KFM 5: Poster Session KFM

Time: Tuesday 16:00–17:00 Location: P

KFM 5.1 Tue 16:00 P

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

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 5.2 Tue 16:00 P

Application of CVD Diamond disks for ECRH systems of fusion reactors — •Sabine Schreck, Gaetano Aiello, Andreas Meier, Theo Scherer, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, D-76021 Karlsruhe, Germany

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

The ITER EC torus window consists of a diamond disk with a diameter of 70mm and a thickness of 1.11mm (resonance thickness for 170GHz). The window serves also as confinement barrier for tritium and is classified as "Protection Important Component". A specific test program is required for its qualification, including prototypical activities. For future fusion machines like DEMO, most likely broadband window solutions as the double disk window or the Brewster window will come into operations. This implies also new requirements for the disks, e.g. large diameters of minimum 180mm for the inclined Brewster-angle disk for a typical aperture of 63.5mm.

KFM 5.3 Tue 16:00 P

Time-Resolved Nonlinear Diffuse Femtosecond-Pulse Reflectometry Using Lithium Niobate Nanoparticles with Two Pulses of Different Colors — •Jan Klenen[1,2], Christian Kijatkin[1,2], Björn Bourdon[1,2], Laura Vittadello[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Osnabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

In the context of biophotonics and material science, harmonic nanoparticles (HNPs) attract elevated interest owing to their versatile nonlinear optical (NLO) properties, such as their broad spectral tunability [C. Kijatkin, *Photonics* **2017**, *4*, 11]. However, the characterization of the time-evolution of light-matter interaction in such nanoscale media is yet to be completed. In this study we are using femtosecond-pulse diffuse reflectometry to investigate the time-resolved sum-frequency generation (SFG) of two differently colored, infrared femtosecond laser pulses in lithium niobate nanoparticle pellets [C. Kijatkin, *Adv. Photonics Res.* **2020**, DOI: 10.1002/adpr.202000019]. The pulse shape of the remitted SFG shows an asymmetry in the temporal domain. This finding can be explained within the framework of light propagation in random media and is generalized on the basis of numerical simulations. As a consequence, ultrashort pulse shapes can now be comprehensively predicted in nanoscale, densely packed media with a NLO response. In this respect we discuss the potential of HNPs as a flexible alternative to crystalline media for the determination of a pulses chirp. Funded by the DFG (IM37/12-1, FOR 5044, INST 190/165-1 FUGG).

KFM 5.4 Tue 16:00 P

Ferroelektrischer Phasenübergang in Mg dotiertem $LiNbO_3$ — •Leonard Verhoff und Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschlnd

Lithiumniobat ($LiNbO_3$) ist besonders in der Optoelektronik ein beliebtes Material und nimmt dort den Stellenwert von Silizium in der Elektronik ein.

Eine Dotierung mit Magnesium kann eine Verminderung von Eigendefekten im Material bewirken, was zu einer geringeren Photorefraktivität führen kann.

$LiNbO_3$ besitzt bei tiefen Temperaturen eine ferroelektrische Phase, allerdings ist der Phasenübergang in die paraelektrische Phase nicht besonders gut bekannt. Wir haben *ab initio* Molekülardynamik im Rahmen der Dichtefunktionaltheorie verwendet, um einen Einblick in die Dynamik des Phasenübergangs von reinem und Mg dotiertem $LiNbO_3$ zu erhalten.

Dabei ergibt sich in beiden Fällen ein Phasenübergang 2. Ordnung. Zudem erhalten wir durch die Dotierung eine Steigerung der Curie-Temperatur und des Absolutwerts der spontanen Polarisation bei 0 K.

KFM 5.5 Tue 16:00 P

Theoretische Bestimmung der minimalen Energiepfade und Energiebarrieren für die Diffusion von Lithium und Sauerstoff in Lithium-Niobat und Lithium-Tantalat — •Brendan Muscutt und Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschland

Lithium-Niobat (LN) und Lithium-Tantalat (LT) sind von herausragender Bedeutung für aktuelle Forschung und Technik, denn sie besitzen u.a. einzigartige ferroelektrische und elektro-optische Eigenschaften.

