Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

Elisabeth Soergel
Physikalisches Institut
Nussallée 12
53115 Bonn
soergel@uni-bonn.de

Overview of Invited Talks and Sessions

(Lecture rooms: EB 107, EB 407 and EB 133C; Posters: C)

Tutorial on Ferroics

DF 1.1	Sun	16:00–16:50	H 0107	**Fundamentals of ferroelectric materials** — •Susan Trolier-McKinstry
DF 1.2	Sun	16:50–17:40	H 0107	**Domain walls in multiferroics as functional oxide interfaces** — •Manfred Fiebig
DF 1.3	Sun	17:40–18:30	H 0107	**Ferroelastic templates for multiferroic domain boundaries** — •Ekhard Salje

Symposium SYDW "Ferroic Domain Walls"

See SYDW for the full program of the symposium.

SYDW 1.1	Mon	9:30–10:00	H 0105	**Domain walls: from conductive paths to technology roadmaps** — •Gustau Catalan
SYDW 1.2	Mon	10:00–10:30	H 0105	**Domain walls and oxygen vacancies - towards reversible control of domain wall conductance** — •Patrycja Paruch
SYDW 1.3	Mon	10:30–11:00	H 0105	**Novel mechanisms of domain-wall formation** — •Andres Cano
SYDW 1.4	Mon	11:30–12:00	H 0105	**Novel materials at domain walls** — •Beatriz Noheda
SYDW 1.5	Mon	12:00–12:30	H 0105	**Controlling and mapping domain wall behaviour in ferroelectrics** — •John Martin Gregg, Jonathan Whyte, Raymond McQuaid, Michael Campbell, Amit Kumar, Roger Whatmore

Invited Talks: Focus Sessions on Ferroic Domain Walls I - III

DF 4.1	Mon	15:00–15:30	EB 107	**Domain walls and phase boundaries - new nanoscale functional elements in complex oxides** — •Jan Seidel
DF 4.4	Mon	16:10–16:40	EB 107	**Field-induced hysteresis of chiral vortices in ferroelectric $SrTiO_3$ twin walls.** — •Ekhard Salje
DF 4.5	Mon	16:50–17:20	EB 107	**Spintronic functionality of $BiFeO_3$ domain walls** — Ji Hye Lee, Ignasi Fina, Dietrich Hesse, •Marin Alexe
DF 4.8	Mon	18:00–18:30	EB 107	**Functional ferroic domain walls - AC & DC transport** — •Lukas M. Eng
DF 7.1	Tue	9:30–10:00	EB 107	**Polarization charge as a reconfigurable dopant in wide-bandgap ferroelectrics** — •Tomas Sluka
DF 7.4	Tue	10:40–11:10	EB 107	**Influence of defects on domain wall mobility in ferroelectrics** — •Susan Trolier-McKinstry, Daniel Marincel, Stephen Jesse, Sergei Kalinin, Huiaruo Zhang, Ian Reaney
DF 7.5	Tue	11:20–11:50	EB 107	**The electronic structure of longitudinal domain walls: a DFT perspective** — •Gustav Bihlmayer, Kourosh Rahmanizadeh, Daniel Wortmann, Stefan Blügel
DF 7.8	Tue	12:30–13:00	EB 107	**Electronic reconstruction and transport at ferroelectric domain walls** — •Dennis Meier
DF 14.1	Wed	15:00–15:30	EB 107	**Low energy consumption spintronics using multiferroic heterostructures** — •Morgan Trassin

Invited Talks: Focus Sessions on GHz Dielectrics: Materials for Mobile Communication I and II

