Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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Overview of Invited Talks, Topical Talks, and Sessions

(Lecture rooms H25 and H26 (Vielberth-Gebäude); Poster E)

Invited Talks

DF 7.1	Tue	9:30–10:10	H25	**Spin and charge transport in multiferroic domain walls** — •Ramamoorthy Ramesh

Topical Talks

DF 6.1	Mon	15:00–15:30	H26	**CVD diamond for nuclear fusion experiments** — •Eckhard Wörner, Christoph Wild
DF 6.2	Mon	15:30–16:00	H26	**Torus Diamond Window for the ITER ECRH Upper launcher** — •Sabine Schreck, Gaetano Aiello, Giovanni Grossetti, Francesco Mazzocchi, Andreas Meier, Peter Spaeh, Dirk Strauss, Alessandro Vaccaro, Theo Scherer
DF 6.4	Mon	16:20–16:50	H26	**Double-disc Diamond Windows for Fusion Applications** — •Alessandro Vaccaro, Gaetano Aiello, Giovanni Grossetti, Francesco Mazzocchi, Andreas Meier, Theo Scherer, Sabine Schreck, Peter Spaeh, Dirk Strauss
DF 6.5	Mon	17:10–17:40	H26	**Dielectric Characterization for Industrial Microwave Applications** — •Sergey Soldatov, Vasileios Ramopoulos, Guido Link, John Jelonnek
DF 7.5	Tue	11:30–12:00	H25	**Conduction and Diode Behaviour in Charged Domain Walls** — •Michael Campbell
DF 8.1	Tue	14:00–14:30	H25	**Microscopic order parameters coupling at domain walls and its effect on macroscopic properties** — •Saeedeh Farokhipoor
DF 9.1	Wed	9:30–10:00	H25	**Functional domain walls in multiferroics** — •Dennis Meier
DF 9.3	Wed	10:20–10:50	H25	**Neutron scattering study of the cycloidal and Néel-type skyrmion lattice phases of GaV_4S_8** — •Sándor Bordács, Jonathan S White, Nicole Reynolds, Charles D Dewhurst, Henrik M Rønnow, Vladimir Tsurkan, Alois Loidl, István Kézsmárki
DF 9.5	Wed	11:30–12:00	H25	**Collective spin excitations at GHz frequencies in Skyrmion-hosting bulk materials** — •Dirk Grundler
DF 9.7	Wed	12:20–12:50	H25	**Skyrmionic states in ferroelectric nanocomposites** — Yousra Nahas, •Sergei Prokhorenko, Lydie Louis, Zhigang Gui, Igor Kornev, Laurent Bellaiche
DF 10.1	Wed	15:00–15:30	H25	**Controlling domain wall motion as a route towards new functionalities in $Pb(Zr,Ti)O_3$ ferroelectric thin films** — •Leo McGilly, Ludwig Feigl, Petr Yudin, Tomas Sluka, Alexander Tagantsev, Nava Setter
DF 10.7	Wed	17:30–18:00	H25	**Domain Glass** — •Ekhard Salje

Invited talks of the joint symposium SYHP

See SYHP for the full program of the symposium.

SYHP 1.1	Mon	9:30–10:00	H1	**Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design** — •David B. Mitzi
SYHP 1.2	Mon	10:00–10:30	H1	**Perovskite Solar Cells: A new Paradigm in Photovoltaics** — •Mohammad Nazeeruddin
SYHP 1.3	Mon	10:30–11:00	H1	**Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites** — •Laura Herz
SYHP 1.4	Mon	11:15–11:45	H1	**Photovoltage losses in perovskite solar cells** — •Kristofer Tvingsted
SYHP 1.5	Mon	11:45–12:15	H1	**Computational screening of perovskite solar energy materials** — •Karsten W. Jacobsen

Invited talks of the joint symposium SYCE

See SYCE for the full program of the symposium.

SYCE 1.1	Mon	15:00–15:30	H1	**Multicaloric effects in metamagnetic Heusler materials** — •Antoni Planes
SYCE 1.2	Mon	15:30–16:00	H1	**Multicaloric effect in biological systems: a case of nerve action** — •Matjaz Valant, Lawrence J. Dunne, Anna-Karin Axelsson, Florian Le Goupil, George Manos
SYCE 1.3	Mon	16:00–16:30	H1	**Optimizing the electrocaloric effect by first-principles simulations: The role of strain and defects** — •Anna Grünebohm
SYCE 1.4	Mon	16:45–17:15	H1	**Giant inverse barocaloric effects in ferrielectric ammonium sulphate** — Pol Lloveras, Enric Stern-Taulats, Maria Barrio, Josep Lluis Tamarit, Sam Crossley, Wei Li, Vladimir Pomjakushin, Antoni Planes, Lluis Mañosa, Neil Mathur, •Xavier Moya
SYCE 1.5	Mon	17:15–17:45	H1	**TiNiCu-based thin films for elastocaloric cooling** — •Eckhard Quandt, Christoph Chluba

Sessions

DF 1.1–1.3	Sun	16:00–18:30	H18	**Tutorial: Hybrid and Perovskite Photovoltaics (CPP with DS, DF, HL)**
DF 2.1–2.5	Mon	9:30–12:15	H1	**SYHP: Fundamentals of Hybrid and Perovskite Photovoltaics (CPP with DS, DF, HL)**
DF 3.1–3.7	Mon	9:30–12:10	H26	**Optical and nonlinear optical properties, photonic**
DF 4.1–4.12	Mon	14:45–18:30	H2	**Photovoltaics (HL with DF)**
DF 5.1–5.5	Mon	15:00–17:45	H1	**SYCE: Caloric effects in ferroic materials (MM with MA, DF)**
DF 6.1–6.8	Mon	15:00–18:40	H26	**Focus Session: Applications of Dielectric Materials in Microwave Technology**
DF 7.1–7.8	Tue	9:30–13:00	H25	**Focus Session: Ferroic Domain Walls I**
DF 8.1–8.6	Tue	14:00–16:00	H25	**Focus Session: Ferroic Domain Walls II**
DF 9.1–9.7	Wed	9:30–12:50	H25	**Focus Session: Skyrmions meet Multiferroicity**
DF 10.1–10.7	Wed	15:00–18:00	H25	**Focus Session: Ferroic Domain Walls III**
DF 11.1–11.32	Wed	18:00–20:00	Poster E	**Poster**
DF 12.1–12.9	Thu	9:30–12:50	H25	**Multiferroics I (DF with MA)**
DF 13.1–13.8	Thu	9:30–12:30	H26	**Nano- and microstructured dielectrics/thin films (DF with KR)**
DF 14.1–14.9	Thu	15:00–17:30	H34	**Multiferroics II (MA with DF)**
DF 15.1–15.2	Thu	15:00–15:40	H26	**Ceramics and Applications (DF with KR)**
DF 16.1–16.4	Thu	15:40–17:00	H26	**Crystallography in Materials Science (KR with DF, MI)**

Annual General Meeting of the Dielectric Solids Division

Donnerstag 17:30–18:00 H25

DF 1: Tutorial: Hybrid and Perovskite Photovoltaics (CPP with DS, DF, HL)

Organizers: Lukas Schmidt-Mende (Universität Konstanz), Vladimir Dyakonov (Universität Würzburg) and Christoph Lienau (Universität Oldenburg)

Tremendous progress has been achieved in the performance of hybrid solar cells, with efficiencies now exceeding 20 % for devices based on organometallic halide perovskites. Aim of this tutorial is to introduce this topic of perovskite solar cells to prepare for the following symposium (SYHP) and allow vivid scientific discussions. A description of current state-of-the-art device fabrication methods and solar cell architectures will be given and their role on the device performance explained. The device physics will be discussed and charge carrier generation and recombination mechanisms in perovskite films explained and compared to other material systems. Additionally the important role of electronic structure of the different layers in hybrid perovskite will be covered.

Time: Sunday 16:00–18:30 Location: H18

Tutorial DF 1.1 Sun 16:00 H18

Perovskite photovoltaics: Synthesis, structure and device architecture — •Pablo Docampo — LMU Munich, Germany

Recently, organic-inorganic hybrid perovskites have been proven to be excellent photovoltaic materials, exhibiting outstanding light absorption, high carrier mobility and facile solution processability. Besides the manufacturing low costs of perovskite thin-films, the power conversion efficiencies demonstrated for this class of materials is already at the same level as poly-crystalline silicon and other thin film photovoltaic technologies. The pursuit of efficiency in the field of metal halide perovskite solar cells has been achieved mainly through the improvement to perovskite deposition processing and optimization of the device architecture.

In this tutorial I will focus on three topics. Firstly, the evolution of the device architecture, starting from sensitized mesoscopic solar cells to planar heterojunction devices employing organic contacts. Secondly, the commonly employed perovskite deposition techniques with special emphasis on the morphological quality of the prepared perovskite films. Thirdly, the perovskite structure and its stability both towards moisture and other factors such as UV-light, temperature and atmosphere. I will link these different aspects with device performance characteristics and introduce recent developments in the field towards surmounting the challenges the technology is currently facing from a materials point of view.

Tutorial DF 1.2 Sun 16:50 H18

Charge Carrier Generation and Recombination in Organic and Perovskite Solar Cells — •Andreas Baumann — Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), Magdalene-Schoch-Str. 3, D-97074 Würzburg

The new star on the photovoltaic (PV) horizon, are the so called organometal halide perovskite solar cells. This new kind of thin-film PV technology has experienced a tremendous, yet not seen increase in power conversion efficiency (PCE) compared to other types of PV technologies. Up to now the solar cell efficiency on lab scale could be improved from 3.8% in 2008 to above 20% in 2015 being already competitive with commercially available PV technologies. Especially this boost in PCE values has attracted attention of many researchers from all different PV research fields. Thereby, perovskite PV is one of the most promising thin film PV technologies regarding low-cost manufacturing combined with high PCE. However, the working principle of these solar cells is yet not completely understood and is strongly discussed in literature. Phenomena, such as the often observed anomalous hysteresis in the current-voltage characteristics or the giant dielectric constant and its impact on charge carrier generation and recombination are highly debated topics with so far different given possible explanations.

In this tutorial, the processes of charge carrier generation and recombination in perovskite solar cells will be highlighted and compared to those in well studied organic solar cells. Thereby, the aim is to give an overview of the published data on these processes in order to present the current status of research.

Tutorial DF 1.3 Sun 17:40 H18

The electronic structure in hybrid perovskite layers and devices — •Selina Olthof — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

The performance of optoelectronic devices strongly depends on the appropriate energetic alignment of the participating transport levels which directly influence the charge transport through the different layers. In order to optimize these interfaces in a non-trial-and-error fashion, one needs to know the conduction band minimum and valence band maximum of the perovskites to be able to select ideal transport layers as well as contact materials. While commonly vacuum level alignment is assumed at the interface to the substrate, this is actually rarely found in devices. Interfacial states, interface dipoles, and band bending can (and do) significantly alter the energy level landscape.

In this tutorial I will discuss the electronic structure of perovskites and introduce common measurement techniques that can shed a light on their energetic properties as well as the interface alignment relevant for devices. Combining reports from literature with our own recent results on the versatile electronic nature of this material I will elucidate the interplay between electronic structure and overall device performance.

DF 2: SYHP: Fundamentals of Hybrid and Perovskite Photovoltaics (CPP with DS, DF, HL)

Time: Monday 9:30–12:15 Location: H1

Invited Talk DF 2.1 Mon 9:30 H1

Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design — •David B. Mitzi — Duke University, Edmund T. Pratt Jr. School of Engineering, Durham, NC 27708-0300 USA

Organic-inorganic and related halide-based perovskites (e.g., those based on Pb halide frameworks) have attracted substantial recent interest for solar cell and other optoelectronic technologies, because of the large optical absorption coefficients, high carrier mobilities, long minority carrier lifetimes, and relatively benign defects and grain boundaries. Indeed, these materials have enabled an unprecedented rapid improvement in photovoltaic (PV) performance to levels above 20% power conversion efficiency. Despite the great promise, challenges for the current generation of PV materials include replacing lead with more environmentally benign metals, improving PV device stability (moisture, UV and air) and controlling hysteresis. This talk will explore beyond the current focus on three-dimensional (3-D) lead(II)-based perovskites, to highlight the outstanding structural, chemical and electronic flexibility of the perovskite family. Particular focus will be afforded to systems in which divalent lead is replaced with other metal cations exhibiting a lone pair of electrons, such as Sn, Bi and Sb, since these systems share some of the beneficial electronic structure characteristics of the Pb-based systems. Further discovery within the perovskite structural and chemical space may offer prospects to solve the current technological challenges for perovskite PV and yield important opportunities for energy materials design.

Invited Talk DF 2.2 Mon 10:00 H1

Perovskite Solar Cells: A new Paradigm in Photovoltaics —

•Mohammad Nazeeruddin — EPFL, GMF, Sion Switzerland

Perovskite solar cells exhibited significant leapfrog in efficiency due to a broad absorption, high optical absorption coefficient, very low exciton binding energy, long carrier diffusion lengths, efficient charge collection, and very high open circuit potential similar to III-IV semiconductors. Unlike silicon solar cells, perovskite solar cells can be developed a variety of low-temperature solution process from inexpensive raw materials. By engineering compositional ratio of perovskite absorber, film formation using anti-solvent, and interface engineering of charge transport materials a remarkable power conversion efficiency of over 21% has been demonstrated, highlighting the unique photovoltaic properties of perovskite materials. In this talk, we present the current progress in perovskite solar cells, various deposition methods for perovskite absorbing layer, synthesis and characterization of novel hole transporting materials, and highlight crucial challenges and prospects

Invited Talk DF 2.3 Mon 10:30 H1

Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites — •Laura Herz — University of Oxford, Oxford, UK

Hybrid metal halide perovskites (stoichiometry AMX_3) have recently emerged as low-cost active materials in PV cells with power conversion efficiencies in excess of 20%. In addition, hybrid perovskites show prospects for applications in low-cost light-emitting diodes and lasers.

Here we discuss how parameters essential for photovoltaic operation, such as charge carrier recombination and diffusion lengths are altered with substitutions of the organic A cation (e.g. methylammonium versus formamidinium), the metal M cation (e.g. Pb^{2+} or Sn^{2+}) and the halide X anion (I versus Br). We analyze distinct charge-carrier recombination mechanisms, such as trap-mediated, bi-molecular (electron-hole) and Auger recombination, which show different dependences on composition and temperature.

We use these insights to predict charge-carrier diffusion lengths and radiative efficiencies in the limit of ultra-low trap-related recombination, which could potentially be reached through further advances in material processing. We find that for hybrid lead iodide perovskites with typical charge-carrier mobilities of $\sim 30 cm^2/(Vs)$, charge-carrier diffusion lengths under solar irradiation are unlikely to exceed $\sim 10 \mu m$ even if all trap-related recombination is eliminated. We further show that if high radiative efficiencies are to be obtained for intermediate charge-carrier densities ($n \sim 10^{14} cm^{-3}$), trap-related recombination lifetimes have to exceed microseconds.

15 min. break.

Invited Talk DF 2.4 Mon 11:15 H1

Photovoltage losses in perovskite solar cells — •Kristofer Tvingsted — Experimental Physics VI, Julius Maximilians Universität, Würzburg, Germany

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage (VOC). The VOC of most solar cells is however far from its potential upper limit due to charge carrier recombination of various types, whose origin must be accurately determined. Herein, I summarize what we have learned about these photovoltage losses by studying the radiative part of recombination in Perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far the solar cells are from their own thermodynamic upper limit and further, how they relate to a reference OPV cell. We evaluate the carrier density dependence of the radiative efficiency and associate it to the ideality factor, which in itself represents a uniform figure of merit for the dominant type of recombination. We show that, as the perovskite steady state photoluminescence is strong at open circuit conditions, but substantially quenched only at short circuit, they perform in this respect just as an ideal solar cell should do, and also very different from most OPVs or DSSC cells studied so far. Substantially improving the radiative efficiency to increase the open circuit voltage is a promising route to put these new photovoltaic converters in efficiency parity with the best inorganic counterparts.

Invited Talk DF 2.5 Mon 11:45 H1

Computational screening of perovskite solar energy materials — •Karsten W. Jacobsen — CAMD, Dept. of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In the talk I shall describe computational efforts to idenfity new materials for efficient light absorption with particular focus on materials in the perovskite structure and water splitting. The materials have to obey a number of criteria in order to work for light absorption and water splitting depending on the particular design of the device. We consider in particular stability, appropriate bandgap and bandstructure for visible light absorption, and an adequate line-up of band edges to the water redox potential. We also identify descriptors to determine defect-sensitivity of the materials.

We have considered several classes of materials with most emphasis on the cubic perovskite structure and derivatives like double perovskites and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with anions O, N, F, or S. Also a range of Sn and Pb based organic and inorganic perovskites have been considered with different combinations of the anions I, Br, and Cl. The possibilities of band gap tuning using atomic-level heterostructures or strain will also be touched upon.

I shall finally mention presently available open databases of relevance for energy materials including the Computational Materials Repository (https://cmr.fysik.dtu.dk) where the discussed data are made publicly available.