Um die Kristalle auf verschiedenste technische Anwendungen optimal anpassen zu können, müssen auch die Stabilität bzw. die Dynamik von Defekten und möglichen Defektstrukturen im Detail verstanden werden.

In unserer Arbeit wurden LN- und LT-Kristalle mit Lithium- und Sauerstoff-Leerstellen simuliert. Auf Basis der Dichtefunktionaltheorie und mit Hilfe der *climbing image nudged elastic band method* wurden dann die Energiebarrieren und minimalen Energiepfade für die Lithium- und Sauerstoff-Leerstellendiffusion *ab initio* berechnet.

Die Ergebnisse lassen in beiden Stoffen auf eine hohe Dynamik der Lithium-Leerstellen bei Temperaturen ab etwa 200 Grad Celsius schließen. Die Sauerstoff-Diffusion findet laut Berechnungen dagegen bereits bei Raumtemperatur statt.

Die Erkenntnisse können bei der Modellierung von Defektstrukturen in LN und LT sowie zur Deutung von entsprechenden Transport-Messungen genutzt werden.

KFM 5.6 Tue 16:00 P

Defect physics in $LiTaO_3$ — •Mike Nico Pionteck, Jonas Fey, and Simone Sanna — Institut 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 5.7 Tue 16:00 P

Vibrational properties of strained $LiNbO_3$ and $LiTaO_3$ crys-

tals — •Mike Nico Piontеck and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

The investigation of Raman frequencies is a widely used non-destructive way to characterize crystalline solids and nanostructures. X-ray diffraction measurements have shown that domain walls in $LiNbO_3$ and $LiTaO_3$ behave like compressed bulk material [1]. Hence, knowledge of the dependence of Raman frequencies on uniaxial strain can help, i.a., to characterize domain walls in $LiNbO_3$ and $LiTaO_3$ crystals.

In our work, we model the vibrational properties of $LiNbO_3$ and $LiTaO_3$ crystals from first principles as a function of compressive and tensile strain in x-, y- and z-direction. The calculations show a roughly linear dependence of the phonon frequencies on the applied strain, which is similar for $LiNbO_3$ and $LiTaO_3$ crystals. The frequencies increase linearly under compressive strain. On the other hand, they decrease linearly under tensile strain. In particular, we observe a strong dependence on strain in x- and y-direction for the E TO_5 and TO_6 modes which can be thus exploited as markers of the strain. While E modes of unstrained $LiNbO_3$ and $LiTaO_3$ crystals are degenerate [2], we predict non-degenerate E modes under strain, due to the breaking of rotational symmetry by strain in x- and y-direction. [1] M. Rüsing et al., Phys. Rev. Mat. **2**, 103801 (2018). [2] S. Sanna et al., Phys. Rev. B **91**, 224302 (2015).

KFM 5.8 Tue 16:00 P

Light-induced transient absorption of lithium niobate as a function of temperature and composition — •Mira Hesselink, Simon Messerschmidt, Laura Vittadello, and Mirco Imlau — Department of Physics, Osnabrueck University, Germany

Small polaron hopping in lithium niobate, $LiNbO_3$ (LN), takes a crucial role in optical process. Its behavior is investigated with a systematic study as a function of temperature, composition and doping. [Messerschmidt, S. *et al. Crystals* **2020**, 10, 109.; Vittadello, L. *et al. Crystals* **2018**, 8, 294.] The number and type of hopping processes are measured by means of light-induced transient absorption spectroscopy. All measurements are performed in a cryostat using a setup with ns-pump and cw-probe. Different sample compositions and dopings (Fe- or Mg-doped LN) go along with different polaron traps inside the crystal. At room temperature, the absorption signals decay in the range of milliseconds, while at lower T the processes are slowed down extensively. The decay rate of the light-induced absorption in Mg:LN appears Arrhenius temperature dependent in range 200K - 120K but this dependence weakens and becomes non-Arrhenius as T is lowered. For the Fe:LN, it is observed that different temperatures lead to different hopping processes by measuring the activation energy. Moreover, the experimental results are in good coincidence with numerical and analytical models based on the Holstein theory. At elevated T ionic diffusion is expected to play a big role and the influence on polaronic charge transport is to be investigated in a next step. Financial support by the DFG (IM3/12-1, FOR 5044) is gratefully acknowledged.