DF 16.1	Thu	9:30–10:00	EB 407	**New application scenarios for dielectric materials in mobile communication systems of the 5th generation** — •Roland Gabriel
DF 16.5	Thu	11:00–11:30	EB 407	**Dielectric-loaded antennas for circular polarisation: their contribution to the information capacity of wireless terminals** — •Oliver Leisten
DF 16.8	Thu	12:30–13:00	EB 407	**Tunable GHz-components with ferroelectric and liquid crystal technologies for mobile terrestrial and satellite-based systems** — •Rolf Jakoby
DF 17.1	Thu	15:00–15:30	EB 407	**Temperature stable low loss ceramics for resonators and filters** — •Ian Reaney
DF 17.5	Thu	16:30–17:00	EB 407	**Low loss flexible and stretchable dielectrics for microwave applications** — •Mailadil Sebastian

Invited Talks

DF 12.1	Wed	9:30–10:00	EB 407	**Holographic microstructuring of liquid-crystalline elastomers** — •Irena Drevensek-Olenik, Martin Čopič, Martin Fally, Valentina Domenici, Antoni Sánchez-Ferrer
DF 13.1	Wed	11:20–11:50	EB 407	**Twisting the anionic-electronic transport kinetics to trigger memristance for resistive switching non-volatile memories: new materials, structering and methods** — •Jennifer Rupp, Felix Messerschmitt, Sebastian Schweiger, Rafael Schmitt, Markus Kubicek
DF 13.4	Wed	12:30–13:00	EB 407	**Investigation of dielectrics under electron irradiation** — •Hans-Joachim Fitting
DF 14.1	Wed	15:00–15:30	EB 107	**Low energy consumption spintronics using multiferroic heterostructures** — •Morgan Trassin

Sessions

DF 1.1–1.3	Sun	16:00–18:30	H 0107	**Tutorial on Ferroics (DF with MA/TT)**
DF 2.1–2.5	Mon	9:30–12:30	H 0105	**Symposium on Ferroic Domain Walls**
DF 3.1–3.7	Mon	11:15–13:00	ER 164	**Photovoltaics: Kesterites and Less Widely used Materials (HL with DF)**
DF 4.1–4.8	Mon	15:00–18:30	EB 107	**Focused Session on Ferroic Domain Walls I (DF with MA)**
DF 5.1–5.30	Mon	19:00–21:00	Poster C	**Poster Session on Ferroic Domain Walls - Multiferroics (DF with KR/MA/TT)**
DF 6.1–6.8	Mon	19:00–21:00	Poster C	**Poster Session DF**
DF 7.1–7.8	Tue	9:30–13:00	EB 107	**Focused Session on Ferroic Domain Walls II (DF with MA)**
DF 8.1–8.4	Tue	11:15–12:15	H 0111	**High-k and Low-k Dielectrics (DS with DF)**
DF 9.1–9.6	Tue	14:00–16:00	EB 107	**Focused Session on Ferroic Domain Walls III (DF with MA)**
DF 10.1–10.13	Wed	9:30–13:00	EB 107	**Multiferroics I (DF with DS/KR/MA/TT)**
DF 11.1–11.10	Wed	9:30–13:00	EB 133C	**Small Polarons in $LiNbO_3$**
DF 12.1–12.4	Wed	9:30–11:00	EB 407	**Optical and Nonlinear Optical Properties I (DF with CPP)**
DF 13.1–13.4	Wed	11:20–13:00	EB 407	**Ceramics and Applications (DF with KR)**
DF 14.1–14.13	Wed	15:00–18:50	EB 107	**Multiferroics II (DF with DS/KR/MA/TT)**
DF 15.1–15.8	Wed	15:00–17:40	EB 407	**Optical and Nonlinear Optical Properties II (DF with KR)**
DF 16.1–16.8	Thu	9:30–13:00	EB 407	**Focused Session on GHz Dielectrics: Materials for Mobile Communication I (DF with HL/MM)**
DF 17.1–17.5	Thu	15:00–17:00	EB 407	**Focused Session on GHz Dielectrics: Materials for Mobile Communication II (DF with HL/MM)**
DF 18.1–18.9	Thu	15:00–17:30	BH-N 128	**Glasses and Glass Transition I (DY with DF/CPP)**
DF 19.1–19.7	Fri	9:30–11:15	C 243	**Glasses and Glass Transition II (CPP with DF/DY)**