DF 3: Optical and nonlinear optical properties, photonic

Time: Monday 9:30–12:10 Location: H26

DF 3.1 Mon 9:30 H26

Scanning nonlinear absorption in lithium niobate over the time regime of small polaron formation — Holger Badorreck, Stefan Nolte, •Felix Freytag, Pia Bäune, and Mirco Imlau — School of Physics, Osnabrueck University,Barbarastr. 7, 49076 Osnabrueck, Germany

Nonlinear absorption is studied in presence of small polaron formation in lithium niobate using the z-scan technique and ultrashort laser pulses with pulse durations of 70 - 1.000 fs. A model for the analysis of the transmission loss as a function of pulse duration is introduced that considers (i) the individual contributions of two-photon and small polaron absorption, (ii) the small polaron formation time and (iii) an offset time between the optical excitation of free carriers by two-photon absorption and the appearance of small polarons. It is shown that the model allows for the analysis of the experimentally determined z-scan data with high precision over the entire range of pulse durations using a two-photon absorption coefficient of $\beta = (5.6 \pm 0.8)$ mm/GW. A significant contribution by small polaron absorption to the nonlinear absorption is uncovered for pulse durations exceeding the characteristic small polaron formation time of ≈ 100 fs. It can be concluded that the small polaron formation time is as short as (70 - 110) fs and the appearance of small polaron formation is delayed with respect to two-photon absorption by an offset of about 80 fs. Financial support by the DFG (IM37/5-2, INST 190/137-1 FUGG, INST 190/165-1) is gratefully acknowledged. [Baddoreck et al., Opt. Mater. Express 5(12) 2729-2741 (2015)]

DF 3.2 Mon 9:50 H26

Luminescence of undoped lithium niobate — •Simon Messerschmidt, Andreas Krampf, and Mirco Imlau — Department of Physics, Osnabrück University, Germany

Luminescence of lithium niobate (LN) was studied for the first time 1973 by Blasse [Blasse, G. Phys. Stat. Sol. (a) 20, K99 – K102 (1973)]. He detected a broadband light emission of LN under UV-excitation at temperatures below 80 K and assumed that the origin of the luminescence lies in the NbO_6-octahedron. Various authors subsequently have found a connection between the ratio of [Li]/[Nb] and the emitted peak wavelengths so that the red-shift in lithium-poor LN is interpreted as a disturbance of the NbO_6-octahedron (Nb_{Li}-antisite defect). The emitted light is independent of the excitation wavelength and has a large

Stokes shift. Therefore, the luminescence is described in a model of a self-trapped exciton (STE) [Wiegel, M., *et al.*, J. Phys. Chem. Solids 55, 773 – 778 (1994)]. Until now, the interplay of STE and small polarons as well as parameters such as duration of the excitation pulse or crystal morphology to control the probability of the luminescence is unknown which is the topic of this work. Two experimental setups are used and initial results are presented. In the first setup, ns-pulses were used to excite a sample cooled to $T = 30\,\mathrm{K}$ whose emitted light is detected with a gated photon counter. In a second setup, a luminescence upconversion detector utilizing ultrashort femtosecond pulses is applied to detect the dynamics of the luminescence light. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

DF 3.3 Mon 10:10 H26

Ultrafast holographic spectroscopy for the study of small polarons in lithium niobate — •Stefan Nolte, Bjoern Bourdon, Felix Freytag, and Mirco Imlau — School of Physics, Osnabrück University, Germany

The optical generation of small bound polarons in lithium niobate can be used to record holographic gratings with a single nanosecond laser pulse and a diffraction efficiency above 20 % [M. Imlau *et al.* Opt. Express 19, 15322 (2011), H. Brüning *et al.* Opt. Express 20, 13326 (2012)]. This finding is explained via the linear electro-optic effect and the space-charge field generated from a small polaron number density modulation with $E \approx 17\,\mathrm{kV/cm}$. For the long-range transport of small polarons, we assume cascaded optical excitation during light exposure, i.e. the pulse duration has a strong impact on the hologram recording process [cf. H. Badorreck *et al.* Opt. Mater. Express 5, 2729 (2015)].

In this contribution, we study the holographic buildup as a function of pulse duration in the femtosecond time regime. Thus, a four-wave pump-probe experiment with continously varied pulse-durations between $\tau = (70 - 500)\,\mathrm{fs}$ is used to record the time-dependent diffraction efficiency from a mixed holographic grating, based on nearly instantaneous nonlinearities $\chi^{(3)}$ and polaron effects. The results are disscussed under consideration of polaron formation.

Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

DF 3.4 Mon 10:30 H26

OH^- as local, vibrational probe for the inspection ofsmall, strong-coupling polarons — •Felix Freytag, Phillip Booker, and Mirco Imlau — School of Physics, Osnabrueck University,Barbarastr. 7, 49076 Osnabrueck, Germany

A *small polaron* is defined by the unit of a self-trapped carrier and the associated displacement of atomic equilibrium positions confined to a single lattice site [Emin, *Polarons*, Cambridge University Press (2013)]. There's an increasing attention to the structural distortion parameters of small polarons for nonlinear optical processes in polar oxides on the ultrafast time-scale [Imlau et al., Applied Physics Reviews **2**, 40606 (2015)]. Even though, a multitude of knowledge has been gathered and a variety of experimental techniques like EPR/NMR measurements were applied, there is still no possibility for direct experimental access to the structural aspects of small polarons within a continuum and at elevated temperatures. Here, we propose a vibrational method to experimentally achieve local information about small polarons at room temperature. The absorption change of the OH^- stretching vibration is applied as local probe for optically excited small polarons with lithium niobate as an example; detected by time-resolved mid-infrared pump-probe spectroscopy. The change is explained straightforwardly by a local change of the lattice environment induced by small polaron formation. By analysis of the vibrational potential of the OH^--stretching bond, we are able to estimate the polaron induced lattice distortion. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

20 min. break

DF 3.5 Mon 11:10 H26

Quadrupolar Bulk SHG from First Principles — •Klaus-Dieter Bauer and Kurt Hingerl — Zentrum für Oberflächen- und Nanoanalytik, Johannes Kepler Universität, Linz, Austria

Second harmonic generation (SHG) has been established as surface sensitive probe by exploiting symmetry-suppression of the otherwise dominant bulk dipole term in centrosymmetric systems. However, bulk quadrupole contributions are not suppressed and can be on the same order of magnitude as surface effects, yet abinitio calculations so far have neglected this term for bulk solids.

We discuss the formal relation of the optical quadrupole SHG response to a microscopic second-order response function $\chi^{(2)}(\mathbf{q}_0; \mathbf{q}_1, \mathbf{q}_2)$ and report our progress towards an implementation in the Vienna Abinitio Simulation Package (VASP).

DF 3.6 Mon 11:30 H26

Nonlinear optical spectroscopy of niobate nanopowders — •Christian Kijatkin[1], Anke Duettmann[1,2], Karsten Koempe[2], Laura Olah[3], Eva Tichy-Racs[3], Zsuzsanna Szaller[3], and Mirco Imlau[1] — [1]School of Physics, Osnabrück University, Germany — [2]Institute of Chemistry of New Materials, Osnabrück University, Germany — [3]Wigner Research Centre for Physics, Budapest, Hungary

Nonlinear optical (NLO) nanocrystals (NCs) excel in a wide spectrum of applications, most notably as optical probes in high-resolution microscopy. This field has incited a multitude of NLO characterization approaches with the ultimate goal of providing comprehensive analysis of NCs. The plethora of available NLO materials in conjunction with different measurement techniques raises the question of comparability. A peculiar case is frequency-doubling which may be attributed to surface- or volume-second harmonic generation (SHG) as well as Hyper-Rayleigh scattering or higher-order multipole contributions. Extensive studies have been performed with little interconnections to each other. We present the results of our examinations on the individual NLO contributions arising from their respective origins by assessing the SHG behavior of niobate nanopowders ($NaNbO_3$, $LiNbO_3$:Yb). Transmittive and reflective techniques are performed to elucidate intensity and dispersion relation. In combination with linear diffuse reflectance scans, a prospective method of comparing NLO investigations is introduced. Financial support (DFG INST 190/165-1 FUGG, DAAD 57139940) is gratefully acknowledged.

DF 3.7 Mon 11:50 H26

Quasi-solitons and rogue waves generation in optical fibers — •Antonino Savojardo[1], Rudolf A. Römer[1], and Marc Eberhard[2] — [1]Department of Physics and Centre for Scientific Computing, The University of Warwick, Coventry CV4 7AL, UK — [2]School of Engineering and Applied Science, Aston University, Aston Triangle, Birmingham B4 7ET, UK

Optical rogue waves are sharp, rare and extremely high power pulses. Experimental and numerical data suggest that these giant waves are due to at least two mechanisms of amplification, modulation instability (that allows the creation of quasi-solitons) and multiple inelastic quasi-soliton collisions. Using a generalized nonlinear Schrödinger equation we calculate the probability distribution function (PDF) for the intensity inside a fiber. We investigate pair-wise quasi-soliton collisions and propose a formula for the energy transfer. This allows us to implement an effective cascade model. The PDFs calculated using the two models are very similar. Our results suggest that once localized pulses are formed because of modulation instability an important contribution to rogue waves generation is quasi-soliton inelastic scattering.

DF 4: Photovoltaics (HL with DF)

Time: Monday 14:45–18:30 Location: H2

Invited Talk DF 4.1 Mon 14:45 H2

Surface chemistry of colloidal semiconductor nanocrystals — •Zeger Hens — Physics and Chemistry of Nanostructures, Ghent University, Krijgslaan 281-S3, B9000 Gent, Belgium

Colloidal semiconductor nanocrystals or quantum dots are hybrid nano-objects composed of an inorganic, crystalline core capped by organic surface ligands. This talk addresses recent advances in the understanding of this ligand shell. First, solution NMR will be introduced as a unique, in-situ analysis technique for identifying and quantifying these ligands and for analysing ligand exchange reactions. This has

recently led to the classification of nanocrystal/ligand nanocrystals based on the ligand binding motif, where use is made of the covalent bond classification scheme that was originally introduced for the classification of metal complexes. It is shown how this classification enables ligand exchange reaction to be rationalized and predicted and how this now provides researchers with an extensive toolbox to tweak nanocrystal properties at will by changing their surface chemistry. In the last part of the talk, the extension of the approach to metal oxide nanocrystals is addressed. It is shown that these feature a markedly different surface chemistry, which enables for example their use as colloidal nanocatalysts.

DF 4.2 Mon 15:15 H2

Combined Black Silicon Textures for Advanced Antireflective Surfaces — •Maria Gaudig[1,2], Jens Hirsch[1,3], Alexander N. Sprafke[2], Dominik Lausch[3], Norbert Bernhard[1,3], and Ralf B. Wehrspohn[2,4] — [1]Anhalt University of Applied Sciences, Technologies of Photovoltaics Group, Bernburger Str. 55, D-06366 Köthen — [2]Martin Luther University Halle-Wittenberg, Institute of Physics, Group microMD, Heinrich-Damerow-Str. 4, D-06120 Halle (Saale) — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeldt-Straße 12, D-06120 Halle (Saale) — [4]Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, D-06120 Halle (Saale)

Black silicon (b-Si) promises with its extremely low reflectivity to become a real alternative to wet chemical textured silicon in the PV industry. In this work, the nano texturing is realized with a maskless SF6/O2 plasma etch process. Compared to the wet chemical texturing, this method provides benefits like reduced silicon waste, independence of prior surface treatment and crystal orientation and the variation of the texture forms by different plasma processes by different plasma processes. We showed two different plasma textures with absorption about 95 %: (I) a needle like texture (needle height/width ~ 500/100-200 nm) with a strong antireflection and (II) parabolic pits (height/width ~ 2/1 micron) with improved light trapping. In this contribution, we want to go one step further and combine these two techniques to exploit the optical benefits of both textures. For this purpose, the two etch processes are applied successively on the wafer. The experimental data will be discussed and advantages will be highlighted.

DF 4.3 Mon 15:30 H2

Improved light harvesting and carrier collection using transparent nano-textured back contacts in sub-micron chalcopyrite absorber solar cells — •Wiebke Ohm[1,2], Wiebke Riedel[1,2], Ümit Aksünger[2], Martha Ch. Lux-Steiner[1,2], and Sophie Gledhill[1,2] — [1]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — [2]Institut für Heterogene Materialsysteme, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

We investigate bifacial Cu(In,Ga)Se_2 (CIGS) solar cells on glass/F:SnO_2 substrates with ZnO nanorods (NR) at the back contact and a reduced absorber thickness ($<1\,\mu m$). Optical simulations of reflection and depth resolved absorption were used to show the potential of ZnO NR in bifacial sub-micron CIGS solar cells to increase the short-circuit current J_{SC}. Next to anti-reflection properties a shift of the absorption closer to the pn-junction was identified for back side illumination enhancing charge carrier collection resulting in an overall J_{SC} increase by up to 30 %. The anti-reflection effect of ZnO NR at the solar cell back contact was observed using optical measurements and the anti-reflection enhancement was estimated resulting in a maximum photo current increase of 2 %. An overall 5 % increase in J_{SC} with NR was achieved, identified in I-V measurements for back side illumination. The external quantum efficiency, however, show that parasitic absorption in the NR-based back contact limits the photo current enhancement, whereas in a wide wavelength range 20 % J_{SC} increase is demonstrated.

DF 4.4 Mon 15:45 H2

Hybrid charge transfer excitons at ZnMgO/P3HT interfaces — •Moritz Eyer, Sergey Sadofev, Joachim Puls, and Sylke Blumstengel — Institut für Physik, Humboldt-Universität zu Berlin

The performance of hybrid photovoltaic devices is strongly related to the efficiency of the charge separation process. In photovoltaic operation excitons generated in the organic and inorganic part diffuse to the interface of the heterojunction. It is suggested that prior to full charge separation a hybrid charge transfer exciton (HCTE) is formed i.e. a coulombically bound charge pair residing on both sides of the interface. Only after dissociation of such a pair a photocurrent is generated.

The formation of HCTE is experimentally verified in planar ZnMgO/poly(3-hexylthiophene) (P3HT) heterojunction devices via electroluminescence (EL) measurements [1]. Radiative recombination across the interface produces EL in the near infrared spectral region. The energy offset ΔE_{IO} between the conduction band minimum of ZnMgO and the P3HT highest unoccupied molecular orbital is tuned systematically by varying the Mg content. Combined analysis of radiative properties and the open circuit voltage V_{OC} in photovoltaic operation shows a clear correlation to the HCTE transition energy.

Investigation of the properties of HCTE yields valuable input for the optimization of the charge separation process at inorganic/organic semiconductor interfaces in order to fully exploit the potential of hybrid devices.

[1] M. Eyer et al., Appl. Phys. Lett. **107**, 221602 (2015).

DF 4.5 Mon 16:00 H2

VUV Pump-Probe Magneto-optical Ellipsometry at ELI Beamlines — •Shirly J. Espinoza-Herrera[1], Bastian Besner[2], Jakob Andreasson[1], and Michael A. Ruebhausen[2] — [1]ELI Beamlines Project, Institute of Physics of the ASCR, 252 41 Dolní Břežany, Czech Republic — [2]Institut fuer Nanostruktur- und Festkoerperforschung, Center for Free-Electron Laser Science, Advanced Study Group APOG, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

A new ellipsometer that is capable of measuring in one run the dielectric function of solid states samples from the IR and the VUV spectral range is being set up at ELI beamlines. ELI is a pillar of the transnational European Extreme Light Infrastructure (ELI) that will hold some of the most intense lasers in the world. The Center for Free Electron Laser in Hamburg is joining this European effort and the work presented here is the development of the pump-probe VUV ellipsometer that will allow the study of materials out of the Fermi level, testing the established tradition of condensed matter physics where most of the phenomena observed are driven the physics close to the Fermi level. Results showing the coupling between the low and high energy levels of freedoms on the case of STO and LAO will be presented.

DF 4.6 Mon 16:15 H2

Synchrotron-based spectroscopy study of the conduction band development in Cu2ZnSn(S,Se)4 with different [S]/([S]+[Se]) ratios — •Tetiana Olar[1], Iver Lauermann[1], Archana Manoharan[2], Lorenzo Pardini[2], Karsten Hannewald[2,3], Claudia Draxl[2,3], Haibing Xie[4], Edgardo Saucedo[4], Binoy Chacko[1], and Martha Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH,Albert-Einstein-Str. 15, 12489 Berlin,Germany — [2]Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, 12489 Berlin, Germany — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [4]Catalonia Institute for Energy Research- IREC, Jadinsde les Dones de Negre 1, 08930 Sant Adrià de Besòs (Barcelona), Spain

Cu2ZnSn(S,Se)4 absorber layers with different [S]/([S]+[Se]) ratios were studied using XPS, UPS, HIKE and NEXAFS. To investigate the band gap transition from the pure sulfide to the pure selenide compound, the valence band maximum (VBM) and conduction band minimum (CBM) were probed. In UPS and HIKE measurements, the relative distance between Fermi level and VBM for the pure sulfide sample was 130 meV larger than for the pure selenide. Using NEXAFS to probe the CBM, a systematic study of the positions of K- and L-absorption edges was done and the observed shifts are proportional to the relative shifts in the CBM. The experimental findings are further validated and analyzed by performing corresponding ab initio calculations using the full-potential all-electron code exciting.

30 min. Coffee Break

DF 4.7 Mon 17:00 H2

Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites — Menno Bokdam[1], Tobias Sander[1], Alessandro Stroppa[2], Silvia Picozzi[2], •D.D. Sarma[3], Cesare Franchini[1], and Georg Kresse[1] — [1]Faculty of Physics, Computational Materials Physics, University of Vienna, Austria — [2]Consiglio Nazionale delle Ricerche - CNR-SPIN, L'Aquila, Italy — [3]Indian Institute of Science, Bangalore, India

The development of high efficiency perovskite solar cells has sparked a multitude of measurements on the optical properties of these materials. For the most studied methylammonium(MA)PbI_3 perovskite, a

large range (6-55 meV) of exciton binding energies has been reported by various experiments. The existence of excitons at room temperature is unclear. For the MAPbX_3 perovskites we report on relativistic GW-BSE calculations. This method is capable to directly calculate excitonic properties from first-principles. At low temperatures it predicts exciton binding energies in agreement with the reported 'large' values. For $MAPbI_3$, phonon modes present in this frequency range have a negligible contribution to the ionic screening. By calculating the polarisation in time from finite temperature Molecular Dynamics, we show that at room temperature this does not change. We therefore exclude ionic screening as an explanation for the experimentally observed reduction of the exciton binding energy at room temperature.

