DF 11: Poster

Time: Wednesday 18:00–20:00 Location: Poster E

DF 11.1 Wed 18:00 Poster E

Excitation and relaxation dynamics of electrons in dielectrics irradiated by intense, ultrashort laser pulses — •Nils Brouwer and Bärbel Rethfeld — Fachbereich Physik und Landesforschungszentrum Optimas, TU Kaiserslautern

Ultrashort laser pulses of high intensity are of increasing importance in material processing and fundamental research. In order to control or avoid laser damage to transparent dielectrics, a proper understanding of the involved microscopic processes is necessary.

When a transparent dielectric is irradiated by an intense laser pulse, electrons are exited to the conduction band first by multiphoton or tunnel ionization. These electrons than absorb more laser energy and can then ionize further electrons by impact ionization. To determine material damage, it is necessary to investigate the coupling of the electrons to the lattice.

We model the electron and phonon non-equilibrium dynamics of laser excited dielectrics using Boltzmann collision integrals to calculate the respective distribution functions[1,2]. We analyse the intra- and interband relaxation dynamics and we calculate the transient non-equilibrium electron-phonon energy transfer rate during intense laser irradiation and compare our results with rates of thermalized electron systems.

[1] A. Kaiser, B. Rethfeld, M. Vicanek, G. Simon, *Phys. Rev. B* **61**, 11437 (2000)
[2] N. Brouwer and B. Rethfeld, *JOSA B* **31**, C28 (2014)

DF 11.2 Wed 18:00 Poster E

Plasmon-enhanced biosensing with polymeric whispering-gallery-mode resonators — •Carolin Klusmann[1], Sarah Krämmer[1], Steffen A. Schmid[1], Tobias Siegle[1], Carsten Rockstuhl[2] und Heinz Kalt[1] — [1]Institute of Applied Physics (KIT), Wolfgang-Gaede-Straße 1, 76131 Karlsruhe — [2]Institute of Theoretical Solid State State Physics (KIT), Wolfgang-Gaede-Straße 1, 76131 Karlsruhe

Polymeric whispering gallery mode (WGM) microresonators are very promising candidates for the label-free detection of biomolecules. They derive their unprecedented sensitivity from very high quality factors in combination with small modal volumes. By exciting plasmonic resonances in metal nanoparticles immobilized within the evanescent field of the WGMs their sensitivity can be enhanced even further. The excitation of plasmonic resonances leads to the formation of hybrid photonic-plasmonic modes within the resonator and greatly elevated field intensities at the nanoparticle site. We present simulations and first experimental results on how a sensitivity enhancement can be achieved by carefully choosing the plasmonic NP's material, size, shape and concentration.

DF 11.3 Wed 18:00 Poster E

Effect of different excitation and collection geometries on the lasing threshold of PM597-doped WGM micro disk cavities — •Tobias Siegle, Marielle Bonenberger, Sarah Krämmer, Carolin Klusmann, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

The rotational symmetry and also the high quality factor of whispering gallery mode (WGM) micro resonators impedes free-space coupling of light to WGM cavities. Lasing modes in dye (pyrromethene 597)-doped WGM micro disks are excited through the free-space excitation of the active material within the cavity (fluorescence coupling). A more efficient excitation method is coupling to the evanescent field of a tapered fiber. Free-space and tapered fiber excitation geometries are compared regarding their effect on the lasing threshold: The localization of the pump energy by fiber excitation leads to a reduction of the lasing threshold by a factor of approximately one hundred as here only the WGM rim region of the cavity is excited.
In the free-space geometry light extraction from the cavity typically relies on impurities scattering the light towards the detector. Using the same tapered fiber for excitation and collection of light leads to a significant increase of the collection efficiency compared to the free-space geometry and does not depend on impurities.

DF 11.4 Wed 18:00 Poster E

Studying the interplay of nanoparticles and dielectric whispering gallery mode resonators using a generalized Mie theory — •Steffen A. Schmid[1,2], Radius N. S. Suryadharma.[1], Martin Fruhnert[1], Carolin Klusmann[2], Heinz Kalt[2], and Carsten Rockstuhl[1] — [1]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Institute of Applied Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

The high quality factors and small modal volumes of whispering gallery mode (WGM) resonators promote their use in sensing applications. Coupling metallic nanoparticles to WGM resonators has recently been suggested to further improve their sensitivity. However, the underlying physical mechanism is currently not fully understood. To answer this question, we consider here a spherically shaped resonator coupled to metallic nanoparticles and use the generalized Mie theory to study all related effects by such quasi-analytical method.

Specifically, we investigate the effect of dielectric and metallic nanospheres on the spectral position and the quality factor of the WGM resonances. To this end, we model the WGM resonator as a large dielectric sphere. Metallic nanoparticles are adjacent to the WGM resonator to improve the sensitivity. The presence of molecules is taken into account by considering them as dielectric nanospheres. Hereby, we obtain a deeper understanding of the physical properties of such a system and deduce engineering guidelines to enhance the sensitivity of WGM resonator based sensors.

