. Eng[1,2] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany — [3]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, United Kingdom

In material science, mechanical strain has an influence on a multitude of material properties. For ferroelectrics, strain can be achieved via standard techniques, such as lattice-mismatched epitaxial growth of thin films, or hydrostatic pressure. However, these methods are either limited to specific material combinations or non-local investigation techniques. Here, we present an alternative approach [1] to study bulk crystals under the influence of uniaxial strain, using a piezo-actuator-based device that is compatible with various local probe techniques. To demonstrate the operation we present the influence of strain on the vibrational properties probed via micro-Raman spectroscopy [1], as well as the influence of strain on the local conductivity of ferroelectric domain walls probed by scanning con-ductance microscopy [2]. [1] E. Singh et.al, arXiv:2210.14120 (2022). [2] E. Singh et.al, Phys. Rev. B 106,144103 (2022).

KFM 14.3 Thu 14:40 POT 106

**Hall effect in conductive ferroelectric domain walls in $BaTiO_3$** — Henrik Beccard[1], Elke Beyreuther[1], Michael Rüsing[1], Benjamin Kirbus[1], Ekta Singh[1], •Samuel Seddon[1], Petr Bednyakov[2], Jiri Hlinka[2], and Lukas M. Eng[1,3] — [1]Institut für Angewandte Physik, TU Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha 8, CZR — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Two dimensional (2D) electronic systems are essential in cutting-edge nano- electronic research. Here, conductive ferroelectric domain walls (DWs) are experiencing a concerted research effort for the last decade. Much of the research, however, did focus onto measuring and tuning the electrical DW conductivity [1], with very little investigations reporting on the very fundamental DW properties such as charge carrier density and mobility. Here, we adapted the 4-point van der Pauw [2] geometry to probe these 2D sheets of ferroelectric DWs in $BaTiO_3$, and were able to determine the aforementioned properties. We find large electron mobilities of 400 $cm^2$ $(Vs)^{-1}$ and decent electron densities [3]. Not only are these results by themselves novel, but also perfectly demonstrate the power of this simple methodology to quantify the charge carrier properties in any low-dimensional system.

[1] C. Godau, et al., ACS Nano **11**, 4816 (2017)
[2] L. J. Van der Pauw, Philips Tech Rev **20**, 220-224 (1958)
[3] H. Beccard, et al., ACS Appl. Nano Mater. **7**, 8717-8722 (2022)

KFM 14.4 Thu 15:00 POT 106

**Thin Patterned Lithium Niobate Metasurfaces by Parallel Additive Capillary Stamping of Aqueous Precursor Solutions** — •Jan Klenen[1], Fatih Alarslan[2], Laura Vittadello[1], Martin Steinhart[2], and Mirco Imlau[1] — [1]Department of Physics, Osnabrück University, Germany — [2]Institute of Chemistry of New Materials, Osnabrück University, Germany

Optical metasurfaces are a rapidly evolving field in the aim to miniaturize optical functionalities and integrated photonics [A. Fedotova et al., *ACS Photonics* **2022**]. However, the large-scale application is still challenging as the preparation of such metasurfaces, i.e., by mechano-chemical wafer thinning or lithographic pattering, is usually complex, time-consuming, and expensive. We try to address this problem and present a novel method of metasurface patterning based on parallel additive capillary stamping of $LiNbO_3$ on an ITO substrate [F. Alarslan et al., *Advanced Engineering Materials* **2021**, 24(6)]. This technique offers the advantage of rapid, easily customizable and cheap structuring of layers with thicknesses on the order of 100 nm. Nonlinear optical investigations performed with the TIGER microscope show a homogeneous second harmonic generation (SHG) of the surface coinciding

with the $LiNbO_3$ film structured by hexagonally arranged macropores. The additional implementation of gold nanoparticles at the position of the macropores allows for a drastic enhancement of the SHG by exploiting plasmonic resonances. Financial support by the ERC (project 646742 INCANA) and DFG (projects IM 37/12-1, FOR 5044 and INST 190/165-1) is gratefully acknowledged.