DF 4.8 Mon 17:15 H2

Stable single-phase Zn-rich $Cu_2ZnSnSe_4$ through In doping — Stefan Hartnauer[1], •Sabine Körbel[2,3], Miguel A L Marques[1,3], Silvana Botti[2,3], and Roland Scheer[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France

Alloying in the system $Cu_2ZnSnSe_4$–$CuInSe_2$–ZnSe (CZTISe) is investigated experimentally and with *ab initio* calculations. The goal is to distinguish stable (single-phase) and unstable (multi-phase) regions within the pseudo-ternary phase diagram. Thin CZTISe films are prepared by co-evaporation of the chemical elements and are investigated in real-time during growth using in-situ angle dispersive X-ray diffraction (XRD). *Ab initio* calculations with density-functional theory are performed to determine the thermodynamic stability of the alloy with respect to the formation of secondary phases. Both in experiment and calculation, we find a surprisingly large single-phase region in the phase diagram for Zn-rich $Cu_2ZnSnSe_4$ if a small amount of In is present, from which we conclude that In doping may help avoiding secondary phase formation under Zn- rich conditions and open up new possibilities for the application of CZTISe thin films in solar cells.

DF 4.9 Mon 17:30 H2

Optical characterization of Cu(In,Ga)Se2 with highly spatially, spectrally, and time resolved cathodoluminescence — •Martin Müller[1], Mathias Müller[1], Frank Bertram[1], Jürgen Christen[1], Torsten Hölscher[2], Setareh Zahedi-Azad[2], Matthias Maiberg[2], and Roland Scheer[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University, Germany — [2]Martin-Luther-University Halle-Wittenberg, Germany

Potential fluctuations and transport parameters are important factors to further improve efficiencies of Cu(In,Ga)Se2 (CIGSe)solar cells. Optical properties of CIGSe absorbers have been studied by means of highly spatially and spectrally resolved cathodoluminescence (CL) to investigate lateral fluctuations and transport parameters. The measurements were performed from low temperature (T = 4.5 K) up to room temperature. CL spectra recorded at 4.5 K, exhibit a dominant emission at 1.06 eV (1170 nm). A shoulder at 1.14 eV (1090 nm) on the low energy side and at 0.99 eV (1250 nm) on the high energy side were observable. In excitation density dependent CL measurements, a blue shift of 25 meV/decade is observed. Additionally, ps-time resolved CL was performed. A dependence of the initial lifetime of more than one order of magnitude from the emission energy could be observed, illustrating relaxation of charge carriers in potential fluctuations. Investigation of panchromatic temperature dependent initial lifetimes reveals a pronounced increase up to 50 K and a subsequent decrease caused by non-radiative recombination. A concept for optical investigations of transport parameters and first results will be presented.

DF 4.10 Mon 17:45 H2

Investigation of shallow defects in $Cu(In,Ga)Se_2$ with time-resolved photoluminescence — •Torsten Hölscher, Matthias Maiberg, Setareh Zahedi-Azad, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle(Saale), Germany

Time-resolved photoluminescence (TRPL) is a powerful method to observe the recombination kinetics of minority carriers in solar cell materials like $Cu(In,Ga)Se_2$ (CIGSe). The influence of a shallow defect (traps) close to the conduction band leads to bi-exponential and curved TRPL-transients due to trapping of minority carriers. TRPL-measurements under increased device temperatures revealed a strong reduction of the second longer decay time, which is may be attributed to the temperature enhanced restitution of the trapped carriers to the conduction band. Saturation of shallow and deep defects became observable by varying the excitation of excess carriers. With Synopsys TCAD® we simulated the recombination behavior of minority carriers in CIGSe as a function of temperature and excitation in the presence of shallow defects. In comparison with the experiments, we obtained in the simulations $E_C - E_t \approx 200$ meV for the energy level, $\sigma_n \approx 10^{-13}$ cm^2 for the electron capture cross-section and $N_t \approx 10^{16}$ cm^{-3} for the density as significant parameters of the trap-state. These trap parameters closely match the N1 admittance signature detected previously - a signature which explanation has been heavily disputed. Our findings now support the explanation of the N1 defect as due to a minority carrier trap. We will discuss the influence of this trap on the solar cell performance.

DF 4.11 Mon 18:00 H2

Plasma-enhanced atomic-layer-deposited MoO_x emitters for silicon heterojunction solar cells — •Johannes Ziegler[1], Thomas Schneider[1], Alexander N. Sprafke[1], Kai Kaufmann[3,4], and Ralf B. Wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg, *μMD Group*, Institute of Physics, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM Halle, Walter-Hülse-Str. 1, 06120 Halle, Germany — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeld-Strasse 12, 06120 Halle, Germany — [4]Hochschule Anhalt Köthen, University of Applied Sciences, Bernburger Str. 55, 06966 Köthen

A method for the deposition of molybdenum oxide (MoO_x) with high growth rates at temperatures below 200 °C based on plasma-enhanced atomic layer deposition (PE-ALD) is presented. The stoichiometry of the of the over-stoichiometric MoO_x films can be adjusted by the plasma-parameters. First results of these layers acting as hole-selective contacts in silicon heterojunction (SHJ) solar cells are presented and discussed.

DF 4.12 Mon 18:15 H2

In-Situ XRD Analysis of the structural Evolution of CZTS Nanoparticles during an Annealing Process — •Marco Brandl[1], Mohamed Sayed[2], Levent Gütay[2], and Rainer Hock[1] — [1]Chair for Crystallography and Structural Physics, Friedrich-Alexander-University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany — [2]Laboratory for Chalcogenide Photovoltaics (LCP), Energy and Semiconductor Research Laboratory (EHF), Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Str. 9-11, 26111 Oldenburg, Germany

A potential method for Kesterite (Cu2ZnSnS4, CZTS) based solar cell production is the synthesis of CZTS nanoparticles by a low temperature wet chemical process. Powders of nanoparticles produced by this process are analysed by X-ray powder diffraction. Initially, these particles have a cubic disordered structure with potential hexagonal stacking faults. With the method of in-situ XRD during an annealing process up to 550°C the recrystallisation to a tetragonal structure of the CZTS as well as the healing of the hexagonal defects can be observed. Furthermore, by mixing the CZTS particles with Selenium powder, the incorporation of Se into CTZS can be studied. The time and temperature resolved observation of the change in unit cell parameters can directly be connected to the Se content in the resulting CZTSSe phase via Vegard's law.

DF 5: SYCE: Caloric effects in ferroic materials (MM with MA, DF)

Time: Monday 15:00–17:45 Location: H1

Invited Talk DF 5.1 Mon 15:00 H1

Multicaloric effects in metamagnetic Heusler materials — •Antoni Planes — Departament d'Estructura i Constituents de la Matèria. Facultat de Física. Universitat de Barcelona. Diagonal 647. 08028 Barcelona. Catalonia.

The talk is aimed at presenting a general thermodynamic framework to deal with multicaloric effects in multiferroic materials. After discussing a number of recently reported examples showing that various caloric effects may occur in the same material interdependently, the formalism will be applied to the study of mulicaloric effects taking place near the magnetostructural transition in metamagnetic Heusler shape-memory materials. This class of metamagnetic materials will be modelled by means of a Landau free energy expansion with appropriate interplay between the corresponding structural and magnetic order parameters. Caloric effects will be quantified by the isothermal entropy changes and the adiabatic temperature changes induced by application of the fields thermodynamically conjugated to the order parameters. It will be shown that multicaloric effects comprise the corresponding contributions from the effects associated with each ferroic property and the cross-contribution arising from the interplay between these properties. Finally, the obtained results will be compared with available experimental data.

Invited Talk DF 5.2 Mon 15:30 H1

Multicaloric effect in biological systems: a case of nerve action — •Matjaz Valant[1], Lawrence J. Dunne[2], Anna-Karin Axelsson[2], Florian Le Goupil[3], and George Manos[4] — [1]University of Nova Gorica — [2]London South Bank University, UK — [3]Imperial College London, UK — [4]University College London, UK

In the recent decades the "caloric community" has demonstrated the technological value of different types of reversible caloric effects induced by pulsing external fields that trigger changes in materials* order parameters. The applied research continues towards first prototypes of refrigeration systems. In addition, we have gained much better understanding of the microscopic processes related to the caloric effects, which enabled us also to recognize their occurrence and role in biological systems. We will discuss a model of nerve action, which is a natural continuation of the soliton model that considers a solitonic type pressure/density pulse propagating along the long axis of the nerve. A special emphasis has been placed on a reversible caloric response during the nerve action, which can be described as a multicaloric effect. We have calculated changes in membrane temperature, thickness, entropy and trans-membrane voltage. All of these calculated parameters are in striking agreement with experimental results. The temperature change is explained with the solitonic propagation that is iso-entropic. This observation is an important biological manifestation of the multicaloric effect, which has hitherto not being described in these terms.

Invited Talk DF 5.3 Mon 16:00 H1

Optimizing the electrocaloric effect by first-principles simulations: The role of strain and defects — •Anna Grünebohm — University of Duisburg-Essen and Cenide, Germany

The electrocaloric effect (ECE) is the adiabatic tempearture change of a material in a varying external electrical field. The ECE is promising for novel cooling devices [1]. However, in many ferroelectrics the large ECE is restricted to a narrow temperature interval.

To model modifications of the ferroelectric and electrocaloric properties of $BaTiO_3$ by defects and epitaxial strain we have combined *ab initio*-based molecular dynamics simulations with a simple model for defects [2]. For polar defects the temperature range of the large caloric response is broadened. Still more striking, a giant inverse caloric effect has been observed for the first time.

Additionally, epitaxial strain can be used to enhance the caloric response and shift the operation range [3,4]. In particular tensile strain is promising to enhance the ECE of $BaTiO_3$ around room temperature.

[1] X. Moya, *et al.*, Nature Mater. **13**,439 (2014)
[2] A. Grünebohm, *et al.*, arXiv:1502.05201
[3] M. Marathe, *et al.*, APL **104**, 212902 (2014)
[4] A. Grünebohm, *et al.*, APL **107**, 102901 (2015).

15 min. coffee break

Invited Talk DF 5.4 Mon 16:45 H1

Giant inverse barocaloric effects in ferrielectric ammonium sulphate — Pol Lloveras[1], Enric Stern-Taulats[2], Maria Barrio[1], Josep Lluis Tamarit[1], Sam Crossley[3], Wei Li[3], Vladimir Pomjakushin[4], Antoni Planes[2], Lluis Mañosa[2], Neil Mathur[3], and •Xavier Moya[3] — [1]Departament de Física i Enginyeria Nuclear, ETSEIB, Universitat Politècnica de Catalunya, Diagonal 647, Barcelona, 08028 Catalonia, Spain — [2]Facultat de Física, Departament d'Estructura i Constituents de la Matèria, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Catalonia, Spain — [3]Department of Materials Science, University of Cambridge, Cambridge, CB3 0FS, UK — [4]Paul Scherrer Institute, WHGA/133, 5232 Villigen - PSI, Switzerland

Giant barocaloric effects driven by hydrostatic pressure have been suggested for cooling applications, but they are only seen in a small range of magnetic materials that are relatively expensive. Here I will present pressure-dependent calorimetry data to demonstrate giant inverse barocaloric effects in ferrielectric ammonium sulphate, which is made of cheap abundant elements [Lloveras et al., Nature Communications, in press].

Invited Talk DF 5.5 Mon 17:15 H1

TiNiCu-based thin films for elastocaloric cooling — •Eckhard Quandt and Christoph Chluba — Chair of Inorganic Functional Materials, Institute for Materials Science, Faculty of Engineering, University of Kiel, Germany

The elastocaloric effect is a promising alternative for the replacement of conventional vapor compression cooling which suffers from a high environmental impact and limited efficiency improvement possibilities. Instead of a vapor-liquid transition in a conventional cooling, the elastocaloric effect is based on a stress induced structural phase transition usually from a high symmetry to a low symmetry phase. At adiabatic conditions this results in a temperature change of the material. For a continuous use of this effect in a cooling cycle, several requirements have to be fulfilled. Transformation temperatures, effect size and efficiency have to be suitable, but most importantly a high functional and structural fatigue resistance is necessary.

Highly fatigue resistant Ti-rich TiNiCu compositions prepared by thin film technology have been found that can withstand 10 million transformation cycles without functional degradation [1]. Within this talk the reasons for the fatigue resistance will be discussed. In situ synchrotron and TEM investigations have been conducted to investigate the underlying microstructural mechanisms that ensure the reversible transformation. Cobalt and iron addition is used to adjust the transformation temperature to a suitable range to enable the use of this compositions at room temperature. The compositional influence on the elastocaloric parameters is investigated by temperature dependent tensile tests, infrared (IR) thermography and differential scanning calorimetry. Due to the small hysteresis of TiNiCu-based compositions an improved elastocaloric cooling efficiency is found in comparison to binary NiTi thin films. Considering also the high fatigue resistance, this class of materials is promising for future elastocaloric cooling applications.

[1] Chluba, C.; Ge, W.; Lima de Miranda, R.; Strobel, J.; Kienle, L.; Quandt, E.; Wuttig, M.: Ultralow-fatigue shape memory alloy films, Science 348 (2015), 1004-1007.

DF 6: Focus Session: Applications of Dielectric Materials in Microwave Technology

Organized by Theo Scherer

Time: Monday 15:00–18:40 Location: H26

Topical Talk DF 6.1 Mon 15:00 H26

CVD diamond for nuclear fusion experiments — •Eckhard Wörner and Christoph Wild — Diamond Materials GmbH, Freiburg, Germany

Its outstanding physical properties make diamond an ideal material for demanding optical and thermal applications and the possibility to grow diamond by Chemical Vapor Deposition (CVD) finally makes it available for industrial use.

While it's common knowledge that diamond is the hardest material only few people know that it is also the material with the highest thermal conductivity, Debye Temperature and atomic density. In addition it's chemically inert, consists of lightweight strongly bound carbon atoms and is optical transparent from the ultraviolet to the far infrared. So it should come as no surprise that fusion experiments take advantage of its unique properties. Inertial confinement fusion uses hollow diamond spheres as capsules to be filled with deuterium and tritium whereas magnetic confinement fusion uses diamond windows to seal the torus from ambient atmosphere while being transparent for ultra-high power microwave radiation.

Diamond Materials GmbH, a Fraunhofer Spin-Off founded about 10 years ago, is one of the leading companies in the world that can grow large area optical grade CVD diamond. In our presentation we will describe growth and processing and focus on the preparation of diamond windows and spheres for nuclear fusion experiments.

Topical Talk DF 6.2 Mon 15:30 H26

Torus Diamond Window for the ITER ECRH Upper launcher — •Sabine Schreck, Gaetano Aiello, Giovanni Grossetti, Francesco Mazzocchi, Andreas Meier, Peter Spaeh, Dirk Strauss, Alessandro Vaccaro, and Theo Scherer — Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

The ITER ECRH window consists of an ultra-low loss CVD diamond disk mounted in a system of metallic parts (Cu/SS). It has to fulfil adequate transmission capability for high power mm-waves, is part of the primary vacuum boundary of the ITER vacuum vessel and has the function of tritium confinement. Being classified as Protection Important Component, high requirements for quality and safety apply to the window. The window assembly cannot be entirely covered by codes and standards and therefore an ad-hoc qualification program is required including the testing of prototypes. Both, structural integrity and the mm-wave transmission capability shall be demonstrated. At KIT, dedicated FABRY-PEROT-resonators are available, to measure the loss tangent of the diamond disk and also its distribution over the disk area. The window design has been improved based on the gained experience with former prototypes of which the second one was already optimized with regard to its mm-wave properties. Recently, the design for two new prototypes has been developed and, after manufacturing, they will be qualified by passing a dedicated test program. First results on the qualification of the bare diamond disks for the prototypes are already available and show a very low dielectric loss.

DF 6.3 Mon 16:00 H26

Requirements for materials in high power mm-wave systems for Nuclear Fusion applications — •Giovanni Grossetti, Gaetano Aiello, Francesco Mazzocchi, Andreas Meier, Theo Scherer, Sabine Schreck, Peter Spaeh, Dirk Strauss, and Alessandro Vaccaro — Karlsruhe Institute of Technology (Institute of Applied Materials), P.O. Box 3640 76021 Karlsruhe Germany

Material science is a key ingredient for granting the success of a complex project like Nuclear Fusion and a great effort is placed to verify and validate components that will work under very harsh conditions in future fusion power plants.

In this paper we present an overview of the requirements for materials which shall be met for ensuring a high reliability, addressing to a specific system called Electron Cyclotron Heating and Current Drive system (hereafter, ECH&CD). Its goals and objectives are to provide heating and driving current into a Deuterium-Tritium plasma, by injecting localized high power mm-wave for plasma assisted breakdown, ramp up/down, pure heating, impurities control, disruption control and to mitigate plasma instabilities like the sawtooth and the Neoclassical Tearing Mode (NTM).

