KFM 15: Postersession KFM

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

KFM 15.1 Thu 16:00 P2/1OG

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

While the defect physics of $LiNbO_3$ has been object of many investigations, the nature of point defects in the isomorphic and isoelectronic $LiTaO_3$ is much less known. Although the existence of small bound polarons [1,2] in $LiTaO_3$ might be expected due to the high lattice polarizability, the verification of this assumption is still missing. In this work we provide the atomistic description of small bound polarons $Ta_{Li}^{5+/4+}$ in $LiTaO_3$ and of many other point defects such as Ta and Li vacancies. The calculations performed within density functional theory with Hubbard corrections predict the large lattice relaxation of the oxygen ligands associated to the electronic capture at the antisite center, which can be interpreted as due to the polaron formation. The relative formation energies of the investigated defects closely mirror those of corresponding defects in $LiNbO_3$ [3], suggesting a rather similar defect physics in the two materials. [1] O. F. Schirmer et al., J. Phys.: Condens. Matter **21**, 123201 (2009). [2] F. Freytag et al., Nature Scientific Reports **6**, 36929 (2016). [3] Y. Li, W. G. Schmidt, S, Sanna, Phys. Rev. B **89**, 094111 (2014).

KFM 15.2 Thu 16:00 P2/1OG

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

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

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

KFM 15.3 Thu 16:00 P2/1OG

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

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

KFM 15.4 Thu 16:00 P2/1OG

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

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

KFM 15.5 Thu 16:00 P2/1OG

Clocking nonlinear optical frequency-mixing in disordered, polar nanoparticles — •Jan Klenen[1,2], Christian Kijatkin[1,2], Bjoern Bourdon[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Osnabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

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

KFM 15.6 Thu 16:00 P2/1OG

Light-induced absorption in Fe:LN by means of ns-pump supercontinuum-probe spectroscopy — •Bjoern Bourdon, Simon Messerschmidt, David Brinkmann, Andreas Krampf, Laura Vittadello, and Mirco Imlau — Department of Physics, Osnabrueck University, Osnabrueck, Germany

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

KFM 15.7 Thu 16:00 P2/1OG

Wide-field real-time nonlinear optical microscope in living organism — •Niklas Bethke[1,2], Dustin Dzikonski[1,2], Laura Vittadello[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Os-

nabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

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

KFM 15.8 Thu 16:00 P2/1OG

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

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

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

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

KFM 15.9 Thu 16:00 P2/1OG

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

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

KFM 15.10 Thu 16:00 P2/1OG

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

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

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

KFM 15.11 Thu 16:00 P2/1OG

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

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

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

KFM 15.12 Thu 16:00 P2/1OG

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

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

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

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

KFM 15.13 Thu 16:00 P2/1OG

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

Due to its UV emission at around 375 nm, its strong photoluminescence and nonlinear optical properties, the wide-gap semiconductor zinc oxide (ZnO) is a current subject in photonics research. ZnO based ring

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

KFM 15.14 Thu 16:00 P2/1OG

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

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

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

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

KFM 15.15 Thu 16:00 P2/1OG

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

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

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

KFM 15.16 Thu 16:00 P2/1OG

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

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

KFM 15.17 Thu 16:00 P2/1OG

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

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

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

KFM 15.18 Thu 16:00 P2/1OG

Ferrimagnetic oxide substrates in the synthesis of multiferroic heterostructures — •Thomas Ruf and Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstraße 2, D-04103, Leipzig

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

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

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

KFM 15.19 Thu 16:00 P2/1OG

Thermal investigation of nonlinear crystals for high power ultrashort MID-IR OPCPA pumped at 1 micrometer — Mahesh Namboodiri[1], •Gregor Indorf[2], Torsten Golz[2], Jan H. Buss[2], Michael Schulz[2], Robert Riedel[2], Tim Laarman[1,3], and

Mark J. Prandolini[2] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]Class 5 Photonics GmbH, Notkestraße 85, 22607 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging CUI, Luruper Chaussee 149, Hamburg 22761, Germany

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

KFM 15.20 Thu 16:00 P2/1OG

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

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

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

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

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

KFM 15.21 Thu 16:00 P2/1OG

Laser-based inspection of technical dielectric thin films — •Simon Podendorf[1], Yannik Toschke[1], Jörg Rischmüller[1], Mirco Imlau[1], Mareike Schlag[2], Kai Brune[2], and Hauke Brüning[2] — [1]School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany — [2]Fraunhofer IFAM, Wiener Strasse 12, 28359 Bremen, Germany

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

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

KFM 15.22 Thu 16:00 P2/1OG

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

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

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

KFM 15.23 Thu 16:00 P2/1OG

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

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

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

KFM 15.24 Thu 16:00 P2/1OG

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

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

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

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

KFM 15.25 Thu 16:00 P2/1OG

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

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

KFM 15.26 Thu 16:00 P2/1OG

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

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

[1] M. Roth, Springer Handbook of Crystal Growth, pp. 691-723 (2010)
[2] S. Neufeld et al., J. Phys.: Matter. 2, 045003 (2019)
[3] A. Bocchini, J. Phys.: Condens. Matter 31, 385401 (2019)

KFM 15.27 Thu 16:00 P2/1OG

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

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

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

[1] M. Roth, Springer Handbook of Crystal Growth (2010).
[2] M. G. Roelofs, J. Appl. Phys. 65, 4976 (1989).
[3] A. Bocchini et al., J. Phys.: Condens. Matter 31 385401 (2019).
[4] S. D. Setzler et al.., J. Phys.: Condens. Matter 15, 3969 (2003)

KFM 15.28 Thu 16:00 P2/1OG

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

Contrary to other transition metal chalcogenides (TMC), TiS_3 has not received attention despite its relative easy exfoliation, and high carrier mobility. In this work, we used DFT investigate the stability, the structural and the electronic properties of vacancy and antisite defects in the transition metal trichalcogenides TiS3. It is found that the formation energy is strongly dependent on which of the symmetrically inequivalent sites the defect is located. In contrast to the dichalcogenide analogs, the energy required to create a sulfur divacancy under Ti-rich conditions are lower than that of the single vacancy independently of the location of the sulfur vacancy. The negative binding energy of the double vacancies is an indication that they will likely depose into the single sulfur defects. Based on both the binding and the formation energy, we also demonstrate that the Ti-rich is the ideal growth condition for the formation of the vacancy complexes. The presence of intermediate states in the bandgap of most of the defects considerably affects the electronic properties of the pristine, with the possibility of n-type and p-type conductivity. With the exception of V_{S^1}, V_{TiS^3}, V_{Ti4S^1}, $V_{Ti4S^14S^3}$, S_{Ti} and $Ti_{S^3}S_{Ti}$, where there is no trace of magnetism as in the pristine system; all other defects acquired some magnetic moment.

KFM 15.29 Thu 16:00 P2/1OG

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

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

KFM 15.30 Thu 16:00 P2/1OG

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

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

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