DF 11.5 Wed 18:00 Poster E

Bio-inspired hierarchical structures for enhanced light harvesting in solar cells — •Raphael Schmager[1,2], Ruben Hünig[2], Guillaume Gomard[2,3], Benjamin Fritz[1,2], Gerald Göring[1], Hendrik Hölscher[3], Heinz Kalt[1], Michael Powalla[2,4], and Michael Hetterich[1] — [1]Institute of Applied Physics, KIT, Karlsruhe, Germany — [2]Light Technology Institute, KIT, Karlsruhe, Germany — [3]Institute of Microstructure Technology, KIT, Eggenstein-Leopoldshafen, Germany — [4]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Stuttgart, Germany

Leaves and petals are shaped to fulfill multiple functionalities, in particular their interaction with light. In this context the surface morphology of rose petals has been reported to be beneficial for producing highly saturated colors, thus increasing the pollination success of those flowers. This morphology consists of disordered micro-cones adorned by nano-scale wrinkles. While previous studies have demonstrated that the larger features act as micro-lenses which focus the incoming light, the specific role and impact of the nano-structures on the global optical properties require further investigations. In our contribution, the topography of this hierarchical surface has first been probed by SEM and AFM, and then modeled in an optical software to study the anti-reflection and scattering properties of the nano-structures in the wave optics regime. We show that understanding the interplay between those micro-and nano photonic structures will enable the design of efficient light harvesting surfaces for solar cells since the latter are also targeting broadband and omnidirectional operation conditions.

DF 11.6 Wed 18:00 Poster E

Whispering gallery mode resonators with varying diameter and thickness for enhanced sensitivity — •Sanaz Rastjoo, Sarah Krämmer, Tobias Siegle, Carolin Klusmann, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

In this work we present our latest results on active polymeric whispering gallery mode resonators. The resonators are dye (pyrromethene 597)-doped PMMA (poly (methyl methacrylate)) disks, exhibiting lasing emission when optically pumped. One of the crucial parameters for sensing is the so-called "bulk refractive index sensitivity" (BRIS). Theory predicts that the sensitivity of the resonators increases with decreasing radius, however the quality factor and thus the lasing threshold are affected when the resonators are operated in an aqueous environment. We fabricated resonators with different radii from 25 μm down to 7.5 μm and performed measurements on the lasing threshold and the BRIS. The theoretical expectations could be confirmed by experiments: Resonators with smaller radii showed higher sensitivities but also higher lasing thresholds. Taking both aspects into account resonators with 10 μm radius show sensitivities up to 46.9 nm/RIU

while still showing comparably low thresholds. Another approach to enhance the sensitivity of disk resonators is by variation of the disk thickness. We investigated this aspect in our work to further optimize the geometry of the disk resonators for sensing applications.

DF 11.7 Wed 18:00 Poster E

Dye-dopped Electrohydrodynamic co-jetted polymeric fibers for optical resonators — •Fabrice Laye[1,2], Sarah Krämmer[2], Alejandro Castillo[1], Joerg Lahann[1], and Heinz Kalt[2] — [1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Applied Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Electrojetting is a low cost high throughput method with a very large material flexibility. Furthermore, electrohydrodynamic co-jetted (EHDCJ) fibers expand the possibilities of structure and material variation of standard procedures[1]. The high surface to volume ratio of a jetted fiber makes them excellent competitors for sensing or filtering applications. In photonic applications, the refractive index is a key parameter; but stiffness, diameter and compatibility with the media also play an important role. Fibers with dyes or fluorescent nanoparticles have been shown as light sources and random polymer fiber cavities have been shown.[2] The possibility of developing new photonic sensors, with very narrow spectral resolution, taking advantage of physical and mechanical properties of complex co-jetted fibers is of great interest. We present our advances in the fabrication of complex polymer such as multi-polymer and multi-dye fiber resonators with this technique.

[1] S. Bhaskar and J. Lahann, Journal of the American Chemical Society 131 (19), 6650 (2009).

[2] S. Krammer, C. Vannahme, C. L. C. Smith, T. Grossmann, M. Jenne, S. Schierle, L. Jorgensen, I. S. Chronakis, A. Kristensen, and H. Kalt, Advanced Materials 26 (48), 8096 (2014).

DF 11.8 Wed 18:00 Poster E

Electrical characterization of domain reversal in thin film lithium niobate — •Kanivar Türk, Michael Rüsing, Peter Mackwitz, Gerhard Berth, and Artur Zrenner — Department Physik, Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany

Lithium niobate is one of the foremost studied materials for applications in integrated, nonlinear optics, such as sum and difference frequency generation or parametric down conversion. The efficiency of these processes can be greatly enhanced by fabricating periodically poled domain structures. Recently, lithium niobate thin films (tf-LN) on insulator have gained great interest, e.g. due to the possibility for strong confinements of optical modes. So far, a lot of devices have been demonstrated in this material system, such as photonic wires, waveguides or ring resonators [1].

Within this work the domain reversal characteristics of tf-LN will be examined. Therefore, in this study a temperature dependent electrical characterization is realized to study the electrical response of domain reversal in tf-LN. The results are compared with previous work on bulk crystal lithium niobate, where it has been found that heat or UV does influence the coercive field and poling characteristics [2].