With respect to materials, the main issues are due to the high neutron flux that can cause material activation, to the high power (MW) of the mm-wave used and to safety, in order to grant Tritium compatibility of components like diamond window assemblies.

Topical Talk DF 6.4 Mon 16:20 H26

Double-disc Diamond Windows for Fusion Applications — •Alessandro Vaccaro, Gaetano Aiello, Giovanni Grossetti, Francesco Mazzocchi, Andreas Meier, Theo Scherer, Sabine Schreck, Peter Spaeh, and Dirk Strauss — Karlsruhe Institute of Technology (Institute of Applied Materials), P.O. Box 3640 76021 Karlsruhe Germany

Diamond windows are employed in Electron-Cyclotron Heating & Current Drive (EC H&CD) systems in fusion devices. By injecting high-power mm-waves beams, these systems heat up the plasma and counteract the formation of instabilities. Acquiring a complete understanding of what happens during operation of diamond windows is an important task. In fact, such units handle powers in the order of Megawatts and therefore small resonant cavities can easily become sources of high-intensity localized heating.

In this paper, we investigate a unit with a double-disc configuration. The study aims to evaluate localized power deposition on the unit's cooling channels and is carried out by developing a ray-tracing code that uses a hybrid approach; our code accounts for the waves' phase and thus reproduces the effects of interference. This goal is achieved by calculating reflection/transmission coefficients under the hypothesis of thin films and applying them only to the incident and back-refracted waves. The results show that mm-wave beams in off-axis position are potentially responsible of high heat flux deposition on the cooling channels that can, in turn, trigger nucleated boiling of the cooling water.

20 min break

Topical Talk DF 6.5 Mon 17:10 H26

Dielectric Characterization for Industrial Microwave Applications — •Sergey Soldatov, Vasileios Ramopoulos, Guido Link, and John Jelonnek — Kalsruher Institute of Technology IHM, Germany

Volumetric and selective heating of dielectric materials is a unique feature of microwave heating technology, that can provided a significant reduction in processing time and increase in energy efficiency. Therefore the use of microwave technology faces growing interest in various fields of industrial applications. As any production technology so also microwave assisted processes typically need process specific and optimized system designs. Those typically can be realized by electromagnetic and multiphysics simulations. The inevitable basis for this is a detailed knowledge about the dielectric behavior of any material involved at the frequency and temperature range of interest. This includes potential tooling materials as well the processed goods. In case the process leads to irreversible modification of those materials, due to phase changes or chemical reactions, than beside the temperature dependence the time dependence of the dielectric properties is of interest as well. Based on this, specific in-situ measurement techniques have been developed at KIT based on the transmission reflection method as well as the cavity perturbation method in the 2.45 GHz ISM-band. The system design of those dielectric test sets will be presented and discussed including some experimental results on specific materials.

DF 6.6 Mon 17:40 H26

A drying and thermoelastic model for microwave ablation of concrete — •benjamin Lepers — KIT, IHM, Hermann von Helmholtz Platz 1, 76344 Eggenstein Leopoldshafen

The use of high power microwaves to perform explosive spalling of concrete surfaces is a promising technique with applications in the area of concrete facilities decommissioning. The mechanism that creates explosive spalling is due to a combination of the thermal stress from high temperature gradients and the pore pressure generated from the water vaporization and water transport through a porous medium. In this

paper a one dimensional model solving the heat and diffusion equations for liquid and vapor phase with the COMSOL Multiphysics finite element software is presented. The modelling of the drying process is based on the spatial reaction engineering approach (SREA). This paper discusses the influence of the relative activation energy parameter and effective diffusion coefficients on the temperature, water content and pore pressure in the case of fast microwave heating of concrete. This model is then used for a 3d geometry with a sealed insulated block of concrete and an conical waveguide antenna to compute the thermal stress, pore pressure and total stress.

DF 6.7 Mon 18:00 H26

Stoichiometry effect on microwave properties of all-oxide BST thin film varactors — •Patrick Salg[1], Arzhang Mani[1], Mohammad Nikfalazar[2], Aldin Radetinac[1], Rolf Jacoby[2], Lambert Alff[1], and Philipp Komissinskiy[1] — [1]Institute of Materials Science, TU Darmstadt, Germany — [2]Institute for Microwave Engineering and Photonics, TU Darmstadt, Germany

We present all-oxide ferroelectric varactors using a bottom electrode of the highly conducting perovskite $SrMoO_3$ [1]. Thin-film epitaxial heterostructures of $SrMoO_3$ with a room-temperature resistivity of 30 $\mu\Omega$cm and the functional tunable dielectric $Ba_xSr_{1-x}TiO_3$ with ($x = 0.2 - 0.6$) were grown by pulsed laser deposition. As top electrode, sputtered amorphous Au/Pt layers were used and patterned by lift-off. The effect of stoichiometry of the $Ba_xSr_{1-x}TiO_3$ layer on the microwave properties of the varactors was investigated at frequencies up to 10 GHz at room temperature. A zero-bias quality factor of the varactors with $Ba_{0.4}Sr_{0.6}TiO_3$ of 110 at 1 GHz and 20 at 10 GHz was achieved. These values are more than 10 times higher than the ones previously reported in the literature for varactors with other oxide electrodes. The capacitance tunability of the varactors is above 50% at 8 V and stable in a broad frequency range from 100 MHz up to 10 GHz. The obtained results suggest a high potential of all-oxide ferroelectric varactors for microwave applications.

[1] A. Radetinac *et al.*, *Highly conducting $SrMoO_3$ thin films for microwave applications*, Appl. Phys. Lett. **105**, 114108 (2014).

DF 6.8 Mon 18:20 H26

Dielectric materials for high frequency detector applications — •Theo Scherer — KIT Karlsruhe, IAM-AWP

Superconducting detectors like Hot-Electron-Bolometers (HEBs) are used for the detection of signals in radioastronomy in the range of several hundrets of GHz up to THz. The dielectric properties and the phonon-conductance of substrate materials is essential for the 3dB-bandwidth of such a device. A comparison of different appropriate dielectrics is shown and the best candidates for real sensor devices will be discussed.

DF 7: Focus Session: Ferroic Domain Walls I

Fascinating correlation physics, such as superconductivity and magnetoelectric coupling, occur at domain walls in complex oxides even when forbidden in the surrounding bulk. These unusual interface phenomena and their hypersensitivity to external stimuli are of great academic and technological interest, and are currently intensively studied. This session focuses on recent and future developments in the rapidly growing field of domain and domain-wall engineering, related functionality, key concepts and materials, as well as advanced characterization methods. In total, the session consists of three parts (DF7, DF9, DF11) and one poster session (DF12)

Organized by Elisabeth Soergel and Dennis Meier

Time: Tuesday 9:30–13:00 Location: H25

Invited Talk DF 7.1 Tue 9:30 H25

Spin and charge transport in multiferroic domain walls — •Ramamoorthy Ramesh — University of California, Berkeley

Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. The basic materials physics of such materials provide the ideal playground for interdisciplinary scientific exploration. Among the large number of materials systems, there exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics. Domain walls may play an important role in future electronic devices, given their small size as well as the fact that their location can be controlled. We reported the observation of room-temperature electronic conductivity at ferroelectric domain walls in the insulating multiferroic BiFeO3. The origin and nature of the observed conductivity were probed using a combination of conductive atomic force microscopy, high-resolution transmission electron microscopy and first-principles density functional computations. Our analyses indicate that the conductivity correlates with structurally driven changes in both the electrostatic potential and the local electronic structure, which shows a decrease in the bandgap at the domain wall. Subsequent work in our program has demonstrated several key features of domain wall transport in manganites. Of course, one dream is to be able to create *metallic* walls in a ferroelectric matrix. I will describe our efforts in this direction.

DF 7.2 Tue 10:10 H25

Roughness, dynamics and conduction at domain walls in $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films — •Philippe Tückmantel[1], Iaroslav Gaponenko[1], Benedikt Ziegler[1], Joshua Agar[2], Lane Martin[2], and Patrycja Paruch[1] — [1]DQMP, University of Geneva — [2]MSE, University of Berkeley

Defects and electrostatic boundary conditions greatly impact the geometry and growth dynamics of polarization domains in ferroelectric thin films. In PZT we have shown that defect pinning and screening by surface water determine the roughness and creep dynamics of 180° domain walls. Surface adsorbates and defects can also reversibly control domain wall conduction. However, there has not been a detailed study considering specifically the interrelation of domain wall roughness and local conductance variations.

Here, we present our results on PZT thin films grown simultaneously on STO, DSO, GSO, and LSAT substrates to address this. Substrate choice provides control over the defect density, while ultra-high vacuum (UHV) thermal annealing allows removal of surface adsorbates, thus providing an opportunity to study the role of defects and adsorbates on the functional and fundamental ferroelectric domain walls.

Using piezoresponse force microscopy at ambient conditions as well as in UHV, we study the effect of the substrate and surface adsorbates on the roughness and growth dynamics of domains as well as on the conduction behaviour of the domain walls, thus providing insight into the effect of the substrate on the intrinsic defect configuration of the overlying films.

DF 7.3 Tue 10:30 H25

Variable arrangement of domain walls in monoclinic $K_{0.9}Na_{0.1}NbO_3$ epitaxial films on $NdScO_3$ substrates — •Jutta Schwarzkopf[1], Dorothee Braun[1], Toni Markurt[1], Michael Hanke[2], and Martin Schmidbauer[1] — [1]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin — [2]Paul-Drude Institute, Hausvogteiplatz 5-7, 10117 Berlin

Many macroscopic characteristics of ferroelectric materials are directly related to the physical properties of domains and domain walls. Therefore it is crucial to investigate structure, size and orientation of domains including their domain walls in order to get a fundamental understanding of formation mechanisms and functionality of domain wall, especially with regard to the incorporated lattice strain. In contrast to films with tetragonal, rhombohedral or orthorhombic symmetry the domain walls of monoclinic phases in $K_xNa_{1-x}NbO_3$ exhibit variable orientation depending on the components of the spontaneous strain tensor allowing the targeted alignment of the domain walls. In this

study $K_{0.9}Na_{0.1}NbO_3$ thin films were grown under anisotropic lattice strain on $NdScO_3$ (NSO) substrates by metal-organic chemical vapor deposition. Lateral PFM images reveal bundles of ferroelectric domains along the $[001]_{NSO}$ direction of the substrate. They are superimposed by smaller domains forming regularly ordered herringbone patterns which can be described by alternately arranged monoclinic M_C/a_1a_2 domains. The in-plane angle $\pm\alpha$ between the twin domain walls and the $[1\text{-}10]_{NSO}$ direction is determined by the incorporated lattice strain and can intentionally be adjusted between 15° and 45°.

DF 7.4 Tue 10:50 H25

Probing the interaction of surface adsorbates with ferroelectric domains — •Iaroslav Gaponenko[1], Nicolas Stucki[2], Albert Verdaguer[3], and Patrycja Paruch[1] — [1]DQMP, University of Geneva, 1211 Geneva, Switzerland — [2]University of Applied Sciences Western Switzerland in Geneva (HES-SO/hepia), 1213 Geneva, Switzerland — [3]Institut Català de Nanociència i Nanotecnologia (ICN2), Campus UAB, 08193, Bellaterra (Barcelona), Spain

Surface adsorbates are an ubiquitous presence on all materials exposed to ambient environmental conditions. Water, in particular, by virtue of its polar nature, has been shown to interact strongly with domains and domain walls in ferroelectric materials. We have previously focused on the influence of water on polarisation switching dynamics in Pb(Zr0.2Ti0.8)O3 thin films, and demonstrated its key role (together with redistribution of oxygen vacancies) in the reversible control of electrical transport at 180° domain walls in this material. However, in these systems the reciprocal effect of polarization also needs to be considered, as it will induce changes in the physics of surface adsorbates.

Here, we present our studies of the interaction of adsorbed water with the surface of thin films of Pb(Zr0.2Ti0.8)O3 by combined topographical and electrostatic force microscopy imaging. Comparing domains written with positive and negative tip voltage, and the as-grown state of the film, we map out the changes in the strength of the electrostatic interactions between the microscopy tip and surface as a function of changing humidity, and demonstrate that the surface arrangement of the water depends on the ferroelectric domain orientation.

20 min. break

Topical Talk DF 7.5 Tue 11:30 H25

Conduction and Diode Behaviour in Charged Domain Walls — •Michael Campbell — Queens University Belfast, Belfast, Northern Ireland, UK

It is now clear that ferroelectric domain walls can have functional properties distinct from bulk. Charged domain walls (or CDWs), at which discontinuities in polarisation occur, have been of particular interest, as they are often associated with strong enhancements in localised conductivity[1-2]. Moveable conducting CDWs could have obvious implications for new forms of *domain wall electronics* and are hence worthy of focused study.

Here we present a multi-faceted investigation into CDWs. We have directly measured dc conduction and used Hall voltage measurements to determine carrier types, densities and mobilities in CDWs in both rare-earth manganites and lithium niobate (LNO). We have probed the properties of naturally forming p-n junctions in domain wall intersection points in ErMnO3 and have directly written CDW p-n junctions using AFM in LNO. 2D diode structures have thus been observed and created within CDWs. We have also seen how direct injection of electrons using Scanning Electron Microscopy can affect the conduction properties of CDWs.

[1]M. Y. Gureev et al. Phys. Rev. B 83, 184104 (2011)
[2]D. Meier et al. Nat. Mat. 11, 284-288 (2012)

DF 7.6 Tue 12:00 H25

A closer look inside out - Domain wall functionalities in $LiNbO_3$ single crystals go 3D — •Alexander Haussmann[1], Thomas Kämpfe[1], Christian Godau[1], Philipp Reichenbach[1], André Gemeinhardt[1], Anna-Sophie Pawlik[2], Andreas Koitzsch[2], Lars Kirsten[3], Edmund Koch[3], and Lukas Eng[1] — [1]Institut für Angewandte Physik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden — [2]IFW Dresden, Helmholtzstr. 20, 01069 Dresden — [3]TU Dresden, Medizinische Fakultät, Klinisches Sensoring und Monitoring, Fetscherstr. 74, 01307 Dresden

Both the discoveries of domain-wall (DW) localized photochemistry and DW conductivity have dramatically broadened the huge interests in ferroelectric $LiNbO_3$ for the last decade. Surprisingly, it turned out that the DW geometries in this material differ consistently from the ideal equilibrium "textbook" arrangement of 180° domain walls: Low inclinations with respect to the polar (z) axis ($< 0.5°$) as well as unexpectedly complex topologies have been regularly observed, depending on composition, doping and subsequent heat treatment of the material. Here, we combined multiple 2D and 3D methods in order to achieve a comprehensive characterization of both the geometry and the resulting electronic properties of DWs in $LiNbO_3$. The portfolio of techniques contributing to this study range from high-resolution surface-sensitive techniques (such as PFM, cAFM, KPFM, PEEM) to complementary optical methods allowing for a full 3D inspection (Cherenkov SHG, interferometric quasi-phase-matched SHG, multiphoton photoluminescence, optical coherence tomography).

DF 7.7 Tue 12:20 H25

Methods to create electronically compensated charged domain walls in ferroelectrics without scanning probe techniques — •Tomas Sluka[1], Arnaud Crassous[1], Petr Bednyakov[1], Igor Stolichnov[1], Ludwig Feigl[1,2], Dragan Damjanovic[1], Alexander Tagantsev[1], and Nava Setter[1] — [1]EPFL - Swiss Federal Institute of Technology, Lausanne, Switzerland — [2]Karlsruhe Instute of Technology, Karlsruhe, Germany

Charged Domain Walls (CDWs) in ferroelectrics were predicted to be metallicaly conducting interfaces that can be positioned inside a monolith of nominally insulating materials. Such CDWs are thus promising elements for the envisaged reconfigurable nanoelectronics. Indeed, highly elevated conductivity was observed at CDWs in several ferroelectric materials. The progress towards CDW exploitation is however hindered by the absence of practical CDW engineering techniques. CDWs were found either locked in as grown patterns, were created locally with scanning probe techniques or stochastically with defect assisted compensation. Here we introduce a set of methods which allow to create electronically compensated CDWs without the need of a scanning probe tip or presence of charged defects. The methods range from the use of superbandgap illumination which generates free carries that compensate appearing CDWs to the use of inhomogeneous electric fields and electron injection inside nanoscale structures. It will be shown that CDWs can be reliably produced in forms of large regular patters or few-nanometes long precisely positioned channels. These methods open the doors to the advanced investigation of CDWs.

DF 7.8 Tue 12:40 H25

Tools in study of abnormal photovoltaic effects at domain walls — Mingmin Yang and •Marin Alexe — University of Warwick, Department of Physics, CV4 7AL, Coventry, UK

In the recent past, the field of anomalous photovoltaic effect in non-centrosymmetric perovskite ferroelectric oxides has been revitalized by the reports of photovoltaic effect (PVE) in BiFeO3 (BFO). The microscopic origins of this effect are still under debate. Initial investigations on BFO films assumed that the PVE in BFO is primarily due to the presence of a potential step at the ferroelectric domain walls (DWs). In order to study the PV effect at DWs we need to use characterisation methods that would deliver information at the same characteristic length as DWs. We have developed local photoelectric measurement such as photo-induced transient spectroscopy (PITS) which bring valuable data regarding generation and recombination of the photo-excited carriers. We will present in detail PITS-SPM and data regarding generation and recombination speed at DWs in BFO.