**15 min. break**

KFM 14.5 Thu 15:35 POT 106

**Optical nonlinearities of lithium tantalate solid solutions** — •Mirco Imlau, Tobias Hehemann, Sören Domke, Niklas Dömer, Fiete Breer, Felix Kodde, Jan Kleenen, Anton Pfannstiel, and Laura Vittadello — Institute of Physics, Osnabrück University

Optical nonlinearities of optical materials, i.e. the nonlinear material response to incident electromagnetic radiation, are the fundamental physical basis for a number of components in nonlinear photonics, such as nonlinear optical Kerr lenses, saturable absorbers or frequency converters. The properties of optical nonlinearities are closely related to the electronic and atomic structure of the material systems used. Against this background, lithium niobate tantalate (LNT, $LiNb_xTa_{1-x}O_3$ with $0 \leq x \leq 1$) solid solutions are promising because the edge compounds themselves (LN, x=1 and LT, x=0) are already extensively used in photonics' components, but especially because the nonlinear optical properties of LNT may be tailored to the specific requirements of the application via composition. We here present the state-of-the-art knowledge of our studies on optical nonlinearities of LNT over the entire composition range, both, for quasi-instantaneous nonlinear responses (absorption & nonlinear index, frequency conversion) and transient responses (time-resolved transient absorption on the temporal multiscale from femtoseconds to seconds & transient index dynamics). The findings are discussed in the framework of emerging applications in (nano-)photonics, particularly for laser systems of the next generation, and will be compared with LN and LT. Financial support by the DFG (project IM 37/12-1, FOR 5044).

KFM 14.6 Thu 15:55 POT 106

**Small polaron absorption centers in lithium noibate-tantalate solid solutions** — •Anton Pfannstiel[1], Simone Sanna[2], Yuriy Suhak[3], and Steffen Ganschow[4] — [1]Inst. Physics, Osnabrück University — [2]Inst. Theoretical Physics, University of Gießen — [3]Inst, Energy Research, Technical university of Clausthal — [4]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin

The study of small polarons in ferroelectric lithium niobate (LN) enabled the understanding of various physical phenomena on a microscopic level, like photo-induced coloration or conductivity and led to the formulation of a robust model of polaronic localization centers and energies [O. F. Schirmer *et al* 2009 J Phys.: Condens. Matter **21** 123201]. So far, for lithium tantalate (LT) and the solid solution, lithium niobate-tantalate (LNT) a respective small polaron model is missing in literature.

For this purpose, this study provides polaron self localization energies for LN, LT and LNT crystals of various composition. Thermally reduced crystals are optically bleached at cryogenic temperatures. The resulting small polaron absorption bands are identified through transmission spectroscopy and modeled within the framework of small polaron absorption theory. The determined polaron energies are interpreted against the background of the known defect models for LN and LT but also in conjunction with ab-initio modeling results for carrier self-localization. Financial support by the DFG [projects IM 37/12-1, SA 1948/3-1, SU 1261/1-1, GA 2403/7-1, FOR5044] is gratefully acknowledged.

KFM 14.7 Thu 16:15 POT 106

**Nonlinear diffuse fs-pulse reflectometry adopted to LNT solid solutions** — •F. Kodde[1], L. Vittadello[1], J. Klenen[1], K. Koempe[2], V. Hreb[3], D. Sugak[3], V. Sydorchuk[4], U. Yakhnevych[5], and M. Imlau[1] — [1]Institute of Physics, Barbarastr. 7, Osnabrück University — [2]Department of Biology and Chemistry, Barbarastr. 11, Osnabrück University — [3]Department of Semiconductor Electronics, Bandery Str. 12, Lviv Polytechnic National University, 79013 Lviv, Ukraine — [4]Institute for Sorption and Problems of Endoecology, NASU, 13 Gen. Naumov St., 03164 Kyiv, Ukraine — [5]Institute of Energy Research and Physical Technologies, Am Stollen 19B, TU Clausthal

Nonlinear diffuse fs-pulse reflectometry is a powerful tool to analyze the spontaneous polarization of polar oxide nano-crystals [Kijatkin *et al.*, Photonics **4**, 11 (2017)]. It profits from the absence of a phase-matching condition for frequency conversion. We present our systematic investigations at the example of nanocrystals of $LiNb_{1-x}Ta_xO_3$ (LNT) solid solutions [Vasylechko *et al.*, Crystals **11**, 755 (2021)], that show a disappearance of the birefringence if the temperature is precisely adjusted [Wood *et al.*, J. Phys.: Condens. Mat. **20**, 235237 (2008)]. Accordingly, we have extended the experimental setup by a temperature controlled pellet holder and determined the harmonic ratio as a function of composition, i.e. Li/Ta-ratio. We find both, a characteristic maximum of the harmonic ratio, and a dependence of the maximum on the composition. Financially supported by the DFG and BMBF [project IM 37/12-1, FOR5044, BMBF, FKZ: 01DK20009].