Annual General Meeting of the Dielectric Solids (DF) and the Crystallography (KR) Divisions

Mittwoch 19:00–20:00 EB 107

DF 1: Tutorial on Ferroics (DF with MA/TT)

This tutorial introduces the field of domain and domain-wall engineering, key concepts and materials, and launches our 3-days focus on ferroic domain walls. The tutorial will provide a forum for non-specialists to get informed / involved and, at the same time, aims at inspiring topical discussions to stimulate a vivid scientific exchange during the following Sypmosium (SYDW), the three Focus Sessions and a Poster Session.

Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Sunday 16:00–18:30 Location: H 0107

Tutorial DF 1.1 Sun 16:00 H 0107

Fundamentals of ferroelectric materials — •Susan Trolier-McKinstry — Penn State University, University Park, PA, USA

This tutorial will cover the fundamental phenomena that underpin the field of ferroelectricity, with an emphasis on the relationship between crystal structure and the allowed domain states. An introduction will be made to ferroelectricity, pyroelectricity, piezoelectricity, and the origins of the dielectric response. The crystal structures of key materials, including perovskites, $LiNbO_3$, the tungsten bronzes, and polymer ferroelectrics will be introduced, along with the link between the loss of symmetry elements and the allowed domain states. The tutorial will conclude with an introduction to the movement of domain walls, and the influence that this has on the properties of ferroelectric materials.

Tutorial DF 1.2 Sun 16:50 H 0107

Domain walls in multiferroics as functional oxide interfaces — •Manfred Fiebig — Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland

The functionality of any ferroic material depends on its domains. Consequently, their shape and manipulation in external fields are of major research interest. In compounds uniting magnetic and electric order in the same phase, the magnetoelectric coupling on the level of the domains is, however, largely unexplored. For such so-called multiferroics it is therefore not known how exactly electric or magnetic fields affect the multiferroic domains and their walls. In my talk I will discuss this issue and focus on the influence of the multiferroic order on the ferroelectric state and its domain walls. Examples I will include are: (i) multiferroics with geometric ferroelectricity such as hexagonal $YMnO_3$ where the domain walls exhibit anisotropic conductance and can therefore be regarded as "tunable oxide interfaces"; (ii) multiferroics with magnetically induced ferroelectricity such as $MnWO_4$ or $TbMnO_3$ where the electric polarization within the wall is expected to rotate instead of passing through zero, as in conventional displacive ferroelectrics; (iii) multiferroics with strain-induced ferroelectricity like $SrMnO_3$ where the interplay of strain and oxygen vacancies leads to polar state in which domain walls act as insulating boundaries to the conducting domains.

Tutorial DF 1.3 Sun 17:40 H 0107

Ferroelastic templates for multiferroic domain boundaries — •Ekhard Salje — University of Cambridge, Cambridge, UK

The field of Domain Boundary Engineering is introduced. Ferroelastic domain pattern are derived and their dynamical behaviour is deducted from experimental observations and computer simulations. It is then shown that twin boundaries are particularly easily modified to possess functional properties that do not exist in the bulk. Such functional properties include (super-) conductivity, ferroelectricity, and ferromagnetism. In addition, chemical mixing inside domain walls can generate novel chemical compounds. This effect is refereed to as 'Chemical Mixing in Confined Spaces'. Functionalities often generate chiralities and vortex structures in domain boundaries. It is shown that chirality (in order parameter space) leads to Bloch lines and vortex points as one- and zero-dimensional domain walls embedded in two-dimensional ferroelastic domain walls and are hence walls in walls. Examples in $CaTiO_3$ and $SrTiO_3$ are discussed.