[1] G. Poberaj, et. al., Laser Photonics Rev. 6, (2012) 488

[2] H. Steigerwald et. al., Appl. Phys. B 101, (2010) 535

DF 11.9 Wed 18:00 Poster E

Growth of epitaxial Ba_2SiO_4 on Si(100) — •Min Huang, Julian Koch, Shariful Islam, and Herbert Pfnür — Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

In search of an alternative gate oxide Barium silicate thin films on Si(100) were investigated. In order to specify the stoichiometry and band gap of these oxides we used X-ray Photoelectron Spectroscopy (XPS) and Electron Energy Loss Spectroscopy (EELS) respectively. The morphology was controlled by Spot Profile Analysis-Low Energy Electron Diffraction (SPA-LEED). To further investigate the crystalline growth, crystal orientation and thickness High Resolution Transmission Electron Microscopy (HRTEM) was used.

In previous work in our group, we investigated Ba_2SiO_4, which was grown by depositing a crystalline BaO_2 layer on Si(100) and heating the sample to 650 °C leading to a diffusion of Si into the BaO_2 layer [1]. The silicate was found to be a very promising candidate as an alternative gate dielectric. It has a high temperature stability up to desorption (approx. 720 °C), a dielectric constant of 20, a band offset of >2eV and a very low hysteresis of <0.5 mV. But due to the growth process the interface was quite rough and the silicate layer was not completely crystalline as confirmed by HRTEM. Thus, the leakage current was comparatively high (0.1 A/cm^2 at 1V). Here we present new results, where we avoid diffusion of Si by co-deposition of Ba and Si in an oxygen atmosphere and show that crystallinity as well as leakage currents were improved.

[1] Islam, S., Ph.D. thesis, Leibniz Universität Hannover (2015)

DF 11.10 Wed 18:00 Poster E

Numerische Simulation von STO mittels Microstrip Geometrie — •Max Pargmann, Daniel Niermann und Joachim Hemberger — 2. Physikalisches Institut Zuelpicherstrasse 77

Dielektrische-Spektroskopie im Mikrowellenbereich erfordert im Allgemeinen erhöhten Aufwand bezüglich Kalibration der residualen Reflexionsbeiträge von Leitungen, Steckverbindungen und Probenhalter. Ein etabliertes Verfahren ist die Messung in Reflexionsgeometrie ("Corbino" [1]) . In unserer Arbeitsgruppe wurde ein Microstrip-Probenhalter zur breitbandigen Spektroskopie in Transmissionsgeometrie entwickelt. In hochpermeablen Proben können Resonanzen im GHz Bereich auftauchen, welche von der Probengeometrie und der Permitivität abhängen [1]. Ein Ansatz zur Bestimmung der Permitivität ist ein Vergleich von gemessenen und simulierten Resonanzfrequenzen. Mittels der Software CST MICROWAVE STUDIO wurde eine Parameter abhängige Eichkurve zur Umrechnung der Resonanzfrequenz in Probenpermeabilität erstellt. Das Verfahren wurde mittels temperaturabhängigen Messungen (300K>T>2K) am Probenmaterial $SrTiO_3$ im Frequenzbereich 1-20GHz bzw. für ϵ im Bereich 300-15000 getestet.

[1] M.Felger et al. Rev. Sci. Instrum. **84**, 114703 (2013)

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DF 11.11 Wed 18:00 Poster E

Simulation of reaction- and diffusion processes in pores of ultra low k materials using the ReaxFF+ method — •Stephan Pfadenhauer, Oliver Böhm, and Roman Leitsmann — AQcomputare GmbH, Annaberger Str. 240, 09125 Chemnitz

The decreasing feature size of integrated circuits results in a smaller distance between the conduction layers, which is accompanied by an increasing resistance capacitance delay. Therefore, the usage of materials with an ultra low dielectric constant is necessary. However, the application of such ultra low k (ULK) materials is connected to several problems, like the formation of OH-groups after the etch process. This results in moisture uptake and a strongly increasing dielectric constant. To restore the k-value, a post-etch treatment with repair chemicals is recommended. The main problem of using such chemicals are the competing processes of diffusion of the molecules and their reaction with the pore walls. To study the correlation of both processes we have developed a ReaxFF+ parametrization which is able to describe the pore structures, the diffusion of the repair chemicals and their reactions with the hydroxyl groups of the pore walls.

DF 11.12 Wed 18:00 Poster E

Coupling between spin and charge degrees of freedom in multiferroic $DyMnO_3$ from dielectric spectroscopy. — •Markus Schiebl[1], Alexey Shuvaev[1], Anna Pimenov[1], Graeme Eoin Johnstone[1], Uladzislau Dziom[1], Thomas Kain[1], Wilfried Schranz[2], Alexander Mukhin[3], Vsevolod Ivanov[3], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, Vienna, Austria — [3]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia

In rare-earth manganites (RMnO$_3$) a non-collinear long range cycloidal spin order of the Mn-spins is present in the ferroelectric phase. Above the magnetoelectric phase transition temperature a collinear sinusoidally-modulated spin order is proposed. Based on results by magneto-capacitance and by dielectric spectroscopy, we provide an experimental evidence that the magnetoelectric phase transition in $DyMnO_3$ follows an order-disorder scenario and that a coupling between spin and charge degrees of freedom exists well above the magnetoelectric phase transition. These results suggest the interpretation of the paraelectric sinusoidal phase in manganites as a dynamical equilibrium of magnetic cycloids with opposite chiralities. We provide a free-energy model describing the magnetoelectric phase transition of cycloidal magnetoelectric multiferroics. The model is based on the assumption of a double-well potential and it includes the symmetry-allowed terms up to the second order.

