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 $T = 0\,\mathrm{K}$, 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 (ϵ). 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 integral 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 ΔT 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 μs 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 ferroelectrics 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 μm height and center-to-center distance of 10 μm 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 sig-

nal 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 De-

partment 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 μs.

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)