[1] E.K.H. Salje, Ferroelastic Materials, Annual Review of Materials Research, 42, 265-283 (2012)
[2] E.K.H. Salje and K.A. Dahmen, Crackling Noise in Disordered Materials, Annual Review of Condensed Matter Physics, 5, 233-254 (2014)
[3] E.K.H. Salje, Multiferroic Domain Boundaries as Active Memory Devices: Trajectories Towards Domain Boundary Engineering, Chem. Phys. Chem., 11, 940-950 (2010)
[4] D.D. Viehland and E.K.H. Salje, Domain boundary-dominated systems: adaptive structures and functional twin boundaries, Advances in Physics, 63, 267-326 (2014)

DF 2: Symposium on Ferroic Domain Walls

Time: Monday 9:30–12:30 Location: H 0105

Invited Talk DF 2.1 Mon 9:30 H 0105

Domain walls: from conductive paths to technology roadmaps — •Gustau Catalan — ICREA-Institucio Catalana de Recerca i Estudis Avançats, Barcelona — ICN2-Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, Bellaterra, Barcelona

In this talk, I would like to give a bird's eye view of the field of domain wall nanoelectronics, starting from some basic physics, through a summary of the state of the art, and finishing with a brief and non-exhaustive discussion of unresolved problems. Topics will include the origin(s) of conductivity in perovskite domain walls, the internal phase diagram of domain walls, the interaction of domain walls with other interfaces, how much do we (not) know about the structure, energy cost and dynamics of domain walls, and some strategies for controlling their nucleation and motion.

Disclaimer: The talk will cover much ground in a short time, and will include many results and ideas that are not mine; important works may be misrepresented or underrepresented. I apologize in advance.

Invited Talk DF 2.2 Mon 10:00 H 0105

Domain walls and oxygen vacancies - towards reversible control of domain wall conductance — •Patrycja Paruch — Department of Quantum Matter Physics, University of Geneva, Switzerland

In ferroelectric materials, domain walls separate regions with different polarisation orientation, and can present novel functional properties quite different from those of the parent phase. The extreme localisation of such properties at these intrinsically nanoscale features makes them potentially useful as active components in future miniaturized electronic devices.

Particularly exciting has been the discovery of domain-wall-specific electrical conductivity, shown first in multiferroic $BiFeO_3$. I will present our observation of conductance at 180° domain walls in the simpler ferroelectric $Pb(Zr,Ti)O_3$, using a range of scanned probe microscopy techniques at different time scales.

Our measurements highlight the key role of surface adsorbates and oxygen vacancies, and show how their density and distribution can be modulated to reversibly control domain wall transport. Exploring the conductance of the domain walls under both direct and alternating current regimes, we also address the question of maximum packing density of individual current channels in epitaxial ferroelectric thin films.

Invited Talk DF 2.3 Mon 10:30 H 0105

Novel mechanisms of domain-wall formation — •Andres Cano — CNRS, Univ. Bordeaux, ICMCB, F-33600 Pessac, France

Domain walls in ferroic materials are inherent interfaces separating different ordered regions. They can exhibit specific properties radically different from those of the corresponding domains. I will discuss

two novel (and, achtung!, unrelated) mechanisms for the formation of domain walls in (multi-)ferroics:

- In conventional ferroelectrics like $BaTiO_3$, the desirable enhancement of ferroelectricity at metal-oxide interfaces can in fact promote the appearance of ferroelectric domain walls in nanoscale capacitors. I will discuss the various factors that control the physics behind this surprising phenomenon (e.g. interfacial energy vs. ferroelectric stiffness).
- In improper ferroelectrics like the hexagonal $RMnO_3$ manganites, I will show that the emergence of multiferroic domain walls (and more complex topological defects) can be rationalized in terms of different residual-symmetry-breaking mechanisms associated to the primary order parameter.