DF 11.13 Wed 18:00 Poster E

Magnetoelectric phase diagrams of $GdMn_2O_5$ — •Thomas Kain[1], Hamad S. Bukhari[1,2], Markus Schiebl[1], Alexey Shuvaev[1], Anna Pimenov[1], Graeme Eoin Johnstone[1], Wlad Dziom[1], X. Wang[3], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, TU Wien, A-1040 Vienna, Austria — [2]Department of Physics, Bahauddin Zakariya University, Multan 60800, Pakistan — [3]University of Science and Technology, Beijing, China

We have measured the temperature dependent dielectric constant ε of $GdMn_2O_5$ under applied magnetic field H to map out complete magnetoelectric phase diagrams. The obtained $\varepsilon(H,T)$ phase diagrams show that except for the antiferromagnetic ordering transition at $T_{N1} \sim 40$ K, all other transitions are strongly field dependent relative to the crystallographic axes. The phase diagram for $H \parallel a$ shows a one-to-one correspondence with the tunable polarization induced by 90° rotation of Gd magnetic moment. Our results support the model of two ferroelectric sublattices Mn-Mn and Gd-Mn with strong R-Mn ($4f$-$3d$) interaction for the polarization in RMn_2O_5. Contrary to other members of the RMn_2O_5 family, the ferroelectric transitions ($T_{N2} \sim 31$ K and $T_C \sim 29$ K) are sensitive to the applied field.

DF 11.14 Wed 18:00 Poster E

Fabrication and characterization of epitaxial $BiAlO_3$ thin films — •Johanna Fischer, Cécile Carrétéro, Vincent Garcia, Stéphane Fusil, Agnes Barthélémy, and Manuel Bibes — Unité Mixte de Physique CNRS/Thales, 1 Av. Fresnel, Univ. Paris-Sud, Université Paris-Saclay, 91767 Palaiseau, France

For applications in information technology ferroelectrics with a high critical temperature are desired [1]. $BiAlO_3$ is such a material and may replace the existing, environmentally harmful lead-based composites in the future [2,3]. This study is dedicated to the epitaxial growth of thin films of $BiAlO_3$ on (001)-oriented single crystalline $LaAlO_3$ and $SrTiO_3$ substrates using pulsed laser deposition. We monitor the thin film growth in situ via reflection high energy electron diffraction (RHEED). To improve the crystalline quality a conductive interlayer of $LaNiO_3$, acting also as a bottom electrode, is deposited between the substrate and the $BiAlO_3$ thin film. We characterize the structural properties, thickness as well as interface and surface roughness of our samples using high resolution X-ray diffractometry and reflectometry. The surface topography is determined by atomic force microscopy and the ferroelectric properties by piezoresponse force microscopy.
[1] J.Zylberberg et al., Chem. Mater. **19**, 6385-6390 (2007)
[2] P. Baettig et al., Chem. Mater. **17**, 1376-1380 (2005)
[3] J.Y.Son et al., Appl. Phys. Lett. **92**, 222911 (2008)

DF 11.15 Wed 18:00 Poster E

Spin-phonon coupling in $ACrO_2$ (A=Cu, Ag, Pd) studied by Raman spectroscopy — •Sebastian Elsässer[1], Anna Pimenov[2], and Jean Geurts[1] — [1]Universität Würzburg, Exp.Physik 3, Würzburg, Germany — [2]Institut für Festkörperphysik, TU Wien, Wien, Austria

The magnetic moments of Cr^{3+} ions in the delafossite $ACrO_2$ systems are coordinated in planes of triangular lattices, which leads to geometric frustration of the spins with an incommensurate proper-screw spin arrangement in the ground state. While multiferroic behaviour was shown, the underlying mechanism is still under debate: The incommensurate order rules out conventional magnetostriction, while inverse Dzyaloshinskii-Moriya interaction does not produce a polarization for the proper-screw pattern. A variation of p-d hybridization was proposed to cause the imbalance in charge transfer between the Cr and O ions on different sites, leading to an electric polarization that depends on the modulation vector **Q**. We study the three compounds with A=Cu^+, Ag^+, and Pd^+ with T-dependent Raman spectroscopy down to 6K. As predicted by group theory (space group $R\bar{3}m$), both Raman-active modes with E_g and A_g symmetry are observed. Especially the E_g mode modulates the Cr-O bond, which mediates the exchange between adjacent Cr ions. Below T=100 K, the E_g mode shows a frequency softening which is therefore ascribed to spin-phonon coupling. In clear contrast, the A_g mode shows no such softening. In $CuCrO_2$ at the high-energy side of the E_g mode an unexplained shoulder peak is observed, which at 300 K nearly coincides with this mode.