KFM 5.9 Tue 16:00 P

In-vivo tracking of potassium niobate nanoparticles by means of the TIGER microscope — •Laura Vittadello[1], Jan Klenen[1], Karsten Koempe[2], and Mirco Imlau[1] — [1]Department of Physics, Osnabrueck University, Germany — [2]Department of Biology/Chemistry, Osnabrueck University

In recent year, remarkable progress in the area of in-vivo harmonic nanoparticle (HNPs)-based nonlinear optical (NLO) microscopy has been reported. From one side the NLO microscopy has emerged as a successful tool within the bio-medical research field enabling the imaging of intact living organisms. From the other side, polar ferroelectric HNPs have been identified as a good marker candidate in such type of technique for their high nonlinear optical coefficients. Despite of this success, realtime in-vivo tracking based on HNPs has not been exploited so far, mainly because of a lack of an appropriate microscopy tool, i.e. a nonlinear optical widefield microscope. We realised this by means of a regeneratively amplified fs-laser coupled to an inverted microscope creating an easy alignable and reproducible Tunable hIGh Energy (TIGER) widefield microscope [Vittadello *et al.* Opt. Mater. Express 11, 1953-1969 (2021)]. This new approach is successfully applied for HNPs tracking in a area up to $1.5\,\mathrm{x}\,1.5\,\mathrm{mm}^2$ in the blood flow of the heart system of a *Drosophila* larvae, a powerful platform to study social relevant diseases, such as congenital heart defects in human beings. The goal is to access the blood circulation in the heart of a larve, a quantity directly linked to the presence of cardiac disease. Financial support (DFG INST 190/165-1) is gratefully acknowledged.

KFM 5.10 Tue 16:00 P

Einsichten in den Phasenübergang von LiNbO3 und LiTaO3 — •Nils André Schäfer und Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschland

Lithiumniobat (LiNbO3, LN) sowie Lithiumtantalat (LiTaO3, LT) sind ferroelektrische Kristalle, die unter anderem in der integrierten Optik oft eingesetzt werden.

Niob und Tantal kommen in der gleichen Nebengruppe vor und sind chemisch sehr ähnlich. Dementsprechend kristallisieren LN und LT in derselben Struktur, sowohl in der ferroelektrischen Phase (mit Raumgruppe R3c) als auch in der paraelektrischen Phase (mit Raumgruppe R-3c). Dennoch weisen diese Stoffe eine um 500 K voneinander abweichende Curie-Temperatur auf.

Der Phasenübergang von der ferroelektrischen in die paraelektrische Phase beider Stoffe ist bisher noch nicht gut verstanden und daher ist der Ursprung dieser überraschend großen Diskrepanz nicht geklärt. Um Ähnlichkeiten und Unterschiede beider Phasenübergänge zu untersuchen, haben wir *ab initio* Molekulardynamik Simulationen im Rahmen der Dichtefunktionaltheorie durchgeführt. Unsere Rechnungen zeigen, dass, obwohl die Mechanismen der Phasenübergänge ähnlich sind, die Temperaturbereiche in denen sie stattfinden sehr voneinander abweichen.