Coffee break

Invited Talk DF 2.4 Mon 11:30 H 0105

Novel materials at domain walls — •Beatriz Noheda — Zernike Institute for Advanced Materials, Groningen, The Netherlands

There is a growing need to control and improve the physical responses of useful electronic materials, as well as to induce additional functionalities of significance for applications. Domain wall nanoelectronics has been proposed as a suitable route to achieve such control at the smallest scales. Addressing the domain wall functionalities, in particular those of ferroelastic domain walls, we take advantage not only the intrinsic symmetry breaking that takes place at the wall but also of the strain gradients that are associated to these walls. The possibility to generate periodic arrays of domain walls by self-assembly during epitaxial growth is an added benefit. I will show that, depending of the chosen thin film material, the local stresses that develop locally around ferroelastic domain walls can either trigger local electrochemistry or give rise to atomic arrangements that cannot be obtained by other existing routes, generating novel 2D materials with distinct nanoscale functionalities.

The works presented here are in collaboration with S. Farokhipoor, C.J.M. Daumont, D. Rubi, C. Magén, E. Snoeck, S. Venkatesan, A. Müller, M. Döblinger, C. Scheu, J. Íñiguez, M. Mostovoy and C. de Graaf.

Invited Talk DF 2.5 Mon 12:00 H 0105

Controlling and mapping domain wall behaviour in ferroelectrics — •John Martin Gregg[1], Jonathan Whyte[1], Raymond McQuaid[1], Michael Campbell[1], Amit Kumar[1], and Roger Whatmore[2] — [1]Queens University Belfast, Belfast, Northern Ireland, UK — [2]Imperial College London, London, England

Over the last decade there has been an explosion of interest in sheet conductors, such as surface states in topological insulators [1], $LaAlO_3$-$SrTiO_3$ interfaces [2] and graphene. Recent research has shown that ferroic domain walls constitute another exciting group of 2D conductors, with probably even greater potential than those already known: after all, domain walls have special properties in that they are mobile, can be controllably shunted from point to point, and can be spontaneously created, or made to disappear. Luckily for the research community, the field of domain wall nanoelectronics [3] is still young and there is consequently a great deal left to discover.

In this talk, the extent to which ideas developed in the nanomagnetics community can be adapted to allow domain wall injection [4] and motion control in ferroelectrics, as needed for domain wall-based devices, will be discussed. In addition, results from experiments to determine the fundamental nature of conduction in both boracite and manganite domain walls will be presented.

[1] H. Zhang et al. Nature Physics 5, 438 (2009)
[2] A. Ohtomo and H. Y. Hwang, Nature 427, 423 (2004)
[3] G. Catalan et al. Rev. Mod. Phys. 84 119 (2012)
[4] J. R. Whyte et al. 26, 293 (2014)

DF 3: Photovoltaics: Kesterites and Less Widely used Materials (HL with DF)

Time: Monday 11:15–13:00 Location: ER 164

DF 3.1 Mon 11:15 ER 164

Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW and the Bethe-Salpeter equation — •Sabine Körbel[1,2], David Kammerlander[2], Rafael Alejandro Sarmiento Pérez[2,3], Miguel Alexandre Lopes Marques[1], and Silvana Botti[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Université Claude Bernard Lyon 1, France — [3]Friedrich-Schiller-Universität Jena, Germany

Self-consistent *GW* and the solution of the Bethe-Salpeter equation are currently the best approaches to accurately simulate electronic excitations in a vast class of materials, ranging from molecules to solids. However, numerical instabilities, caused by a vanishing band gap in density-functional theory, make it impossible to use the common implementations of these techniques to calculate optical absorption spectra of the best-known thin-film absorbers for solar cells: $Cu(In,Ga)(S,Se)_2$ chalcopyrites and $Cu_2ZnSn(S,Se)_4$ kesterites/stannites. Here we solve this problem by using a finite-difference method in k-space to evaluate the otherwise diverging dipole matrix elements, obtaining excellent agreement with experiment. Having established the validity of this approach, we use it then to calculate the optical response of the less-studied, but promising, $Cu_2ZnGe(S,Se)_4$ compounds, opening the way to predictive calculations of still unknown materials.