DF 8: Focus Session: Ferroic Domain Walls II

Time: Tuesday 14:00–16:00 Location: H25

Topical Talk DF 8.1 Tue 14:00 H25

Microscopic order parameters coupling at domain walls and its effect on macroscopic properties — •Saeedeh Farokhipoor — Device Materials Group, University of Cambridge, Cambridge, UK

Domain and domain wall (DW) engineering provides an alternative model to tune the physical properties of materials, typically done via conventional materials chemistry. The interplay of coexisting non-ferroelectric structural order parameters, ferroelectric and magnetic order parameters at the DWs in hexagonal manganites provides a new pathway to determine macroscopic properties by tuning the DW characteristics [1]. Here, I report different types of domain structures and DW types associated with the crystal growth conditions in hexagonal manganites. I show that differences in the DW polar state manifest themselves as variations in the conductivity measured macroscopically. In addition, local piezo force microscopy and X-ray diffraction enable us to determine the plane of the DWs and hence, their strain state. The latter findings are in very good agreement with the topographical study. Finally, these results show that DWs under strain lower the critical field of the magnetic phase transition compared to samples with strain-free DWs. In conclusion, I show that among all the complexity in the behavior and response of nano-features, it is possible to tune macroscopic responses by understanding the local state properties, which can be adjusted as easily as by thermal annealing and/or by the crystal growth method. [1] S. Artyukhin et al., Nat. Mater. 13 (2014)

DF 8.2 Tue 14:30 H25

Low-temperature study of semiconducting domain walls in hexagonal manganites — •Peggy Schönherr[1], Jakob Schaab[1], Andres Cano[2], Manfred Fiebig[1], and Dennis Meier[1] — [1]ETH Zürich, Switzerland — [2]CNRS, University Bordeaux, France

Unusual electronic properties arise at domain walls in semiconducting ferroelectrics due to the local electrostatics, their low symmetry and strain. The hexagonal manganites are a particularly interesting example as their improper ferroelectricity naturally leads to simultaneous formation of neutral side-by-side and charged head-to-head and tail-to-tail domain walls. These domain-wall states allow for accessing a wide variety of phenomena, so that the hexagonal manganites represent an ideal playground for studying domain-wall nanoscale physics.

Here, we will discuss temperature-dependent variations in the electronic domain-wall transport in the semiconductor $Er_{1-x}Ca_xMnO3$. Using low-temperature atomic force microscopy we monitor the ferroelectric domain pattern and investigate changes in the electronic properties of the domain walls for temperatures between 295 K and 4.2 K. Our data demonstrate that the domain walls adopt the basic p-type semiconducting properties of the host materials. Additional modulations in the Schottky barrier, electronic conductance and screening arise according to the local domain-wall charge state. Our result clarify pending questions about the low-temperature performance and stability of charged domain walls and provide new insight to the general domain-wall physics in semiconducting ferroelectrics.

DF 8.3 Tue 14:45 H25

Controlling electronic domain-wall conductance by charge-carrier doping — •Jakob Schaab[1], Andres Cano[2], Hatice Doganay[3], Daniel Gottlob[3], Ingo P Krug[4], Claus M Schneider[3], Ramamoorthy Ramesh[5], Manfred Fiebig[1], and Dennis Meier[1] — [1]ETH Zürich — [2]CNRS, Univ. Bordeaux — [3]FZ Jülich — [4]TU Berlin — [5]UC Berkeley

The electronic transport at ferroelectric domain walls bears great application potential in the field of nano-electronics. The precise control and optimization of domain-wall properties towards technologically useful regimes, however, remains a major challenge. A promising but largely unexplored route is to implant specific acceptor or donor atoms, as known from conventional semiconductor physics, and thereby tailor the performance of the domain-wall transport. Here, we discuss to the perspectives of charge-carrier doping for tuning the electronic transport properties at ferroelectric domain walls. In $Er_{1-x}Ca_xMnO_3$ we modify the domain-wall conductance by replacing trivalent Er^{3+} for divalent Ca^{2+}. A doping level of 1% is found to enhance the local conductance by a factor of ≈ 50. In addition, leakage effects at the domain walls are suppressed, reducing their effective width by about 50%. The higher conductance, together with the reduced domain-wall width, leads to a significant enhancement of the current density carried by the walls, which we characterize using scanning probe and photoemission electron microscopy. Our study demonstrates chemical charge-carrier doping as powerful and easily controllable approach for engineering and improving the functionality of ferroelectric domain walls.

DF 8.4 Tue 15:00 H25

Anisotropic Domain Wall Conductivity in $LiNbO_3$ single crystals — •Shuyu Xiao[1,2], Thomas Kämpfe[2], Yaming Jin[1], Alexander Haussmann[2], Xiaomei Lu[1], and Lukas Eng[2] — [1]Physics School, Nanjing University, 210093 Nanjing, P. R. China — [2]Institution of Applied Photophysics, Technical University of Dresden, 01062 Dresden, Germany

Nowadays, investigating the origin and nature of domain wall conductivity (DWC) in different ferroelectric materials such as BFO [1,2] and PZT thin films [3], but equally in $LiNbO_3$ (LNO) single crystals [4,5] are of broad scientific interest. The work presented here reports on anisotropic DWC found between head-to-head (h2h) and tail-to-tail (t2t) 180° DWs in z-cut PPLN single crystal, as measured with Tunneling AFM (ICON) and Optimized Resistance Conductance Amplifier (Cypher). The three dimensional polarization distribution is analyzed at the same position via Piezoresponse Force Microscopy and Cherenkov Second Harmonic Generation. The origin of the different DWC between h2h and t2t is studied by both phenomenological theories and dipole modeled tunneling simulations. As a conclusion, the different conductivities might arise due to the differently charged DWs, as results from the DW inclination with respect to the z-axes.

[1] J. Seidel et al., Nat. Mater. **8**, 229 (2009).
[2] S. Farokhipoor et al., Phys. Rev. Lett. **107**, 127601 (2011).
[3] J. Guyonnet et al., Adv. Mater. **23**, 5377 (2011)
[4] M. Schröder er al., Mater. Res. Express. **1**, 035012 (2014)

DF 8.5 Tue 15:20 H25

Enhancing the domain wall conductivity in lithium niobate single crystals — •Christian Godau, Thomas Kämpfe, Andreas Thiessen, Alexander Haussmann, and Lukas Eng — Institute of Applied Physics, Technische Universität Dresden, D-01062 Dresden, Germany

Highly conductive ferroelectric domain walls (DWs) were found for thin films [1] as well as single crystals [2]. In lithium niobate (LNO) this effect was forecast by theoretical considerations [3]. However, such a high conductivity has so far only been reported under support super band-gap illumination [4]. We show here that high voltage treatment of domain walls in bulk lithium niobate single crystals when applying voltage ramps of up to 1 kV to macroscopic electrodes, results in the desired high conductivity as well. An increase in domain wall conduction of several orders of magnitude can then be measured. High voltage treatment also affects the 3-dimensional domain wall shape, which was complementary delineated Cerenkov second harmonic generation (C-SHG) [5]. As a result, we are able to correlate the local domain wall conductive paths (measured by cAFM) to the DW inclination angle as deduced by C-SHG.

[1] J. Seidel et al., Nat. Mater. 8, 229 (2009)
[2] T. Sluka et al., Nat. Comm. 4, 1808 (2013)
[3] E. A. Eliseev et al., Phys. Rev. B 83, 235313 (2011)
[4] M. Schroeder et al., Adv. Funct. Mater. 22, 3926 (2012)
[5] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014)

DF 8.6 Tue 15:40 H25

Imaging of conducting domain walls in lithium niobate with energy filtered photoelectron microscopy — •Anna-Sophie Pawlik[1], Andreas Koitzsch[1], Thomas Kämpfe[2], Andreas Haussmann[2], Martin Knupfer[1], Lukas Eng[2], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, D-01069 Dresden, Germany — [2]Institute for Applied Photo Physics, Technical University Dresden, D-01069 Dresden, Germany

Conductive domain walls (CDWs) in ferroelectrics are an intensively investigated novel topic in solid state research. However, up to now the chemical structure of CDWs and the microscopic origin of conductance is still hidden. The conducting behaviour of the material

is investigated by means of energy filtered photoelectron microscopy (PEEM).

We confirmed that head-to-head domain walls are more conducting than the hosting bulk insulator by means of secondary electron emission upon x-ray illumination. Yet tail-to-tail domain walls are insulating, in accordance to theory. The conductive property depends considerably on the DW inclination angle relative to the polar axis: the more the angle deviates from 90°, the lower the conductance.

Additionally we investigated 180° domain walls with energy filtered PEEM. We could resolve a contrast for different domains due to a work function difference of c^+ and c^- surfaces. The domain walls itself were not visible in PEEM measurements. With this we confirmed the insulating properties of the 180° domain walls

DF 9: Focus Session: Skyrmions meet Multiferroicity

Bridging the gap between multiferroicity and skyrmions, which are themselves of high importance for new electronic building blocks, is an upcoming challenge. Recently, magnetoelectric effects and ferroelectric phases were demonstrated in insulating skyrmion crystals comprising novel mechanisms of complex magnetic and unconventional ferroelectric order. The focus session introduces the new field of skyrmion dielectric solids and aims at an inspiring interdisciplinary discussion.

Organized by Stephan Krohns

Time: Wednesday 9:30–12:50 Location: H25

Topical Talk DF 9.1 Wed 9:30 H25

Functional domain walls in multiferroics — •Dennis Meier — ETH Zürich, Switzerland

During the last decade a wide variety of novel and fascinating correlation phenomena has been discovered at domain walls in multiferroic bulk systems, ranging from unusual electronic conductance to inseparably entangled spin and charge degrees of freedom. The domain walls represent quasi-2D functional objects that can be induced, positioned, and erased on demand, bearing considerable technological potential for future nanoelectronics. Most of the challenges that remain to be solved before turning related device paradigms into reality, however, still fall in the field of fundamental condensed matter physics and materials science. In my talk I will provide an overview of seminal experimental findings gained on electric and magnetic domain walls in multiferroic bulk materials. A special focus is put on the physical properties that emerge at so-called charged domain walls and the added functionality that arises from coexisting magnetic order. The goal is to draw attention to the persistent challenges and identify future key directions for the research on functional domain walls in multiferroics.

DF 9.2 Wed 10:00 H25

Dielectric properties of the spin driven multiferroic linarite — •Alexander Ruff, Theresa Mack, Stephan Krohns, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

In the last decade various mechanisms for coupled polar and magnetic ordering, so called multiferroicity, were discovered. Among various multiferroic systems, spin-driven ferroelectrics are in the scientific focus due to a close coupling of spin and charge leading to cross-link control of magnetic and electric order. These systems have noncollinear spin structures, e.g., magnetic phases with spiral or helical order. Thus, two canted neighbouring spins S_i and S_j allow for inverse Dzychaloshinskii-Moriya interaction resulting in spin-driven ferroelectric polarization P via $P = Q \times (S_i \times S_j)$, where Q denotes the propagation vector of the spin spiral. Those complex magnetic phases often reveal unconventional magnetic behaviour, which can be found in frustrated quantum spin systems, like $LiCuVO_4$ or the naturally grown single crystal linarite, $PbCuSO_4(OH)_2$.

Here we present the dielectric properties as well as the ferroelectric polarization obtained via pyro- and magnetocurrent measurements, both in applied magnetic fields up to 9 T. Their analysis allows validating the theoretical prediction of $P = Q \times (S_i \times S_j)$. Compared to prototypical $LiCuVO_4$, linarite crystallizes monoclinic leading to a more complex relation of crystallographic direction, ferroelectric polarization and spin spiral axis. Finally, we provide (H,T)-diagrams for the multiferroic phase of linarite.

Topical Talk DF 9.3 Wed 10:20 H25

Neutron scattering study of the cycloidal and Néel-type skyrmion lattice phases of GaV_4S_8 — •Sándor Bordács[1], Jonathan S White[2], Nicole Reynolds[2,3], Charles D Dewhurst[4], Henrik M Rønnow[3], Vladimir Tsurkan[5], Alois Loidl[5], and István Kézsmárki[1] — [1]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [2]Laboratory for Neutron Scattering and Imaging, PSI, Villigen, Switzerland — [3]Laboratory for Quantum Magnetism, EPFL, Lausanne, Switzerland — [4]Institut Laue-Langevin, Grenoble, France — [5]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

Recently, it was shown that not just whirlpool-like i.e. Bloch-type skyrmions but also Néel-type skyrmions formed by spin cycloids can exist in nature and the polar crystal symmetry of the Mott-insulator GaV_4S_8 can host this new kind of topological magnetic structures [1].

Here, we report the results of polarized small angle neutron scattering (SANS) experiments in the magnetically ordered phases of GaV_4S_8. We could experimentally demonstrate that the modulated magnetic states of GaV_4S_8 are formed by spin cycloids, thus, the helicity state of the skyrmions is compatible with the Néel type. Based on SANS experiments we also revealed that the orientation of the cycloidal wave vector is weakly pinned within the rhomboheral plane. Furthermore, the temperature vs. magnetic field phase diagram of GaV_4S_8 is systematically studied.

[1] I. Kézsmárki, et al., Nature Materials 14, 1116 (2015).

DF 9.4 Wed 10:50 H25

Real-space inspection of Skyrmion lattices with confined orientation in the multiferroic semiconductor GaV_4S_8 — •Erik Neuber[1], Peter Milde[1], Istvan Kézsmárki[2], and Lukas Eng[1] — [1]Institut für Angewandte Physik, TU Dresden, D-01069 Dresden, Germany — [2]Department of Physics, Budapest University of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, Hungary

Following early predictions, skyrmion lattices (SkL) constituting a periodic array of spin vortices have now been reported to exist in various magnetic crystals mostly with chiral structure. Although non-chiral but polar crystals with C_{nv} symmetry were identified as ideal SkL hosts, this archetype of SkL has remained experimentally unexplored. In this contribution, we report on the discovery and real-space exploitation of a SkL in the multiferroic polar magnetic semiconductor GaV_4S_8 (GVS) that possesses rhombohedral (C_{3v}) symmetry and easy axis anisotropy [1]. The SkL exists over an unusally broad temperature range compared to other bulk SkL crystals, while the orientation of vortices is pinned along the magnetic easy axis and can not be controlled via external magnetic fields. Our investigation focuses on the real-space inspection of SkL in GVS using various scanning probe techniques.

[1] Kézsmarki et al., Nature Materials **14**, 1116-1122 (2015)

20 min. break

Topical Talk DF 9.5 Wed 11:30 H25

Collective spin excitations at GHz frequencies in Skyrmion-hosting bulk materials — •Dirk Grundler — Laboratoire des Matériaux Magnétiques Nanostructurés and Magnoniques, Institut des Matériaux, Faculté Science et Technique de l'Ingénieur, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Skyrmion-hosting materials have generated great research efforts in fundamental and applied sciences. Collective spin excitations in the

GHz frequency regime are in particular interesting as they provide information about the system's free energy and define response times in possible applications, respectively. We report on GHz spectroscopy performed on different bulk materials. For cubic chiral helimagnets supporting Bloch-type Skyrmions, such as insulating Cu_2OSeO_3 and semiconducting $Fe_{0.8}Co_{0.2}Si$, we found a universal behavior when studying the GHz response throughout the magnetic phase diagram (T. Schwarze *et al.*, Nat. Mater. **14**, 478 (2015)). Comparing with data from the polar magnetic semiconductor GaV_4S_8 supporting Néel-type Skyrmions (D. Ehlers *et al.*, arXiv:1512.02391), characteristic changes in the spectra are encountered that we attribute to an additional uniaxial magnetic anisotropy. We acknowledge financial support by the DFG via TRR80. The reported works are performed in cooperations with A. Bauer, H. Berger, D. Ehlers, T. Fehér, M. Garst, I. Kézsmárki, H.-A. Krug von Nidda, A. Leonov, A. Loidl, C. Pfleiderer, T. Schwarze, I. Stasinopoulos, V. Tsurkan, J. Waizner, and S. Weichselbaumer.

DF 9.6 Wed 12:00 H25

Skyrmions carrying electric polarization in multiferroic GaV_4S_8 — •Eugen Ruff[1], Sebastian Widmann[1], Peter Lunkenheimer[1], Vladimir Tsurkan[1,2], Sandor Bordács[3], Istvan Kézsmárki[1,3], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg 86135, Germany. — [2]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau 2028, Republic of Moldova. — [3]Department of Physics, Budapest University of Technology and Economics and MTA-BME Lendület Magneto-Optical Spectroscopy Research Group, Budapest 1111, Hungary.

As predicted by Bogdanov *et al.*[1], recently a skyrmion lattice (SkL) was found in the magnetic semiconductor GaV_4S_8. Skyrmions, topologically protected spin textures, have a big potential for future applications in data storage. A crucial question is whether the SkL causes a ferroelectric polarization, which can be controlled by an electric field. In this contribution we study the magnetic and polar properties in the lacunar spinel GaV_4S_8. The system shows a structural transition at 44 K, associated with orbital order, and is known to have a complex magnetic phase diagram below 13 K. We show that already below 44 K the system reveals a sizable polarization[3] of 1 $\mu C/cm^2$. Furthermore also the magnetically ordered phases show spin driven excess polarizations, so GaV_4S_8 is multiferroic below 13 K.

[1]A. N. Bogdanov and A. Hubert, J. Magn. Magn. Mater. **138**, 255 (1994). [2]I. Kézsmárki *et al.*, Nat. Mater. **14**, 1116 (2015). [3]E. Ruff *et al.*, Sci. Adv. **1**, e1500916 (2015).