DF 11.16 Wed 18:00 Poster E

Impact of temperature-dependent local and global ordering in $RMnO_3$ for electromagnons and spin-phonon coupling. — •Sebastian Elsässer[1], Markus Schiebl[2], Alexey Shuvaev[2], Alexander Mukhin[3], Jean Geurts[1], and Andrei Pimenov[2] — [1]Universität Würzburg, Exp.Physik 3, Würzburg, Germany — [2]Institut für Festkörperphysik, TU Wien, Wien, Austria — [3]General Physics Institute of the Russian Academy of Sciences, Moscow, Russia

The perovskite-like rare-earth manganites $RMnO_3$ are among the most widely studied compounds in multiferroics. The inverse Dzyaloshinskii - Moriya (DM) interaction with cycloidal spin ordering is generally accepted as the driving mechanism of magnetically induced ferroelectricity in compounds with e.g. R=Dy^{3+}, Tb^{3+}, $(Eu_x{:}Y_{1-x})^{3+}$, $(Eu_x{:}Ho_{1-x})^{3+}$. This DM coupling leads to the emergence of electromagnons (EM), i.e. electro-active spin waves that can be excited by a.c. electric fields. The magnetic order also induces shifts of specific phonon frequencies due to spin-phonon coupling (SPC). After usual view, the EM should only occur for the ferroelectric state with cycloidal magnetic order at $T < T_{FE} \approx 25$K, and the SPC below $T_N \approx 45$K. However, we observe the EM and SPC already far above T_N. The occurrence of the EM for $T > T_{FE}$ can be explained in terms of cycloids with opposite chirality and T-dependent correlation lengths, which simulate a sinusoidal magnetization pattern for $T_{FE} < T < T_N$, and a disorder-order transition at T_{FE}. Along the same line, the gradual occurrence of SPC already far above T_N can be understood in terms of an onset of locally spin-ordered areas already in this T-range.

DF 11.17 Wed 18:00 Poster E

Tilt engineering of spontaneous magnetisation and polarisation at room temperature in an oxide — •Michael Pitcher, Pranab Mandal, Matthew Dyer, Jonathan Alaria, Pavel Borisov, Hongjun Niu, John Claridge, and Matthew Rosseinsky — Department of Chemistry, University of Liverpool, Liverpool, UK

Combining spontaneous, switchable polarisation and magnetisation into a single phase multiferroic material is a major challenge in materials chemistry. Such materials with coupled electric and magnetic polarisation could provide the basis for low-energy high-density information storage devices, but are unlikely to be viable unless they can operate at (or close to) ambient temperatures. We have demonstrated a new strategy inspired by recent theoretical work on hybrid improper ferroelectrics, which describes how specific combinations of octahedral tilt distortions in layered $(AO)(ABO_3)_n$ perovskites may be used to break inversion symmetry. We have applied these structural principles to a carefully selected $(AO)(ABO_3)_2$ parent phase with a strongly magnetic B-site sublattice, using chemical control to produce the desired polar distortion in a new series of compounds which order magnetically above room temperature. In this series, electrical polarisation and spontaneous magnetisation are induced simultaneously by control of the same structural distortion (an octahedral tilt). These properties are therefore coupled, as demonstrated by a linear magnetoelectric response, and are shown to coexist at temperatures of up to 330 K across a range of compositions.

DF 11.18 Wed 18:00 Poster E

Therahertz Study of Ultrafast carrier Dynamics in Ca-doped Praseodymium Manganite — •Matteo Montagnese[1], Agung Nugroho[2], and Paul H. M. van Loosdrecht[1] — [1]II. Physikalishes Institut der Universität zu Köln, Germany — [2]Faculty of Mathematics and Natural Science, Bandung Institute of Technology, Bandung, Indonesia

Manganites show a number of exotic phenomena such as charge- and obital-ordering, the formation of striped phases, colossal magnetoresistance, and metal-to-insulator transitions. Here we report on nature of a photoinduced metal-to insulator transition in the manganite $Pr_{1-x}Ca_xMnO_3$ (PCMO) induced by the coherent excitation of a cubic perovskite structure vibration as revealed by ultrafast measurements of the optical conductivity in the terahertz range. The ultrafast coherent modulation of the Mn-O bond distance modulates the electronic overlap, thereby causing a bandgap collapse leading to substantial changes in the low frequency optical conductivity. The aim of this research is to clarify the coupling mechanism between the structural and the electronic degrees of freedom in this vibrationally-induced phase transition.

DF 11.19 Wed 18:00 Poster E

New multiferroic composite consisting of barium calcium zirconate titanate with large magnetoelectricty — •Muhammad Naveed-Ul-Haq[1], Vladimir Shvartsman[1], Soma Salamon[2], Heiko Wende[2], and Doru Lupascu[1] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE),

University of Duisburg-Essen, Universitätsstraße 15, 45141 Essen, Germany. — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany.

The lead-free composite multiferroics are the focus of current day research. The composites consist of a piezoelectric/ferroelectric part and a magnetostrictive part and the product property of the composites is utilized for the extraction of magnetoelectricity out of these composites. There are several composites in which barium titanate or its derivatives were used as the piezoelectric part. However, due to its excellent piezoelectric properties, the composition 50Ba(Zr, Ti)O_3 - 50(Ba, Ca)TiO_3 commonly known as BZT-BCT, is an excellent candidate for piezoelectric properties as it lies at the morphotropic phase boundary between orthorhombic and tetragonal polymorphic phases. BZT-BCT has an excellent room temperature piezoelectric constant, d_{33} , of 600 pC/N. As a magnetostrictive phase we used cobalt ferrite due to its high value of magnetostriction. The composite so formed gives a value of converse magnetoelectric constant 6 ps/m which is excellent for piezoelectric-magnetostrictive composites.