KFM 5.11 Tue 16:00 P

Comparative evaluation of polar oxide $LiTaO_3$ and $LiNbO_3$ by means of ultrafast transient absorption and luminescence spectroscopy — •Anton Pfannstiel, Andreas Krampf, and Mirco Imlau — Univ. of Osnabrück, School of Physics, Germany

The two model systems $LiNbO_3$ (LN) and $LiTaO_3$ (LT) are commonly assumed to show equivalent (nonlinear) optical and electrical response and that the possibility to generate self-localized quasiparticles, such as polarons and self-trapped excitons exists in both systems. The latter are thoroughly studied in LN however, for LT there is nearly no information available in literature so far. We have adressed this topic by a systematic study on pulse induced transient absorption and luminescence of LN and LT [A Krampf *et al* 2021 *New J. Phys.* 23 033016].

As a result, a qualitatively similar behavior is found that can be attributed to the presence of Nb_{Li}^{4+} and Ta_{Li}^{4+} polarons as-well-as to the formation of excitonic states localized at Nb-O-octahedra. But, a more closer inspection of the data set reveals significant differences in the temporal behavior. In particular, specific time constants are found for short- and long term relaxation.

Discussion of the results is based on the individual crystallographic characteristics, defects, optical features, but also in conjuncture with *ab-initio* modeling results for carrier self-localization in both systems. A conclusion for the ultrafast optical response in $LiNb_xTa_{1-x}O_3$ mixed crystals is deduced. Financial support by the DFG (IM 37/12-1, FOR5044, INST FUGG) is gratefully acknowledged.

KFM 5.12 Tue 16:00 P

High pressure and temperature X-ray emission and diffraction studies of iron containing minerals at the European XFEL — •Johannes Kaa[1,2], Christian Sternemann[2], Christian Albers[2], Karen Appel[1], Valerio Cerantola[1], Mirko Elbers[2], Lélia Libon[3], Mikako Makita[1], Thomas Preston[1], Sylvain Petitgirard[4], Christoph Sahle[5], Georg Spiekermann[3,4], Christian Plückthun[1], Vladimir Roddatis[6], Metin Tolan[2], Max Wilke[3], Ulf Zastrau[1], and Zuzana Konopkova[1] — [1]European X-ray Free-Electron Laser Facility GmbH, Holzkoppel 4, 22869 Schenefeld, Germany — [2]TU Dortmund Fakultät Physik DELTA, Maria-Goeppert-Mayer-Straße 2, 44227 Dortmund, Germany — [3]University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — [4]ETH Zürich, Rämistrasse 101, 8092 Zürich, Switzerland — [5]European Synchrotron Radiation Facility ESRF, 71 Avenue des Martyrs, 38000 Grenoble, France — [6]Geoforschungszentrum Telegrafenberg, 14473 Potsdam, Potsdam, Germany

Data on the spin state of iron bearing minerals are scarce at high temperatures and pressures found in the deep Earth's interior, due to limitations of the commonly used techniques to heat and probe the spin state in situ. To overcome these limitations, we conducted an experiment with a different approach. We used the unique properties of a pulsed and highly brilliant XFEL beam that allowed us to heat samples contained in a DAC via X-ray heating, while measuring X-ray emission and X-ray diffraction on $FeCO_3$ pressurized within a diamond

anvil cell at the HED instrument at the Eu-XFEL.

KFM 5.13 Tue 16:00 P

X-ray emission scanning imaging setup to study electronic structure of iron bearing compounds in-situ at conditions of the Earth's mantle — •Christian Albers[1], Georg Spiekermann[2], Lélia Libon[3], Robin Sakrowski[1], Max Wilke[3], Johannes Kaa[4], Nicola Thiering[1], Hlynur Gretarrson[5], Martin Sundermann[5], Metin Tolan[1], and Christian Sternemann[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Dortmund, Germany — [2]Institut für Geochemie und Petrologie, ETH Zürich — [3]Institut für Geowissenschaften, Universität Potsdam, Potsdam, Germany — [4]HED Group, European XFEL GmbH, Hamburg, Germany — [5]Deutschen-Elektronen-Synchrotron DESY, Hamburg, Germany