Topical Talk DF 9.7 Wed 12:20 H25

Skyrmionic states in ferroelectric nanocomposites — Yousra Nahas[1], •Sergei Prokhorenko[1,2], Lydie Louis[3], Zhigang Gui[4], Igor Kornev[5], and Laurent Bellaiche[1] — [1]University of Arkansas, Fayetteville, Arkansas, USA — [2]University of Liege, Liege, Belgium — [3]University of Connecticut, Storrs, Connecticut, USA — [4]University of Delaware, Newark, Delaware,USA — [5]Ecole Centrale Paris, Chatenay-Malabry, France

Non-coplanar swirling field textures, or skyrmions, are now widely recognized as objects of both fundamental interest and technological relevance. So far, skyrmions were amply investigated in magnets, where due to the presence of chiral interactions, these topological objects were found to be intrinsically stabilized. Ferroelectrics on the other hand, lacking such chiral interactions, were somewhat left aside in this quest. Here we demonstrate, via the use of a first-principles-based framework, that skyrmionic configuration of polarization can be extrinsically stabilized in ferroelectric nanocomposites. The interplay between the considered confined geometry and the dipolar interaction underlying the ferroelectric phase instability induces skyrmionic configurations. The topological structure of the obtained electrical skyrmion can be mapped onto the topology of domain-wall junctions. Furthermore, the stabilized electrical skyrmion can be as small as a few nanometers, thus revealing prospective skyrmion-based applications of ferroelectric nanocomposites.

DF 10: Focus Session: Ferroic Domain Walls III

Time: Wednesday 15:00–18:00 Location: H25

Topical Talk DF 10.1 Wed 15:00 H25

Controlling domain wall motion as a route towards new functionalities in $Pb(Zr,Ti)O_3$ ferroelectric thin films — •Leo McGilly[1], Ludwig Feigl[1], Petr Yudin[1], Tomas Sluka[1,2], Alexander Tagantsev[1], and Nava Setter[1] — [1]Ceramics Laboratory, EPFL - Swiss Federal Institute of Technology, Lausanne, CH-1015 Switzerland — [2]DPMC-MaNEP, University of Geneva, 24 Quai Ernest Ansermet, 1211 Geneva 4, Switzerland

Ferroelectric domain walls offer the exciting prospect of truly nanoscale reconfigurable circuits owing to their small thickness, typically 1-5 nm, their inherently mobile nature and the functional properties they exhibit. However, to fully harness their potential as nanoscale functional entities, it is essential to achieve reliable and precise control of their nucleation, location, number and velocity. In this work we demonstrate an ability that allows extensive control of individual and multiple 180° domain walls in PZT thin films. Furthermore advances towards readout of domain wall position, via a read-restore technique will be presented. This method involves measurement of partial switching currents due to domain wall perturbations from an initial position through sub-switching voltage pulses. Finally, understanding the interaction of domain walls with defects is crucial to tailoring their properties. For future devices based on individual domain walls and their motion, defects could potentially kill or create functionality. We show that local nanoscale defect regions can be used to modify imprint and domain wall motion. This adds an additional dimension to the domain-wall-control toolbox.

DF 10.2 Wed 15:30 H25

Growth temperature as a tuning parameter for internal screening in ferroelectric thin films — •Christian Weymann, Céline Lichtensteiger, Stéphanie Fernandez-Pena, Jean-Marc Triscone, and Patrycja Paruch — DQMP, University of Geneva

In ferroelectric ultrathin films, the depolarization field arising from bound interface/surface charges must be compensated. This can be achieved by screening either by external screening, or by internal mobile charges from within the ferroelectric itself. In the absence of sufficient free charges, the ferroelectric can also form domains of opposite polarization.

Another frequently observed feature in ferroelectric thin films is built-in voltage, originating from asymmetrical screening, trapped charges, or strain gradients leading to flexoelectricity, and modifying the properties of the films. The resulting residual field will not only shift P-E hysteresis, but will also modify the intrinsic polarization configuration and domain stability.

By modulating the growth temperature of $PbTiO_3$ thin films, we engineered several series of ferroelectric samples with the same external electrical boundary conditions, but distinctively different internal screening. We used piezoresponse force microscopy to investigate the intrinsic domain configuration, written domain stability, and local ferroelectric switching loops of these samples. Our results open up a straightforward method to control the built-in field in such ferroelectric oxide thin films, which is crucial to applications.

DF 10.3 Wed 15:50 H25

Magnonic magnetoelectric coupling and domain wall formation in composite multiferroics — Alexander Sukhov[1], Chenglong Jia[1,2], and •Jamal Berakdar[1] — [1]Martin-Luther Universität, Halle-Wittenberg, 06099 Halle — [2]Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, Lanzhou 730000, China

Control of magnetization by an external electric field or, vice versa, ferroelectric (FE) polarization by magnetic fields entails a clear understanding of the underlying coupling. For a multiferroic nanostructure composed of metallic ferromagnetic (FM) (e.g., Fe or Co) attached to a FE (e.g. BaTiO3), we predicted recently [1] the formation in FM of a non-collinear magnetic order in the FM/FE contact area extending to distances on the spin-diffusion length of the FM. Our predictions were recently confirmed in subsequent experiment and offer also an explanation for earlier findings [3]. Here we present further resutls and suggestions that structuring the FE offers the possibility to generate

and control multiferroic domains.

[1] C.-L. Jia, T.-L. Wei, C.-J. Jiang, D.-S. Xue, A. Sukhov, and J. Berakdar, Phys. Rev. B 90, 054423 (2014).

[2]C.-L. Jia, F. Wang, C. Jiang, J. Berakdar, and D. Xue, Sci. Rep. 5, 11111 (2015).

[3] N. Jedrecy, H.J. Von Bardeleben, V. Badjeck, D. Demaille, D. Stanescu. H. Magnan, and A. Barbier, Phys. Rev. B 88, 121409(R) (2013).

20 min. break

DF 10.4 Wed 16:30 H25

Theoretical study of domain wall dynamics in multiferroic hexagonal manganites — •Urko Petralanda and Sergey Artyukhin — Istituto Italiano di Tecnologia. Via Morego 30, Genova (Italy)

Multiferroic hexagonal manganites are antiferromagnetic improper ferroelectrics where unit-cell-tripling buckling of oxygen bipyramids induces polarization and, in some compounds, weak ferromagnetism. Understanding the dynamical effects controlling motion of clamped structural, ferroelectric and magnetic domain walls (DW) in these materials is critical to design devices based on controlled switching of DWs. However, the study of DW dynamics in realistic multiferroics has been mainly focused on proper ferroelectrics and ferromagnetic materials so far, and for multiferroics was mostly limited to estimating switching barriers [1,2]. We develop a model Hamiltonian to describe the driven dynamics of DWs in hexagonal manganites, with parameters extracted from ab-initio calculations.

[1] Yu Kumagai, N. A. Spaldin Nature Communications 4, 1540 (2012)

[2] N. A. Benedek and C. J. Fennie, Phys. Rev. Lett. 106, 107204 (2011)

DF 10.5 Wed 16:50 H25

Landau theory of domain walls revisited — •Wilfried Schranz — University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria

Domain walls and twin boundaries currently attract enormous attention, since they can host functional properties that are not present in the bulk crystal [1,2]. CaTiO3 is the first example, where it was succeeded in observing a ferroelectric polarization [2] inside a ferroelastic twin wall while the rest of the crystal remained centrosymmetric. There are many more examples demonstrating the application potential of functional domain walls in future information technologies. Modelling of functional twin walls ranges from ab-initio calculations [3] to phenomenological descriptions based on Ginzburg-Landau-Devonshire free energies [4]. The possibility of an electric polarization in ferroelastic twin walls was already predicted long time ago by V. Janovec [5,6], based on a group theoretical symmetry approach. In the present talk we show how we may use the layer-group approach of domain twins [7] to describe corresponding functional properties of domain walls.

Supported by the Austrian FWF (P28672-N36).

[1] Seidel, et al., R. Nature Materials 8, 229 Vol 34 (2009). [2] Van Aert, S., et al., Adv. Mater. 24, 523 (2012). [3] B. Meyer and D. Vanderbilt, Phys. Rev. B 65, 104111 (2002). [4] P. Marton, I. Rychetsky, and J. Hlinka, Phys. Rev. B 81, 144125 (2010). [5] V. Janovec, L. Richterová and J. Prívratská, Ferroelectrics 222, 73 (1999). [6] V. Janovec, W. Schranz, H. Warhanek and Z. Zikmund, Ferroelectrics 98, 171 (1989). [7] V. Janovec, Ferroelectrics 35, 105 (1981).

DF 10.6 Wed 17:10 H25

Ferroelectric Bloch walls and ferroelectric Ising lines — Vilma Stepkova, Pavel Marton, and •Jiri Hlinka — Institute of Physics, Czech Acad. Sci., Prague

In this contribution we would like to address geometry and properties of plausible topological defects chiral ferroelectric domain walls of perovskite ferroelectrics, in particular linear defects analogous to dislocations or disclination lines known from liquid crystals. We will present our investigations of the properties of such one dimensional objects obtained within the Ginzburg-Landau-Devonshire theory using phase-field simulations.

Topical Talk DF 10.7 Wed 17:30 H25

Domain Glass — •Ekhard Salje — Cambridge University, Cambridge UK

Ferroelastic materials often develop complex domain structures, which have properties of glassy systems (non-ergodicity, glass dynamics, glass transitions, and freezing). Four characteristic temperatures are defined for such domain glasses: the dynamical nucleation temperature Td where local correlated clusters can form glass states within a (tweed-) nano structure, To the Vogel Fulcher temperature of these precursor nano- structures, Tpt the phase transition temperature where the (ferroelastic) transition occurs, and TK the Kauzmann temperature where the complex domain structure freezes. Td exists in most ferroelastic materials whereas the other transitions depend on the complexity of the domain patterns and hence on their thermal history. Shear collapse and rapid thermal quench of ferroelastic crystals preferentially lead to domain glasses whereas slow anneal produces mostly highly correlated pattern such as stripe patterns or single domain crystals. Domain glasses are compared with structural glasses and several examples for domain glass features are discussed.

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 ($R$$MnO_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 $R$$Mn_2O_5$. Contrary to other members of the $R$$Mn_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 incom-

mensurate 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 $R$$MnO_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 $R$$MnO_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, magneto-mechanical, 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, magneto-

mechanical, 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 de-

tection 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.

DF 12: Multiferroics I (DF with MA)

Time: Thursday 9:30–12:50 Location: H25

DF 12.1 Thu 9:30 H25

Room-temperature electric-field-induced magnetic anisotropy rotation in multiferroic heterostructures — •Gabriele De Luca, Peggy Schönherr, Manfred Fiebig, and Morgan Trassin — ETH Zürich, Department of Materials

The possibility to control magnetic anisotropy by using only an electric field has rendered compounds with interacting ferromagnetic and ferroelectric order a prime target of materials research. However, both orders hardly coexist at room-temperature in a single material phase, thus efforts focused on artificial heterostructures and magnetoelectric coupling as a composite effect. Here we design a multiferroic heterostructure Pt/CoFe/BiFeO3 (BFO) and we use a combination of magnetic force microscopy (MFM) and second harmonic generation (SHG) to detect the distribution of the ferromagnetic domains in CoFe and the buried ferroelectric domain state in BFO. With SHG we establish a unique relation between the BFO domains distribution and the nonlinear response and we perform the read-out without invading the system [1]. MFM reveals the one-to-one coupling of the ferroelectric/ferromagnetic domains. With an external electric field, we induce changes in the BFO ferroelectric state and we use magnetic field dependent MFM to probe the resulting effect on the CoFe domains and magnetic anisotropy. Previous work has unveiled in such systems that the net CoFe magnetization can be electrically reversed. Here we show that local magnetic anisotropy rotation can be achieved and correlated with the underlying ferroelectric domain state after voltage application. [1] M. Trassin, G. De Luca et al., Adv. Mater. 27, 4871 (2015)

DF 12.2 Thu 9:50 H25

Design and synthesis of a room temperature multiferroic bulk oxide — Pranab Mandal[1], •Michael Pitcher[1], Jonathan Alaria[2], Hongjun Niu[1], Pavel Borisov[1], Plamen Stamenov[3], John Claridge[1], and Matthew Rosseinsky[1] — [1]Department of Chemistry, University of Liverpool, Liverpool, UK — [2]Department of Physics, University of Liverpool, Liverpool, UK — [3]CRANN, Trinity College Dublin, Ireland

A new generation of low-power high-density information storage would be enabled by the development of multiferroic materials that combine switchable electrical polarisation (conventionally arising from second order Jahn-Teller distortion of d^0 cations) with spontaneous magnetisation (from long range ordering of unpaired d electrons) within a single phase material. Combining these properties at room temperature is very challenging due to their antagonistic electronic requirements and the need to maintain long range magnetic ordering to such high temperatures. We have demonstrated a new route to such materials,

first by engineering competitive ferroelectric performance in a Bi-based perovskite by creating a PZT-like morphotropic phase boundary in the solid solution [1-x] $BiFe_{2/8}Mg_{3/8}Ti_{3/8}O_3$ - [x]$CaTiO_3$ ($0 < x < 0.40$); and then introducing long range magnetic order to this ferroelectric platform by increasing the concentration of Fe^{3+} above the threshold required for a percolating superexchange network. The resulting materials are magnetoelectric, ferromagnetic and ferroelectric above 300 K.

DF 12.3 Thu 10:10 H25

Multiferroic clusters: a new perspective for relaxor-type room-temperature multiferroics — •Leonard Henrichs[1,2], Oscar Cespedes[3], Wolfgang Kleemann[4], and Andrew Bell[2] — [1]Karlsruher Institut für Technologie, Institut für Angewandte Geowissenschaften, Germany — [2]University of Leeds, Institute for Materials Research, United Kingdom — [3]University of Leeds, School of Physics and Astronomy, United Kingdom — [4]University of Duisburg-Essen, Faculty of Physics, Germany

Multiferroics are promising for sensor and memory applications. However, no single-phase material displaying both ferroelectricity and large magnetization at room-temperature has hitherto been reported. This situation has substantially been improved in the novel relaxor ferroelectric (BiFe0.9Co0.1O3)0.4-(Bi1/2K1/2TiO3)0.6, where polar nanoregions (PNR) transform into static-PNR (SPNR) and simultaneously enable congruent multiferroic clusters (MFC) to emerge from inherent Bi(Fe,Co)O3 rich regions. The MFC supposedly are ferrimagnetic. On these MFC, exceptionally large direct and converse magnetoelectric coupling coefficients, α * 1.0 x 10-5 s/m at room-temperature, were measured by PFM and MFM respectively. We expect the non-ergodic relaxor properties which are governed by the Bi1/2K1/2TiO3 component to play a vital role in the strong ME coupling. The extremely high Neel temperature of approx. 690 K, as verified by neutron diffraction, further underlines the exceptional magnetic properties of the material. This new class of non-ergodic relaxor multiferroics bears great potential for applications.

DF 12.4 Thu 10:30 H25

Imaging of electric-field-induced magnetization reversal in $Dy_{0.7}Tb_{0.3}FeO_3$ — •Ehsan Hassanpour Yesaghi[1], Yusuke Tokunaga[2], Thomas Lottermoser[1], Yasujiro Taguchi[3], Yoshinori Tokura[3,4], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, Zürich, Switzerland — [2]Department of Advanced Materials Science, University of Tokyo, Kashiwa, Chiba 277-8561, Japan — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan — [4]Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), University of Tokyo, Tokyo 113-8656, Japan

Full control of the magnetic state via electric field was recently reported in $Dy_{0.7}Tb_{0.3}FeO_3$. This material undergoes several magnetic phase transitions, including a multiferroic phase in which the polarization is induced by the symmetric exchange interaction of the rare earth moments and Fe spins. It was shown that the magnetization reversal in this material depends on both the magnitude and the time-derivative of the electric field, such that the switching occurs only if the E-field is applied sufficiently fast. Such behavior, however, was never investigated at the level of domains, which is crucial for its understanding and application in devices. Here we investigate the underlying physics of the time-dependent switching process using Faraday imaging technique in order to spatially resolve magnetic domains and domain walls. The observation of two distinct types of domains and their relation to the magnetic Fe/Dy sub-lattices will be discussed. The electric field dependence on the magnetic ordering will be presented.

DF 12.5 Thu 10:50 H25

Influence of ferroelectric electron emission in BTO layer systems on measurements of core-level binding energies — •Paula Huth[1], Martin Welke[1], Alireza Bayat[2], Karl-Michael Schindler[2], Angelika Chassé[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut, Universität Leipzig — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Barium titanate (BTO) is a well-known ferroelectric material with perovskite-like structure. During the phase transition from tetragonal to cubic crystal system at 120 °C, the spontaneous electrical polarization vanishes. In conventional x-ray photoelectron spectroscopy measurements, sudden shifts ("jumps") in core-level binding energies have been observed at the Curie temperature. This was proposed to originate from surface charge build-up[1], but by using high-kinetic energy XPS, the effect could be shown to occur for deeper layers and in the presence of covering non-conducting oxide layers, as well. Since the effect occurs at the ferroelectric-to-paraelectric phase transition, ferroelectric electron emission[2] is proposed as origin. Iron and Cobalt layers of different thicknesses have been prepared in-situ on BTO(001), to show that the effect vanishes if a conducting layer is present. Such core-level shifts have been found for all elements in BTO, except in the presence of thick metal overlayers. Additionally, a general difference of the electronic binding energy between the tetragonal and the cubic phase has been observed and confirmed by DFT calculations. [1] L. Makhova et al.: Phys. Rev. B, 83 (2011) 11540. [2] G. Rosenman et al.: J. Appl. Phys., 88 (2000) 6109.