DF 11.20 Wed 18:00 Poster E

Macroscopic characterization of magneto electric materials — •Ahmadshah Shahab Nazrabi — ahmadshah.nazrabi@uni-due.de

The class of multiferroic materials combine two ferroic ordering phenomenas, the ferromagnetic and ferroelectric. Magneto-electric materials have two main potential applications: Precise sensors for magnetic measurement technology in medicine and fatigue non-volatile memory for the electronics. In both cases the coupling between electric and magnetic variables must be still optimized. The coupling mechanism is due to stress and strain property of these materials. The experimentally obtained macroscopic characterization data is important in order to gain a guideline for the development of modeling tools for mechanics. The essence of the characterization for these materials is a detailed description of the mechanical, electromechanical, magnetomechanical, and over all of the three fields coupled constitutive laws. A set up is constructed to apply simultaneously electrical, magnetic and mechanical field in order to quantify the interactions between fields and specimen. Further, in order to quantify the magnetic properties has been developed a special pressure cell, which allows magnetic measurement under load.

DF 11.21 Wed 18:00 Poster E

Macroscopic characterization of magneto electric materials — •Ahmadshah Shahab Nazrabi — ahmadshah.nazrabi@uni-due.de

The class of multiferroic materials combine two ferroic ordering phenomenas, the ferromagnetic and ferroelectric. Magneto-electric materials have two main potential applications: Precise sensors for magnetic measurement technology in medicine and fatigue non-volatile memory for the electronics. In both cases the coupling between electric and magnetic variables must be still optimized. The coupling mechanism is due to stress and strain property of these materials. The experimentally obtained macroscopic characterization data is important in order to gain a guideline for the development of modeling tools for mechanics. The essence of the characterization for these materials is a detailed description of the mechanical, electromechanical, magnetomechanical, and over all of the three fields coupled constitutive laws. A set up is constructed to apply simultaneously electrical, magnetic and mechanical field in order to quantify the interactions between fields and specimen. Further, in order to quantify the magnetic properties has been developed a special pressure cell, which allows magnetic measurement under load.

DF 11.22 Wed 18:00 Poster E

Piezoresponse force microscopy of domain wall motion in thin film ferroelectrics — •Robert Roth[1], Er-Jia Guo[1,2], Martin Koch[1], Kathrin Dörr[1], and Thomas Thurn-Albrecht[1] — [1]Martin Luther University Halle-Wittenberg, Institute of Physics, 06099 Halle, Germany — [2]Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Ferroelectric domain wall motion is often studied in an atomic force microscope (AFM) by writing ferroelectric domains under a conductive voltage-biased AFM tip and subsequent imaging by recording the local piezoresponse signal [1]. Next to the writing voltage and time, parameters like temperature, ambient atmosphere and elastic strain [2] strongly influence the domain growth and the stability of grown remanent domains. We show results on domain stability and velocity of 180° domain walls in a 24 nm thick epitaxial $BaTiO_3$ (BTO) film. BTO is a strong candidate material for the ferroelectric tunnel barrier in multiferroic tunnel junction devices, but its domain dynamics in thin epitaxial films is yet rarely investigated. As second example, domain growth in a prototype ferroelectric polymer, polyvinylidene fluoride trifluoroethylene (PVDF-TrFE 70/30) has been studied. A strong impact of microstructure parameters such as the orientation and the thickness of the polymer lamellae on domain wall velocity has been observed. These microstructure parameters have been controlled to some degree by the choice of substrate and an optimized annealing procedure.

[1] T. Tybell et al., Phys. Rev. Lett. 89, 097601 (2002), [2] E.-J. Guo, R. Roth, et al., Adv. Mater. 27, 1615 (2015)

DF 11.23 Wed 18:00 Poster E

Domain walls in SrMnO3 thin films under epitaxial tensile strain — •Lokamani Lokamani[1], Carina Faber[3], Peter Zahn[1], Nicola Spaldin[3], and Sibylle Gemming[1,2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR e.V., 01314 Dresden, Germany — [2]Instiute of Physics, Technische Universität, 09107 Chemnitz, Germany — [3]Materials Theory, ETH, 8093 Zürich, Switzerland

Strontium manganate ($SrMnO_3$), a perovskite polymorph, exhibits cubic structure at low temperatures, which transforms into a hexagonal one at high temperatures. Density-functional calculations showed earlier, that under tensile strain the ground state of bulk SrMnO3 corresponds to a G-type-antiferromagnetic (G-AFM) cubic structure. If deposited as epitaxially strained thin film a rearrangement of the MnO_6 coordination polyhedra was calculated, which is antiferrodistortive in the plane parallel to the substrate[1]. Recently, ferroelectric domains have been observed experimentally in thin films of $SrMnO_3$ (20nm) on (001)-oriented LSAT with a 1.7% tensile strain[2]. Strikingly, the domain walls were found to be electrically insulating, rendering the domains to form stable nano-capacitor.

Here, we present a first-principle investigation of the domain wall formation in thin films of $SrMnO_3$, their non-conductive behaviour and the effect of vacancies and defects on the conductance properties of such domain walls.