The determination of the electronic structure in iron-bearing compounds under high pressure and high temperature (HPHT) conditions is of crucial importance for the understanding of the Earth's interior and planetary matter.
We present a setup to investigate the electronic structure of iron-bearing compounds *in-situ* at HPHT conditions using X-ray emission spectroscopy (XES) and show first results for tetracarbonate phases emerged from laser heated siderite ($FeCO_3$) at about 80 GPa and 3000 K. Information on the spin state are obtained by *in-situ* XES of the iron's Kβ-emission. A dedicated sample preparation together with highly intense synchrotron radiation shortens the duration of the measurements to an extend that *in-situ* XES, including valence-to-core XES, as well as *in-situ* spin state imaging becomes feasible.

KFM 5.14 Tue 16:00 P

Investigation of the Electronic Structure of Iron in Bridgmanite at Deep Mantle Pressure Conditions by (Resonant) X-ray Emission Spectroscopy — •Robin Sakrowski[1], Georg Spiekermann[2], Christian Albers[1], Nicola Thiering[1], Lélia Libon[3], Hlynur Gretarsson[4], Martin Sundermann[4], Jean-Pascal Rueff[5], James Ablett[5], Metin Tolan[1], Max Wilke[3], and Christian Sternemann[1] — [1]Faculty of Physics/DELTA, TU Dortmund University — [2]Institute of Geochemistry and Petrology, ETH Zurich — [3]Institute of Geosciences, University of Potsdam — [4]Deutsches-Elektronen-Synchrotron DESY — [5]Synchrotron SOLEIL

We study the controversially discussed iron spin state in pressurized ferrous (Fe^{2+}) and ferric (Fe^{3+}) bridgmanite, as well as coordination state and oxidation state. For that, we use a combination of novel approaches like in situ resonant X-ray emission (RXES) at the iron K-pre-edge region, iron Kβ- and valence-to-core (vtc) X-ray emission spectroscopy (XES). We evaluate the Fe K pre-edge feature position and intensity from Kα HERFD XANES. Consequently, these methods help to further constrain the observed gradual (ferrous) or sharp (ferric) change in spin state, local coordination and oxidation state of iron in ferrous- (up to 140 GPa) and ferric- (up to 75 GPa) bridgmanite, aiming to solve the controversy on the iron's spin state in bridgmanite.

KFM 5.15 Tue 16:00 P

Spatially-resolved lithium and electrolyte distribution in cylindrical 18650-type lithium-ion batteries — •Dominik Petz[1,2], Anatoliy Senyshyn[2], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Garching, Deutschland — [2]Heinz Maier-Leibnitz Zentrum, Garching, Deutschland

Extensive cycling of lithium-ion batteries leads to a partial loss of their capacity due to various side effects like formation of the solid-electrolyte-interphase (SEI), loss of active lithium etc. Typical profiles of side reactions, instantaneous temperature and current density display non-uniform distributions throughout the volume, which leads to a stabilization of intrinsic heterogeneous state in the Li-ion battery. The loss of active lithium is typically correlated with the formation of SEI during cycling, whereas the quantitative role of electrolyte in the cell operation and cell fatigue remains not fully quantified yet.

In the current study we report an attempt of non-destructive quantification of lithium and electrolyte, their spatial distribution throughout the cell and concentration changes vs. cell fatigue. Combined experimental studies including electrochemistry, X-ray computed tomography, and neutron diffraction are applied for 18650-type cylinder cell with NCA|C chemistry. High-resolution neutron diffraction independently reveals a direct volume-averaged correlation between losses of active lithium in the graphite anode and these of the liquid electrolyte. The 3D lithium distribution is mapped by spatially resolved neutron powder diffraction, displaying the non-trivial character of active lithium and electrolyte losses.