20 min. break

DF 12.6 Thu 11:30 H25

Kibble-Zurek mechanism in hexagonal $RMnO_3$ — •Quintin Meier[1], Andres Cano[2], and Nicola Spaldin[1] — [1]ETH Zürich, Department for Materials Theory, Zürich, Switzerland — [2]CNRS, Université de Bordeaux, ICMCB, UPR 9048, 33600 Pessac, France

We present a theoretical study of the effect of cooling rate on the ferroelectric domain formation in the multiferroic hexagonal manganites, RMnO3 (R is Y or a small rare-earth atom). The hexagonal manganites are of interest because of their unusual improper ferroelectricity, which allows multiferroism and promotes conducting domain walls. In addition, the associated structural phase transition has recently been shown to form topological defects according to the Kibble-Zurek scaling law [1], which describes the number of topological defects formed as a function of cooling rate. Here we investigate the Kibble-Zurek scaling for a range of compounds in the RMnO3 series by using first principles density functional theory to calculate trends in the scaling parameters. We present possible models that describe the experimentally observed deviations from Kibble-Zurek scaling at both very fast and very slow cooling rates.

[1] Griffin, S. M., Lilienblum, M., Delaney, K. T., Kumagai, Y., Fiebig, M., & Spaldin, N. A. (2012) Physical Review X, 2(4), 041022.

DF 12.7 Thu 11:50 H25

Theory of colossal magnetoelectric responses in Ni_3TeO_6 — •Sergey Artyukhin[1], Sang-Wook Cheong[2], and David Vanderbilt[2] — [1]Italian Institute of Technology, Genova, Italy — [2]Department of Physics and Astronomy, Rutgers University, USA

The manipulation of magnetic ordering with applied electric fields is of pressing interest for new spintronic and information storage applications. Recently, such magnetoelectric control was realized in multiferroics [1]. However, their magnetoelectric switching is often accompanied by significant hysteresis, resulting from a large barrier, separating different ferroic states. Hysteresis prevents robust switching, unless the applied field overcomes a certain value (coercive field). I will discuss the role of a switching barrier on magnetoelectric control, in particular, in a collinear antiferromagnetic and pyroelectric Ni_3TeO_6 [2,3]. The barrier between two magnetic states in the vicinity of a spin-flop transition is almost flat, and thus small changes in external electric/magnetic fields allow to switch the ferroic state through an intermediate state in a continuous manner, resulting in a colossal magnetoelectric response. This colossal magnetoelectric effect resembles the large piezoelectric effect at the morphotropic phase boundary in ferroelectrics.

[1] T. Kimura, T. Goto, H. Shintani et al., Nature 426, 5 (2003)

[2] Y.-S. Oh, S. Artyukhin J. J. Yang et al., Nature Communications 5, 3201 (2014)

[3] J. W. Kim, S. Artyukhin, E. D. Mun et al., Phys. Rev. Lett. 115, 137201 (2015)

DF 12.8 Thu 12:10 H25

Ab initio calculation of ARPES and SPLEED spectra for the multiferroic heterostructure $Co/BaTiO_3$ — •Stephan Borek[1], Jürgen Braun[1], Jan Minár[1,2], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]University of West Bohemia Pilsen

Multiferroic heterostructures possess promising properties concerning technical applications. It has been shown recently that the combination of x-ray absorption spectroscopy (XAS), x-ray magnetic circular dichroism (XMCD) and x-ray magnetic linear dichroism (XMLD) can be used to determine the magnetic properties of the Co surface layers of the multiferroic system $Co/BaTiO_3$ [1]. In this way an indirect investigation of the coupling mechanisms between the ferroelectric and

the ferromagnetic materials gets possible. In our work we consider complementary spectroscopic methods which are suitable for the determination of the properties of multiferroic heterostructures. For this purpose we used the theoretical description of angle-resolved photoemission spectroscopy (ARPES) and spin-polarized low energy electron diffraction (SPLEED) to investigate the coupling mechanisms at the Co/BTO interface. We will show that both methods provide detailed insight into the behaviour of the electronic structure during a switching of the electric polarization of $BaTiO_3$.

[1] M. Hoffmann et al., Journal of Phys: Cond. Matter **27**, 426003 (2015)

DF 12.9 Thu 12:30 H25

Chaos and stochastic resonance during ferroelectric switching — •Martin Diestelhorst — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, 06120 Halle, Germany

The Landau theory of second-order phase-transitions being taken into account, it gives motivation to look for effects like bifurcations, chaos and stochastic resonance in ferroelectrics. The main features of these effects may be understood based on the quartic double-well potential $V(x) = \frac{a}{2}x^2 + \frac{b}{4}x^4$, which is of the same form as the thermodynamic potential of a ferroelectric with second-order phase-transition near the Curie temperature. The predicted effects could be in principle found in ferroelectric TGS. It is shown that these effects are related to complicated regimes of domain switching and give rise to peculiarities which may not be understood in terms of the simple double-well potential. These effects must be attributed to the real processes which occur during switching.

DF 13: Nano- and microstructured dielectrics/thin films (DF with KR)

Time: Thursday 9:30–12:30 Location: H26

DF 13.1 Thu 9:30 H26

Fabrication of periodically patterned domain structures in x-cut thin film $LiNbO_3$ — Peter Mackwitz[1], Michael Rüsing[1], Gerhard Berth[1,2], and •Artur Zrenner[1,2] — [1]1Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]2Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Within the field of nonlinear optics $LiNbO_3$ represents an important material with outstanding nonlinear optical properties. It is possible to achieve a highly efficient frequency conversion in $LiNbO_3$ with periodic poled structures which preserve the quasi phase matching condition. Bulk $LiNbO_3$ represents one of the major materials for frequency conversion with periodically poled pattern. Concerning the different scattering geometries of $LiNbO_3$ x-cut samples offer favorable properties regarding the fabrication of periodically pattern and the frequency conversion. For example the most intense tensor element d_{33} can directly be triggered. Scores of previous works [1] have shown the fabrication and application of periodically poled domain pattern in bulk $LiNbO_3$. In this work we have processed x-cut thin film $LiNbO_3$ samples in order to create a periodically poled pattern. The transferred domain structures were studied with nonlinear microscopy. Concerning the nonlinear measurements the domain structures could clearly be resolved and the poling process was successful. These results hint to the possibility of homogeneous poled domains allowing novel applications in the framework of photonics and integrated optics. [1] L. Gui, H. Hu et al., Opt. Exp. 17, 3923 (2009)

DF 13.2 Thu 9:50 H26

Nanostructuring of dielectric surfaces using nanosecond laser radiation assisted by metallic absorber layer — •Pierre Lorenz[1], Michael Klöppel[1,2], Christoph Grüner[1], Frank Frost[1], Joachim Zajadacz[1], Martin Ehrhardt[1], and Klaus Zimmer[1] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — [2]Institute of Scientific Computing, Department of Mathematics, TU Dresden, 01062 Dresden, Germany

The laser-induce structuring of different dielectrics assisted by self-organisation of a molten thin metal layer during laser heating with a 248 nm, 25 ns KrF excimer laser was studied. The nanopattern formation at low laser fluence is caused by instabilities of thin molten metal layer on dielectric surfaces within the laser pulse driven by the surface tension of the liquid metal layer. As dielectric substrate and metallic absorber film SiO_2, Al_2O_3, and diamond as well as Cr and Mo were used, respectively. Homogenous and pre-structured metal film were irradiated and specific features of the self-organization process found. For instance, the high laser fluence irradiation of the pre-structured films can result in forming different structures. The resultant structures o the film or in the substrate were investigated by atomic force (AFM) and scanning electron microscopy (SEM). These laser-induced nanoholes were imaged by SEM after cross sectioning by focussed ion beam (FIB). The hole-forming process was simulated using a heat equation to describe the laser-heating of the solid and a kind of Navier-Stokes equation to describe the mass transport in the liquid.

DF 13.3 Thu 10:10 H26

Production yield of rare-earth ions implanted into an optical crystal — •Thomas Kornher[1], Kangwei Xia[1], Roman Kolesov[1], Nadezhda Kukharchyk[2], Hans-Werner Becker[3], Bruno Villa[1], Rolf Reuter[1], Andreas D. Wieck[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]RUBION, Ruhr-Universität Bochum, 44780 Bochum, Germany

Rare-earth (RE) ions doped into desired locations of optical crystals might enable a range of novel integrated photonic devices for quantum applications. With this aim, we have investigated the production yield of cerium and praseodymium by means of ion implantation. As a measure, the collected fluorescence intensity from both, implanted samples and single centers was used. With a tailored annealing procedure for cerium, a yield up to 53% was estimated. Praseodymium yield amounts up to 91%. Such high implantation yield indicates a feasibility of creation of nanopatterned rare-earth doping and suggests strong potential of RE species for on-chip photonic devices. Additionally, the potential of evanescently coupling RE ions in YAG to photonic structures is investigated.

DF 13.4 Thu 10:30 H26

Circular dichroism of the distorted Gyroid photonic crystal — •Johannes Hielscher[1], Sebastian C. Kapfer[1], Caroline Pouya[2], Peter Vukusic[2], and Gerd E. Schröder-Turk[3] — [1]FAU Erlangen-Nürnberg, Institut für Theoretische Physik — [2]University of Exeter, School of Physics — [3]Murdoch University, School of Engineering & IT, Maths & Stats

The single Gyroid is a bi-continuous triply-periodic network with chiral $I4_132$ cubic symmetry. When realised with two phases of dielectric contrast, it acts as a photonic crystal. As a such, it has been found in butterfly wings. Due to its chirality, it exhibits circular dichroism in reflectance.

We show that the introduction of a long-wavelength variation of the lattice constant ("sinusoidal chirp") tunes the coupling of light waves at the interface of the photonic crystal differently depending on circular polarisation, i. e. changes the circular dichroism [1]. Reflectance spectra are gathered from numerical electrodynamics simulations, and are in good agreement with microwave optics measurements on selected 3D-printed replicas. Studying model systems, as the tetragonally distorted Gyroid and its photonic band structure, contributes to our understanding of the intricate geometrical contributions on the reflectance properties of photonic crystals, beyond the unit-cell scale.

[1] J. Hielscher; C. Pouya; P. Vukusic & G. E. Schröder-Turk: Harmonic long-range distortions of Gyroid photonic materials enhance circular dichroism. *In preparation, 2016*

DF 13.5 Thu 10:50 H26

Flexible formation of coupled active polymeric whispering gallery mode cavities on an elastomer substrate — •Stefan Schierle[1], Tobias Siegle[1], Sarah Krämmer[1], Benjamin Richter[2], Sentayehu Wondimu[3], Peter Schuch[3], Christian Koos[4], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karl-

sruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Zoological Institute, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [3]Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [4]Institute of Photonics and Quantum Electronics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Optical modes in whispering gallery resonators are classified in analogy to electronic orbitals in atoms. Coupling between multiple resonators allows a photon exchange among them and leads to the formation of so-called photonic molecules.
Dye (pyrromethene 597)-doped active micro disk and goblet cavities are structured in a linear configuration by direct laser writing on a flexible elastomer substrate. Stretching the substrate and using its lateral contraction allows a fine tuning of the inter-cavity gaps. This enables the formation of photonic molecules consisting of two and three micro cavities. Spatially resolved spectroscopy demonstrated both the localization of super-modes, e.g. modes being resonant in the coupled system, and also the extinction of non-resonant modes in the photonic molecules. Relaxation of the substrate shows a change back to the uncoupled modal spectrum.

20 min. break

DF 13.6 Thu 11:30 H26

Electrospun dye-doped polymeric fiber networks for alcohol vapor detection — •Sarah Krämmer[1], Fabrice Laye[1], Christoph Vannahme[2], Minh Tran[1], Pascal Kiefer[1], Felix Friedrich[1], Cameron L. C. Smith[2], Ana C. Mendes[3], Ioannis S. Chronakis[3], Anders Kristensen[2], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Department of Micro- and Nanotechnology, Technical University of Denmark (DTU), 2800 Kgs., Lyngby, Denmark — [3]Nano-BioScience Research Group, DTU-Food, Technical University of Denmark (DTU), 2800 Kgs., Lyngby, Denmark

Recently we have shown that random resonators within dye-doped electrospun polymeric fiber networks lead to lasing emission [1]. Here, we demonstrate that the narrow laser emission lines can be used as sensor signal. When the fiber networks are exposed to alcohol vapors, the alcohol molecules diffuse into the polymer and cause swelling of the fibers. This swelling process changes the effective refractive index of the fiber resonator and thus causes a spectral shift of the laser mode. In various sensing experiments we analyzed the spectral shift of the lasing modes for different concentrations of ethanol and methanol. For the investigated concentration range we found a linear dependency of the shift on the alcohol concentration. The time resolved signal reveals different saturation times for the different alcohols which are related to the different diffusion constants and allow a differentation of ethanol and methanol.

[1] Krämmer et al., Adv. Mater., 26, 8096-8100, 2014

DF 13.7 Thu 11:50 H26

Implanted Strontium Titanate Single Crystals for Energy Storage Applications — •Max Stöber[1], Charaf Cherkouk[1], Juliane Walter[1], Matthias Schelter[2], Jens Zosel[2], Ralph Strohmeyer[1], Slawomir Prucnal[3], Tilmann Leisegang[1], and Dirk Carl Meyer[1] — [1]TU Bergakademie Freiberg — [2]Kurt Schwabe Institute Meinsberg — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf,

A rapid increase of the demand on efficient energy storage solutions requires new approaches beyond the Li-ion technology. In particular, metal-air batteries as well as solid-state fuel cells offer a great potential for high-energy-density storage devices. Since the efficiency of such devices is significantly limited by the activation of both the oxygen reduction reaction (ORR) and the ionic and electronic conductivities, an adequate porosity as well as a controlled doping are required. The ion implantation is a key technology to achieve this goal. In this work, p- and n-doped strontium titanate ($SrTiO_3$) single crystals were used as oxidic materials. The oxygen exchange kinetics as well as the structural changes of the $SrTiO_3$ crystal surface induced by the ion implantation were investigated. On one hand, the depth profile of dopant concentration and dopant valence state were determined using sputtered X-ray photoelectron spectroscopy (XPS). On the other hand, the overall oxygen exchange kinetic of the implanted $SrTiO_3$ crystal was quantitatively described by means of coulometric titration using Zirox system (ZIROX GmbH, Germany). Furthermore, the surface morphology of the samples was investigated using atomic force microscopy (AFM).

DF 13.8 Thu 12:10 H26

Die wahre Definition der Lichtgeschwindigkeit — •Adolf Bablitzka — 88682 Salem Baden, Alpenblick 6

Der Vortrag beschreibt den mathematischen Weg vom cosinusquadrat des sog. "Magic Angle" bzw. "Zauberwinkel" (1/3) zur Lichtgeschwindigkeit. Bekanntlich spielt dieser Winkel bei Versuchen mit magnetischen Momenten eines Festkörpers eine wichtige Rolle.

DF 14: Multiferroics II (MA with DF)

Time: Thursday 15:00–17:30 Location: H34

DF 14.1 Thu 15:00 H34

Skyrmionic and ferromagnetic resonances in magnetoelectric Cu_2OSeO_3 - magnetic vs electric fields — •S. Harms[1], M. Belesi[2], H. Berger[3], J.-F. Ansermet[3], C. Grams[1], P. Becker[1], and J. Hemberger[1] — [1]University of Cologne, Germany — [2]IFW, Dresden, Germany — [3]ICMP, EPFL, Lausanne, Switzerland

Magnetic Skyrmions are topologically stable spin whirls stabilized by spin-orbit interaction in chiral cubic magnets. It has been shown, that skyrmionic structures can be efficiently manipulated by small forces, such as e.g. currents in metallic host materials [1]. It was also shown, that the skyrmion phases in general can be excited by AC magnetic fields in the microwave range. [2].
The magnetoelectric helimagnetic insulator Cu_2OSeO_3 is one of the up to now rare cases of an insulating chiral magnets showing a stable skyrmion lattice embedded in between helical and ferrimagnetic phases. In this compound the lack of magnetic inversion symmetry leads to the occurrence of electric polarization and correspondingly to a magnetoelectric response. We present results of broadband spectroscopy up to 5 GHz trying to disentangle the different influence of electric and magnetic fields.

Funded through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] T. Schulz et al., Nature Physics 8, 301-304 (2012).
[2] Y. Onose et al., Phys. Rev. Lett. 109, 037603 (2012).

DF 14.2 Thu 15:15 H34

Multiferroic vs. magnetoelectric properties of the dilution series $[(NH_4)_{1-x}K_x]_2[FeCl_5(H_2O)]$ — •Daniel Brüning[1], Matthias Ackermann[1], Ladislav Bohaty[2], Petra Becker[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Insitut für Kristallographie, Universität zu Köln, Germany

Recently we found that $(NH_4)_2[FeCl_5(H_2O)]$, a member of the antiferromagnetic erythrosiderites $A_2[FeX_5(H_2O)]$ (A = K, Rb, Cs or NH_4 and X = Cl or Br) is multiferroic with a spontaneous polarization at T_C = 6.87K, slightly below the magnetic ordering at T_N = 7.25K. Additionally we found a high-temperature structural phase transition T_{st} = 79K, related to a monoclinic distortion (Pnma to $P11\frac{2}{a}$) due to a rearrangement of the hydrogen atoms. In contrast to $(NH_4)_2[FeCl_5(H_2O)]$, the related erythrosiderites with A = K, Rb or Cs are not multiferroic, but show linear magnetoelectric coupling with $P_i = \alpha_{ij}H_j$ below T_N. Investigating the dilution series with $A = (NH_4)_{1-x}K_x$ provides information on the stability of the multiferroic versus magnetoelectric behavior. Based on dielectric and magnetic measurements we present detailed magnetic-field versus temperature phase diagrams. Interestingly, the mixed crystals develop a finite pyroelectric polarization at T_{st}, whereas there is no indication of pyroelectricity above T_N, neither in the pure (NH_4)-based nor in the pure K-based compound.