[1] J. H. Lee et. al., PRL **104**, 207204 (2010).
[2] C. Becher et. al., Nature Nanotechnology **10**, 661 (2015).

DF 11.24 Wed 18:00 Poster E

Domain boundary contributions to the dielectric response — •Pavel Marton, Antonin Klic, Ivan Rychetsky, Petr Ondrejkovic, and Jiri Hlinka — Institute of Physics, Czech Acad. Sci., Prague

Importance of domain boundaries for application-related high-response ferroelectric perovskite oxides is widely accepted. Recent developments of the domain-engineering techniques allows to acquire domain sizes as small as only several tens of nanometers. Then the domain boundaries become true functional part with interesting properties, which significantly influence the behaviour of the material as a whole. In this contributions we investigate 180- and 90-degree layered domain structures within the Ginzburg-Landau-Devonshire model.

DF 11.25 Wed 18:00 Poster E

Electronic structure of $LiNbO_3$: Many-body interactions and spin-orbit coupling — •Arthur Riefer, Michael Friedrich, Simone Sanna, Uwe Gerstmann, Arno Schindlmayr, and Wolf Gero Schmidt — Department Physik, Universität Paderborn, Warburger Str. 100, 33095 Paderborn, Germany

Lithium niobate ($LiNbO_3$, LN) is one of the most important ferroelectric materials and the most important nonlinear optical material. Since the theoretical understanding of the electronic properties is still incomplete, in this work we extend previous theoretical studies [1-3] and provide a detailed analysis of the electronic properties of LN in the frozen-lattice approximation. Starting from semilocal and hybrid DFT, we include self-energy corrections within the non-self-consistent G_0W_0 approximation as well as the QSGW_0 and QSGW [4,5] variants with partial and full quasiparticle self-consistency. In this way we obtain a reliable value for the LN frozen-lattice band gap. Additionally, with a numerically very efficient and recently implemented method by one of the authors [6], we examine the effect of combined atomic spin-orbit coupling and Coulomb-potential asymmetry (Rashba effect).

[1] W. G. Schmidt *et al.*, Phys. Rev. B **77**, 035106 (2008)
[2] C. Thierfelder *et al.*, phys. stat. sol. (c) 7, 362 (2010)
[3] A. Riefer *et al.*, Phys. Rev. B **87**, 195208 (2013)

[4] M. Shishkin *et al.*, Phys. Rev. Lett. **99**, 246403 (2007)
[5] M. van Schilfgaarde *et al.*, Phys. Rev. Lett. **96**, 226402 (2006)
[6] U. Gerstmann *et al.*, Phys. Rev. B **89**, 165431 (2014)

DF 11.26 Wed 18:00 Poster E

Zero-point renormalization and temperature dependence of the $LiNbO_3$ band gap from first principles — •Michael Friedrich, Arthur Riefer, Simone Sanna, Wolf Gero Schmidt, and Arno Schindlmayr — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Lithium niobate ($LiNbO_3$, LN) is a dielectric crystal with outstanding electro-optical properties that is widely used for optical waveguides and other commercial applications. As previous experimental and theoretical studies have mostly concentrated on the ground-state properties, the variation of technologically important material parameters with the temperature, which stems from the coupling to phonons, has received little attention until now.

Here we perform quantitative calculations within density-functional perturbation theory as well as ab initio molecular dynamics in order to evaluate the vibrational contributions to the LN fundamental band gap. Our results indicate a large shift of 0.4 eV due to the zero-point renormalization and predict a temperature-dependent variation of the band gap that are both in excellent agreement with the available experimental data.

[1] M. Friedrich *et al.*, J. Phys.: Condens. Matter **27**, 385402 (2015).

DF 11.27 Wed 18:00 Poster E

Low temperature luminescence of current commercial LED-phosphors — •Sergej Bock and Dirk Berben — South Westphalia University of Applied Sciences, Hagen, Germany

In terms of quality improvement of LEDs we present our investigations on low temperature luminescence properties of current commercial LED-phosphors, i.e YAG:Ce. Therefore, spectral and lifetime measurements were made at very low temperatures, from 10 K up to 318 K. The aim is to identify degradation induced shallow defect centers which are frozen out at low temperatures and are being analyzed by means of thermoluminescence spectroscopy. Using Arrhenius plots, the activation energies can be determined and statements about the energy structure of the presented samples can be made. Comparison of different composition and doping levels allow identification of optimization levers.