KFM 5.16 Tue 16:00 P

Polar oxides: Electrical conductivity of LiNb1-xTaxO3 solid solutions from 400 to 800 °C in air — •Ahsanul Kabir, Vanik Sargsyan, Yuriy Suhak, Stepan Hurskyy, and Holger Fritze — Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Am Stollen 19 B, 38640 Goslar, Germany

The electrical conductivity of lithium niobate-lithium tantalate (LNT, LiNb0.5Ta0.5O3) solid solutions is studied in air at temperatures ranging from 400 to 800 °C. The results were compared with lithium niobate (LN) and lithium tantalate (LT) reference samples grown by the Czochralski method, received from the Institute of Microelectronics Technology and High Purity Materials (IMT), Russia, and Precision Micro-Optics (PMO), USA, respectively. Electrical conductivity was measured by impedance spectroscopy in the frequency range of 1 MHz-1 Hz. Over the studied temperature range, LNT sample displays similar electrical conductivity to LN/LT (IMT), e.g. with a value of 2.9*10-4 S/m at 600 °C. In contrast, LN/LT (PMO) compounds illustrate conductivity that is nearly 2 times higher than that of their counterparts. As noticed, the conductivity follows an Arrhenius relation, uncovering a single thermally activated process. The activation energy ranges from 1.20-1.25 eV which is a typical value for the ionic migration in the lithium niobate family and is governed by mobile lithium (Li) vacancies. This result is consistent with theoretical modeling, which predicts the spontaneous formation of Li vacancies in the band gap for a wide range of Fermi energy values. The research is funded by the German Research Foundation and done within the research unit 5044.

KFM 5.17 Tue 16:00 P

Tracking ferroelectric domain formation during epitaxial growth of $PbTiO_3$ films — •Martin F. Sarott, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zurich, Switzerland

The pronounced impact of growth conditions on the formation of domains in ferroelectric thin films obstructs the effective design of devices based on ferroelectrics that require controlled polarization states. Here, we overcome this notorious difficulty by tracking in-situ, during growth, the ferroelectric domain formation in ultrathin films of the tetragonal ferroelectric model system $PbTiO_3$. By combining in-situ optical second harmonic generation (ISHG) with post-growth piezoresponse force microscopy and ex-situ SHG imaging, we identify the thickness threshold for the epitaxial strain-driven partial conversion of out-of-plane polarized c-domains into in-plane oriented a-domains during the deposition. Furthermore, we find that in the strongly compressive regime the formation of a-domains is triggered during the early stages of growth, which favors a remarkable randomization in the distribution of a- and c-domains upon further deposition. This extraordinary heterogeneity is reminiscent of the domain distribution at the morphotropic phase boundary in technologically relevant PZT and thus highlights the significance of control over the c-to-a domain interconversion for applications.

KFM 5.18 Tue 16:00 P

Impact of domain walls on ferroelectric switching: an ab initio based MD study on orthorhombic $BaTiO_3$ — •Yijing Yang, Ruben Khachaturyan, and Anna Grünebohm — ICAMS, RUB, Bochum, Germany

Ferroelectric switching by domain walls motion is very important for many applications. In this work, we explore the coupling between the external electric field and domain walls in the so far rarely explored orthorhombic phase of $BaTiO_3$. Therefore, we employ molecular dynamics simulations using the effective Hamiltonian approach [1, 2] to study the electric field induced domain wall motion and the local polarization on the walls. In particular, we find polarization vortices on 180° nonelastic domain wall which can minimize the charge density.

[1] A. Grünebohm and M. Madhura, Phys. Rev. Mater. 4, 114417 (2020)

[2] T. Nishimatsu et al. Phys. Rev. B 82.13, 134106 (2010)

KFM 5.19 Tue 16:00 P

Second-harmonic microscopy in optically confining nanostructures — •Zeeshan Hussain Amber[1], Benjamin Kirbus[1], Michael Rüsing[1], and Lukas M Eng[1,2] — [1]Technische Universität Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062, Dresden, Germany

Second-harmonic (SH) microscopy is a very power tool for investigating material properties and noninvasively visualising domains and domain walls in ferroelectic materials [1,2]. Contrary to the conventional assumption when working with a confining structure such as a thin film, the co-propagating phase matched SH signal may also be detected in back-reflection. Interference effects further affect the SH response. Therefore understanding the effects of geometrical confinement is necessary.