M. Ackermann et al., J. Phys.: Condens. Matter, **26**, 506002, (2014)
M. Ackermann et al., New J. Phys., **15** 123001, (2013)

DF 14.3 Thu 15:30 H34

Optical switching of multiferroic domains in $TbMnO_3$ — •Sebastian Manz[1], Masakazu Matsubara[1,2], Jonathan Büchi[1], Thomas Lottermoser[1], Ayato Iyama[3], Tsuyoshi Kimura[3], Dennis Meier[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, 8093 Zurich, Switzerland — [2]Department of Physics, Tohoku University, Sendai 980-8578, Japan — [3]Division of Materials Physics, Osaka University, Osaka 560-8531, Japan

Multiferroics with spin-spiral-driven ferroelectricity possess a strong coupling between electric and magnetic domains, rendering them interesting for future technological devices. Controlling these domains on the local scale is an essential prerequisite, e. g. for data storage applications. Current discussions on spin-spiral multiferroics, however, focused on the conversion of one domain state into the other but reversible local manipulation has not been shown yet. As presently demonstrated in ferri- and ferromagnets, all-optical switching offers a promising route to achieve localized control. Here, we demonstrate spatially-resolved optical switching of antiferromagnetism in multiferroic $TbMnO_3$. We manipulate the antiferromagnetic order via the coupled ferroelectric state using a unique relation between the wavelength of the light and the induced polarization change. This allows us to realize reversible switching of multiferroic domains without any external bias fields. To further understand our results, we performed Monte-Carlo simulations which confirmed our findings. Our proof-of-principle experiments show that multiferroic domains and therefore domain walls can be generated and erased entirely optically on the local scale.

DF 14.4 Thu 15:45 H34

Investigation of the photostriction effect in $BiFeO_3$ by means of infrared and optical spectroscopy — •Florian Burkert and Christine Kuntscher — Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany

It has been reported that $BiFeO_3$ crystals change their size during illumination with visible light or ultraviolet radiation [1,2]. We studied the impact of this photostrictive effect on the optical properties of a $BiFeO_3$ single crystal in the infrared up to the ultraviolet frequency range by using an FTIR spectrometer and a CCD spectrograph. During illumination with various radiation sources we observe the appearance of additional absorption features in the optical spectra. We will discuss possible origins of these new features.

[1] B. Kundys et al., Nat. Mater. **9**, 803 (2010)
[2] B. Kundys et al., Phys. Rev. B **85**, 092301 (2012)

15 min. break

DF 14.5 Thu 16:15 H34

Epitaxial engineering of ferrimagnetic 3*d*-5*d* double perovskites as templates for single phase multiferroics — •Vikas Shabadi[1], Ashish Kulkarni[1,2], Philipp Komissinskiy[1], Ivetta Slipukhina[3], Robert Paria Sena[4], Joke Hadermann[4], Rajeev Gupta[2], Hongbin Zhang[1], Marjana Ležaić[3], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]Materials Science Programme, IIT Kanpur, India — [3]Peter Grünberg Institut, Forschungzentrum Jülich and JARA, Germany — [4]Electron Microscopy for Materials Science (EMAT), University of Antwerp, Belgium

3*d*-5*d* double perovskites ($A_2BB'O_6$) are of high interest due to the possible large magnetic ordering temperatures [1], multiferroicity, and the influence of spin-orbit coupling. We have for the first time synthesized in thin film form double perovskites with Mn^{2+}/Re^{4+} and Ni^{2+}/Re^{4+} cations at the B/B'-sites and La^{3+} at the A-site, previously predicted by density functional theory (DFT). We have shown the almost perfect ordering at the B-site by X-ray diffraction and high-angle annular dark field scanning transmission electron microscopy. The magnetic properties of the compounds studied by SQUID magnetometry and element specific X-Ray magnetic circular dichroism (XMCD) confirm a robust ferrimagnetic order in agreement with the DFT calculations. The results provide a valuable framework for engineering new single-phase multiferroics with ferroelectrically active A-site cations.

[1] Y. Krockenberger *et al.*, Phys. Rev. B **75**, 020404(R) (2007).

DF 14.6 Thu 16:30 H34

Structural and magnetic properties of orthorombic $ErFeO_3$ from first principles — •Dominik M. Juraschek and Nicola A. Spaldin — Materials Theory, ETH Zürich, Switzerland

We investigate the structural and magnetic properties of orthorhombic $ErFeO_3$ using density functional theory.

Rare-earth orthoferrites ($RFeO_3$) show complex coupled lattice and magnetic properties leading to interesting multifferoic, magnetoelectric and spin-dynamic behaviour.

We find that the PBEsol implementation of the generalized gradient approximation plus Hubbard U (GGA+U) method gives structural properties in good agreement with experiment. Using this approximation, we calculate the lattice dynamical properties, the magnetic ground state and the spin-phonon coupling. Our DFT calculations with erbium's 4f electrons frozen in the pseudopotential cores reproduce the G_x-type antiferromagnetic ordering with weak ferromagnetic F_z canting that is observed experimentally at high temperatures. This lends support to the proposal that the observed spin reorientation transition at 100 K to a G_z ordering is mediately coupling to erbium's 4f moments.

DF 14.7 Thu 16:45 H34

First-principles calculations on anion doped GaFeO3 — •Jacqueline Atanelov and Peter Mohn — Technische Universität Wien, Institut für Angewandte Physik, Computational Materials Science

We present ab initio DFT calculations performed on stoichiometric and anion doped GaFeO3 substituting O by a C, N and S atom, respectively. Stoichiometric GaFeO3 has an antiferromagnetic (AFM) ground state. The Fe atoms of the sublattices Fe1 and Fe2 couple antiferromagnetically via the O atoms through the superexchange mechanism. Exchanging the for the superexchange important O atom with p-elements of a different valence electron configuration changes the underlying magnetic exchange mechanism and influence the ground state properties which can be used for tuning properties interesting for technical applications. Four different doping configurations were examined revealing a cell site dependent influence on the magnetic properties. Carbon, for example, changes the AFM coupling present in the Fe1-O-Fe2 configuration into a ferrimagnetic exchange for the Fe1-C-Fe2 bond. Depending on the respective cell site C substitution introduces a ferrimagnetic or AFM ground state. Nitrogen alters the ground state magnetic moment as well and Sulfur introduces large structural distortions affecting the, band gap and the overall AFM coupling inside the doped GaFeO3 simulation cell. We give a detailed discussion on the respective magnetic exchange mechanisms and electronic properties with regard to applications as photocatalysis and use the predictive power of ab initio DFT simulations that may trigger future experiments.

DF 14.8 Thu 17:00 H34

Multiferroicity in off-stoichiometric $Ga_xFe_{1-x}O_3$ — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently reported observation of room-temperature mutiferroic behavior in $Ga_{0.6}Fe_{1.4}O_3$ (GFO) [1] and ϵ-Fe_2O_3 (eFO) [2] offers new perspectives for electronic devices whose operation is based on the switching of magnetic and electric ferroic ordering, as well as on the strong interaction between the magnetic and ferroelectric order parameters, such as multistate non-volatile memory cells. Unfortunately, the realistic microscopic switching mechanism in still not known for either of these materials. They are isostructural with polar $Pna2_1$ crystalline symmetry. In GFO, disorder in the occupancy of Ga and Fe sites is present, whereas eFO is a fully ordered compound. Their parallel study allows us to understand the influence of disorder on possible ferroelectric properties, and develop criteria to maximize the effect. We will present the results of an evolutionary-algorithm [3] based study of $GaFeO_3$-Fe_2O_3 solid solutions, (i.e., with increasing iron content). We will show the condition at which the proper ferroelectricity arises in GFO multiferroics and characterize the parameters of the ferroelectric phase transition. – We acknowledge financial support by Helmholtz Young Investigators Group Programme VH-NG-409 and through DFG-ANR (GALIMEO Consortium).

[1] A. Thomasson *et al.*, J. Appl. Phys. **113**, 214101 (2013); [2] M. Gich *et al.*, Adv. Mater., **26**, 4645 (2014); [3] http://uspex.stonybrook.edu

DF 14.9 Thu 17:15 H34

Fine-tuning ferroic properties: an X-ray diffraction study of type-II multiferroics — •Yoav William Windsor[1], Mahesh Ramakrishnan[1], Kenta Shimamoto[2], Aurora Alberca[1], Laurenz Rettig[1], Elisabeth Monica Bothschafter[1], Yi Hu[2],

Thomas Lippert[2], Christof Schneider[2], and Urs Staub[1] — [1]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [2]General Energy Research Department, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

We present a complete X-ray diffraction study of high-quality crystalline films of a prototypical multiferroic, using soft and hard X-rays. With the prospect of future multiferroic functionalities in mind, we show that epitaxial strain directly controls both of the system's ferroic properties. We demonstrate that strain can be used to "push" the system between different multiferroic phases, and even to fine-tune the magnetic ordering periodicity. We generalize this to show that manipulating the crystal structure by other means allows fine-tuning the ferroic properties in a similar manner.

DF 15: Ceramics and Applications (DF with KR)

Time: Thursday 15:00–15:40 Location: H26

DF 15.1 Thu 15:00 H26

Crystallization in luminescent borate glass for use in white LEDs — •A. Charlotte Rimbach[1], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Luebecker Ring˜2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Luebecker Ring˜2, 59494 Soest

The majority of white LEDs is comprised of a blue light emitting diode and a yellow phosphor. The phosphor powder, which converts a part of the blue light to yellow light, is embedded in an organic polymer and directly coated onto the LED chip. Heat-induced degradation of the polymer-based encapsulate, however, results in an efficiency decrease and color temperature change. Luminescent glasses and glass ceramics might represent an interesting alternative due to their higher thermal and chemical stability. For optical activation, the glasses are doped with rare-earth ions such as europium and terbium. Due to the relatively low absorption coefficient of the rare-earths the blue LED light is only absorbed by a small amount resulting in a too high color temperature. To increase the optical absorption by multiple scattering and reflection the glasses are subsequently processed to glass ceramics. This work focuses on the crystallization process in europium-doped lithium-aluminium-borate glass upon annealing at different temperatures for different periods of time. Differential scanning calorimetry and X-ray diffraction are the methods chosen to monitor the crystal growth and to identify the crystal phases.

DF 15.2 Thu 15:20 H26

Small-scale Dislocation Plasticity in Strontium Titanate — •Alexander Stukowski, Farhan Javaid, Karsten Durst, and Karsten Albe — Technische Universität Darmstadt

Strontium titanate (STO) is an optically transparent perovskite oxide ceramic material. In contrast to other ceramics, single crystal STO plastically deforms under ambient condition, without showing a phase transition or early fracture. This remarkable ductility makes it a prime candidate for different technological applications. However, while the mechanical behavior of bulk STO has been studied extensively using uniaxial compression testing techniques, little is known about the local, small-scale behavior and the details of dislocation-based nanoplasticity in this perovskite material.

In this contribution we compare results obtained from new nanoindentation experiments and corresponding large-scale molecular dynamics simulations. The evolution of the plastic zone and dislocation structures that form underneath the indenter is investigated using etch-pit methods in experiments and a novel three-dimensional defect identification technique in atomistic computer models. The latter allows tracing the evolution of the complete dislocation line network as function of indentation depth, quantifying the activity of different slip systems, and correlating this information with the recorded load-displacement curves and hardness data.

DF 16: Crystallography in Materials Science (KR with DF, MI)

Time: Thursday 15:40–17:00 Location: H26

DF 16.1 Thu 15:40 H26

Low temperature synthesis of $CuFeO_2$ (delafossite) between 50°C and 90°C: A new process solely by precipitation and ageing — •Melanie John[1], Aladin Ullrich[2], and Soraya Heuss-Assbichler[1] — [1]Ludwig-Maximilians-Universität München, München, Deutschland — [2]Universität Augsburg, Augsburg, Deutschland

Due to the large variability of technical applications of delafossite compounds e.g. as a catalyst, in p-type conduction oxides or as a cathode in Li-ion batteries, the synthesis of ABO_2 structures have received much attention the last years. Delafossite syntheses have been reported via solid state reaction and sol-gel processes using high temperatures between 900-1200°C or hydrothermal synthesis methods using at least autogenous pressure so far. We now synthesized $CuFeO_2$ nanoparticles, the parent mineral of the Delafossite group, solely by precipitation and subsequent ageing at temperatures between 50°C and 90°C and without any additives controlling the oxidation state of copper for the first time. With this method, it is possible to synthesize a mixture of 2H (space group (SG): $P6_3/mmc$) and 3R polytype (SG: R-3m) of delafossite showing hexagonal morphology within 10 hours. The experimental conditions regulate the phase assemblage, size and the necessary ageing time. The synthesized material was analyzed by ICP-OES, FTIR, XRD, SEM, TEM and magnetic measurements.

DF 16.2 Thu 16:00 H26

Investigation of the sodium solid electrolyte $Na_5YSi_4O_{12}$ — •Wolfram Münchgesang[1], Anastasia Vyalikh[1], Falk Meutzner[1], Tina Nestler[1], Dörte Wagner[2], Axel Rost[2], Ulrike Langklotz[2], Jochen Schilm[2], Tilmann Leisegang[1], and Dirk C. Meyer[1] — [1]Technische Universität Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg, Germany — [2]Fraunhofer Institute für Ceramic Technologies and Systems IKTS, Winterbergstraße 28, 01277 Dresden, Germany

Beside the well-known sodium solid electrolytes β-Alumina and NASICON, $Na_5YSi_4O_{12}$ (NYS) is another promising crystal structure with a high ionic conductivity. Its main advantage over the two abovementioned structures is the reduced production complexity and the associated costs. However, very little is known about its complex crystal structure and properties. Starting from a crystallographic point of view, sodium ion conduction pathways have been considered with the Voronoi-Dirichlet and the energy-scaled bond valence approaches, and compared with the pathways in other ion conductors.

In the present work, the crystal structure and ionic conductivity in polycrystalline NYS-materials, obtained by a glass-ceramic process, has been analysed using solid-state NMR and Electrical Impedance Spectroscopy respectively, and interpreted in respect to the theoretical predictions.

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DF 16.3 Thu 16:20 H26

Measuring electron-phonon coupling by RIXS: the showcase of anatase TiO2 — •Simon Moser[1], Sara Fatale[1], Peter Krüger[2], Helmuth Berger[1], Philippe Bugnon[1], Arnaud Magrez[1], Hideharu Niwa[3,4], Jun Miyawaki[3,4], Yoshihisa Harada[3,4], and Marco Grioni[1] — [1]Ecole Polytechnique Federale de Lausanne, Switzerland — [2]University of Chiba, Japan — [3]University of Tokyo, Japan — [4]SPring-8, Japan

Anatase TiO2 has been proposed for many applications from trans-

parent conducting panels to photovoltaic- and photocatalytic- devices, as well as memristors. However, little is known about the dynamics of the doped-in charge carriers in this textbook insulator. Recently, we have shown by angle resolved photoemission (ARPES) that these populate the bottom of the conduction band and strongly couple to an optical phonon mode, forming so called large polarons (Moser et al., PRL 110, 196403, 2013).

In the present study, we take the point of view of the phonon. By means of bulk-sensitive resonant inelastic X-ray scattering (RIXS) at the Ti L3 edge. We find that the formation of the polaron cloud involves a single 95 meV phonon along the $c-$axis, besides the 108 meV ab-plane mode previously identified by ARPES. The coupling strength to both modes is the same within error bars, and it is unaffected by the carrier density. This establishes RIXS as a directional and bulk-sensitive probe of electron-phonon coupling in solids (Moser et al. PRL 115, 096404, 2015).

DF 16.4 Thu 16:40 H26

Polycrystalline organic semiconductors studies by X-ray nano diffraction — •Clemens Liewald[1,2], Simon Noever[1,2], Stefan Fischer[1], Janina Roemer[1], and Bert Nickel[1,2] — [1]Fakultät für Physik & Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München — [2]Nanosystems Initiative Munich, Schellingstrasse 4, 80799 München

The efficiency and reliability of organic semiconducting devices depends strongly on the knowledge of the nanoscale arrangement in the active organic layers. Here, we report on the possibilities of X-ray nanodiffraction to characterize polycrystalline organic thin films at beamline ID01, ESRF, before and after its upgrade. The beam diameter in our measurements is 110 nm at 8.9 keV and 350 nm at 20 keV. We find a high beam damage at 8.9 keV compared to only little damage at 20 keV. First, we apply the focused X-ray beam to a multilayer device, with different organic and inorganic layers, and demonstrate the possibility to measure buried microstructures in e.g. the active organic layer under and next to gold electrodes. Second, we explore the local distribution of two polymorphs in a single pentacene thin film. The lateral shape and distribution of these polymorphs can be mapped with infrared (IR) scanning near-field optical microscopy (SNOM) and is compared to the amplitude from the focused X-ray beam at ID01. In future, the combination of X-ray nanodiffraction with e.g. IR-SNOM as a correlated microscopy will allow to gain various new insights to the influence of the nanoscale crystallinity on the efficiency of organic electronics devices.