DF 11.28 Wed 18:00 Poster E

Optical Riblet Sensor: Beam Parameter Requirements for the Probing Laser Source — •Juliane Tschentscher[1], Sven Hochheim[1], Hauke Brüning[2], Kai Brune[2], Kay-Michael Voit[3], and Mirco Imlau[1] — [1]School of Physics, Osnabrück University, Germany — [2]Fraunhofer IFAM, Bremen, Germany — [3]Caesar Research Center, Bonn, Germany

Microstructured grooves on turbulent boundary layers (riblets) have a major impact on drag engineering of aircrafts in the context of kerosine consumption as they reduce skin friction considerably. Great demands are made on the geometry as deviations from theoretically designed riblets of a few percent already reduce the drag-reducing functionality drastically. A suitable optical sensor concept for deviation detection has been published previously. [Imlau *et al.*, EU Project's Report(2013)] We present the results of our studies on the beam parameters of the probing laser source in the riblet sensor by taking the high demands on a sensor's precision and reliability for the determination of degradation of the riblet geometry into account. Mandatory requirements, such as minimum intensity and light polarization, are obtained by means of detailed inspection of the optical response of the riblet using ray and wave optics. Novel measures for analyzing the riblet shape without the necessity of a measurement with a reference sample are derived and values for an ideal riblet structure obtained with the riblet sensor are given. We show that a low-cost $Nd:YVO_4$ laser pointer is sufficient to serve as a reliable laser source in an appropriate optical riblet sensor. We thank the Clean Sky Initiative (SP1-JTI-CS-2011-02).

DF 11.29 Wed 18:00 Poster E

Optical and electrooptical properties of PZT studied by Muller matrix ellipsometry — •Jakub Havlicek[1], Vladimir Foldyna[1], Jaroslav Hamrle[1], Jaromir Pištora[1], Yoichiro Hashizume[2], and Soichiro Okamura[2] — [1]VSB-Technical University of Ostrava, 17. listopadu 15, Ostrava, Czech Republic — [2]Tokyo University of Science, 6-3-1 Niijuku Katsushika-ku, 125-8585 Tokyo, Japan

The optical and electrooptical properties of $Pb[Zr_{0,44}Ti_{0,56}]O_3$ (PZT) thin film have been investigated using Muller matrix ellipsometry. The studied structure consists of Au(10 and 20 nm)/PZT(1000 nm)/Pt(100 nm)/Si, where contacted top Au electrode of diameter 3 mm allows to apply voltage (up to 60V per 1 ms, i.e. up to 0.6 MV/cm) in order to electrically polarize PZT crystal.

The investigations were done using Mueller matrix ellipsometry [1,2], working in spectral range 0.8 - 6.2 eV. From those measurements, we determine both optic spectra of PZT (contribution to permittivity independent on PZT polarization) and spectra of Pockels effect (contribution to permittivity linear with polarization).

[1] H. Fujiwara, Spectroscopic Ellipsometry: Principles and Applications (Willey) (2007). [2] D.H. Goldstein, Mueller matrix dual-rotating retarder polarimeter, Applied Optics, 31, 6676-6683 (1992).

DF 11.30 Wed 18:00 Poster E

Impact of ion-implantation on the nonlinear susceptibility in $LiNbO_3$: A basic study — •Kai Jürgen Spychala[1], Lei Wang[2], Michael Rüsing[1], and Gerhard Berth[1] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]School of physics, Shandong University, 250100 Shandong, China

One of the key elements on the way to integrated optical structures (IOS) are high quality optical waveguides. However, the process of waveguide construction itself is accompanied by a violation of the crystal structure of the used material. Especially when the nonlinear optical properties play a major role in the IOS [1], the impact of ion implantation on the material becomes important. Within this work the effective nonlinear coefficient in ion implanted LiNbO3 waveguides has been studied via surface-near Second-Harmonic (SH) analysis. As in previous work of P. Günter et al. [2], the nonlinear analysis was carried out on wedge shaped samples to acquire depth information in backscattering geometry. Our experimental data shows that a characteristic SH-signal drop is produced for all samples in the implanted region. A comparison with simulation data calculated with the software package "SRIM" by Ziegler et al., suggests that the characteristic drop can be traced back to the induced defects and therefore fits into the simulation curves. In a further step we also examined annealed samples with the same method and obtained that the induced damage can be healed partially.

[1] Daniel Sjörberg: "Nonlinear waveguides" (2001)
[2] P.Günter: "Nonlinear optical effects and materials" (2000)

DF 11.31 Wed 18:00 Poster E

Electrostatic force microscopy at domain walls of $LiNbO_3$ — •Manuel Becker and Elisabeth Soergel — Physikalisches Institut, University of Bonn

The polar z-faces of $LiNbO_3$, usually investigated by PFM for mapping the domain patterning, can not be imaged using non-contact scanning force microscopy; the electrostatic forces owing to the surface polarization charges being to strong. It is, however, possible to access the domain walls via the non-polar faces. Here, electrostatic force microscopy (EFM) can be employed to record the local charge distribution accumulated at the walls which, by means of light or heat, can be modified on demand. Investigations using EFM, thus gaining information on the density of free charge carriers, might allow for a better understanding of the origin for the domain wall conductivity.

DF 11.32 Wed 18:00 Poster E

Analysis of the frequency spectra in PFM — •Sarmed Hussain and Elisabeth Soergel — Physikalisches Institut, Bonn, Germany

Piezoresponse force microscopy (PFM) has emerges as a key-method for mapping domain patterns in ferroelectric materials with high lateral resolution an impressive sensitivity. For recording quantitatively reliable data (in terms of the magnitude of the piezomechanical response), however, a method for calibration is still missing. Besides the need for a calibration standard, there is in addition the difficulty of the frequency dependence of the data recorded, most prominent when investigating samples with small piezoelectric coefficients. Although it might eventually not be possible to get rid of this frequency dependence, its origin is of interest for a better evaluation of the, presumably quantitative PFM-data obtained.