We performed SH experiments on wedge-shaped samples of 5% Mg-doped congruent Lithium tantalate, un-polled & Periodically polled Lithium niobate and compared them with full-vectorial numerical calculations of the SH process [1,3]. We found that the coherent interaction length obtained from the back-reflected SH signal is that of co-propagating phase matched signal. The excellent agreement between the simulated and experimental data confirms that co-propagating signal is detected in back-reflection geometry.

[1] M. Ruesing et al., J. Appl. Phys. 126,114105 (2019).
[2] S. Cherifi-Hertel et al., Nat. commun 8,15768 (2017).
[3] D. Sandkuijl et al., J. Opt. Soc. Amer. B 30, 382 (2013)

KFM 5.20 Tue 16:00 P

Colossal dielectric constant in h-$ErMnO_3$ — •Lima Zhou[1], Lukas Puntigam[1], Markus Altthaler[1], Dennis Meier[2], István Kézsmárki[1], Donald M. Evans[1], and Stephan Krohns[1] — [1]University of Augsburg, 86159, Augsburg, Germany — [2]NTNU Norwegian University of Science and Technology, 7034, Trondheim, Norway

Ferroelectric domain walls can be in some specific cases created, erased and rewritten making them interesting as functional nanoscale object in electronics. In the improper ferroelectric system h-$ErMnO_3$ memristive switching and rectification of charged domain walls has been shown. Here, we explore if also the more insulating domain walls provide functionality in terms of an internal barrier layer capacitance leading to colossal dielectric constants. A recent work [1] already demonstrated via bulk dielectric spectroscopy that insulating domain walls are responsible for a dielectric relaxation-like feature. Our approach is to reveal the dielectric properties for a h-$ErMnO_3$ single crystal before and after a distinct heat treatment leading to an increase in domain size by a factor of 10. Interestingly, the dielectric constant most likely ascribed to the internal barrier layers increases also by a factor of 10 according to the decrease of the volume fraction of the insulating domain walls (overall decrease in insulating barrier thickness giving rise to higher capacitance). With this work we provide a strategy of designing colossal dielectric constant based on internal insulating domain wall barriers. [1] Puntigam et al., *Journal of Applied Physics* **129**, 074101 (Feb. 2021)

KFM 5.21 Tue 16:00 P

Quantitative mapping of nanotwin variants and elastic energy in the bulk — •Jan Schultheiss[1], Lukas Porz[2], Lalitha Kodumudi Venkataraman[2], Marion Höfling[2], Can Yildirim[3], Phil Cook[3], Carsten Detlefs[3], Semen Gorfman[4], Jürgen Rödel[2], and Hugh Simons[5] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Technical University of Darmstadt, Darmstadt, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Tel Aviv University, Tel Aviv, Israel — [5]Technical University of Denmark, Lyngby, Denmark

Most state-of-the-art high-resolution imaging techniques are limited to probing the sample surface. This is a particular drawback for the characterization of twinned materials as the strain state changes from biaxial at the surface to triaxial in the bulk, dramatically influencing the functional properties. Here, we demonstrate mapping of nanotwin variants highly localized in the bulk utilizing the full reciprocal space intensity distributions obtained from Dark-Field X-Ray micorscopy. We demonstrate our method for a high-performance polycrystalline ferroelectric/ferroelastic (Ba,Ca)(Zr,Ti)O_3 model system whose excellent piezoelectric properties originate from domain sizes of 10-100 nm. We find that the density of twin variants inside the grain is 30% smaller compared to the density in the vicinity of the grain boundary, following the trend of the elastic energy. The obtained elasto-morphological correlations are crucial for many twinned materials, ranging from complex oxides to martensitic materials or high entropy alloys.

KFM 5.22 Tue 16:00 P

X-ray emission spectroscopy setup at beamline BL9 of DELTA — •Nicola Thiering[1], Eric Schneider[1], Kevin Lehninger[1], Christian Albers[1], Florian Otte[1,2], Johannes Kaa[1,2], Michael Paulus[1], Christian Sternemann[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund, Germany — [2]European XFEL, Holzkoppel 4, D-22869 Schenefeld, Germany

Beamline BL9 is a multi-purpose X-ray scattering and spectroscopy beamline at the synchrotron radiation facility DELTA located at the TU Dortmund, Dortmund, Germany. The beamline is served by a new superconducting wiggler which provides X-rays in the energy range between 5 and 30 keV. Recently, a setup for X-ray emission spectroscopy was implemented exploiting a von Hamos type spectrometer by combination of cylindrically bent analyzers with a Pilatus 100k area detector. This setup allows to study electronic valence and core hole excitations of low Z elements as well as transition metals. The current experimental setup will be presented along with selected samples of typical applications and the first experimental results.

KFM 5.23 Tue 16:00 P

Nested mirror systems for neutron extraction, transport and focusing — •Christoph Herb[1], Oliver Zimmer[2], Robert Georgii[1,3], and Peter Böni[1] — [1]Physics Department E21, Technical University Munich, 85748 Garching, Germany — [2]Institute Laue-Langevin, F-38042 Grenoble, France — [3]Heinz Maier-Leibnitz Zentrum, Technical University Munich, 85748 Garching, Germnay

The investigation of small samples by neutron scattering is usually very time consuming due to the low neutron flux of contemporary sources and small signals from the sample. Elliptic neutron guides are used to transport neutrons over large distances to make room for additional beamlines and for improving the signal-to-noise ratio by focusing the available neutrons onto the sample. However, elliptic guides do not image objects properly due to coma aberrations. We propose using nested arrays of short elliptic mirrors to reduce the coma aberrations.

We report on the investigation of a nested mirror optic at the MIRA beamline. The key properties of the optic are a large brilliance transfer of approximately 72% and the possibility of adjusting the beam size and the divergence of the neutron beam at the sample position by apertures placed before the nested mirror optic. Therefore, no beam shaping devices are required close to the sample position, thus reducing the background.

Nested mirrors will also be particularly useful for the efficient extraction of neutrons from small, highly brilliant moderators such as at the ESS, since common illumination losses associated with using neutron guides are mitigated.

KFM 5.24 Tue 16:00 P

Intrinsic electronic structure of TiCoSb half-heusler single crystals by ARPES — •Federico Serrano-Sanchez[1], Mengyu Yao[1], Suchitra Prasad[1], Andrei Gloskovskii[2], Alexander Fedorov[3], Gudrun Auffermann[1], Ulrich Burkhardt[1], Gerhard Fecher[1], Claudia Felser[1], Yu Pan[1], and Chenguang Fu[1] — [1]MPI-CPfS, Dresden, Germany — [2]DESY, Hamburg, Germany — [3]HZB fur Materialien und Energie, Berlin, Germany

In half-Heulser thermoelectric TiCoSb, defects yield elusive intrinsic properties and a wide range of properties reported in the literature[1-3]. To tackle these inconsistencies, single crystals of TiCoSb have been grown and their crystallographic and electronic properties characterized. The crystals display an almost perfect stoichiometry, while XRD display the half-Heusler $F\bar{4}3m$ structure only. Electrical resistivity shows a metallic behaviour due to the intrinsic p-type nature of the crystals, while the temperature evolution of the conductivity indicates the presence of point defects. Nevertheless, no in-gaps states in the valence band top are detected by HAXPES, suggesting the absence of interstitial defects. ARPES displays a diffusive surface state above the VBM and the band convergence at the L and Γ band maxima points, which is compared to previous theoretical calculations and gives a further hint on the excellent electronic performance of this family of materials.

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