DF 3.2 Mon 11:30 ER 164

Formation of Single-Phase Cu_2ZnSnS_4 Thin Films by Control of Secondary Phases in a Solid State Reaction — •Justus Just[1,2], Jan-Christoph Hebig[1,2], Roland Mainz[1], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Bergische Universität Wuppertal, Gaußstraße 20, 42109 Wuppertal, Germany

The conversion efficiency of Cu_2ZnSnS_4(CZTS) based solar cells significantly depends on deposition conditions and specifically the composition of the material. Although best material qualities are observed for Cu-poor and Zn-rich conditions, it has been shown that the compositional region of single phase CZTS is rather small, inevitably leading to a segregation of secondary phases, especially ZnS for Zn-rich material. To overcome this, but still maintain Cu-poor and Zn-rich growth we have developed a two stage co-evaporation process including a thermal treatment. In this process CZTS is formed by a cation interdiffusion process during a solid state reaction of ZnS with ternary Cu_2SnS_3. By oversupplying ZnS the chemical potential of Zn is higher than needed for stoichiometric CZTS, while an uncontrolled segregation of ZnS within the CZTS layer is avoided. This method allows the synthesis of single phase CZTS as shown by X-ray absorption spectroscopy. The final absorber layers show a homogenous distribution of atoms indicating that the solid state reaction is fully completed. To investigate the diffusion kinetics as well as the recrystallization mechanism in-situ real-time X-ray diffraction measurements were performed.

DF 3.3 Mon 11:45 ER 164

Reversible band gap changes in $Cu_2ZnSn(S,Se)_4$ solar cells induced by post-annealing — •Christoph Krämmer[1], Christian Huber[1], Christian Zimmermann[1], Mario Lang[1], Thomas Schnabel[2], Tobias Abzieher[1,2], Erik Ahlswede[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany

The absence of the environmentally problematic and expensive metals indium and gallium makes the kesterite $Cu_2ZnSn(S,Se)_4$ (CZTSSe) material system a promising alternative to the established $Cu(In,Ga)Se_2$. Recent publications demonstrated that the amount of Cu_{Zn}+Zn_{Cu} antisite defect pairs can be influenced by post-annealing experiments. This has a direct impact on the band gap E_g of the material. We demonstrate that this effect can be used to reversibly tune E_g within a range of over 100 meV – even in finished solar cell devices. These reversible band gap shifts are detected using electroreflectance. We demonstrate that the band gap of the material is directly correlated to the amount of Cu–Zn disorder and follows the stochastic Vineyard model.

DF 3.4 Mon 12:00 ER 164

Effect of post-annealing on $Cu_2ZnSn(S,Se)_4$ solar cells studied by photoluminescence spectroscopy — •Christian Zimmermann[1], Christoph Kraemmer[1], Christian Huber[1], Mario Lang[1], Thomas Schnabel[2], Tobias Abzieher[1,2], Erik Ahlswede[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

In contrast to the established absorbers for thin-film solar cells such as Cu(In,Ga)Se_2 and CdTe, thin-film solar cells based on kesterite absorbers like $Cu_2ZnSn(S,Se)_4$ (CZTSSe) require less toxic and scarce constituents. Recently it has been shown by Scragg *et al.*, that a thermal processing can lead to a change in the ordering of the kesterite Cu–Zn planes (Appl. Phys. Lett. **104**, 041911 (2014)), which could lead to a change in the density of the defect pair Cu_{Zn}+Zn_{Cu}. The density and nature of intrinsic defects have a huge influence on the recombination characteristics of kesterites. Hence we use photoluminescence spectroscopy to investigate the influence of post-annealing of solar cells based on solution-processed CZTSSe. Our results lead to the conclusion, that electrostatic potential fluctuations still play a major role in CZTSSe solar cells regardless of the Cu–Zn ordering.

DF 3.5 Mon 12:15 ER 164

Theoretical and experimental approach to optoelectronic study of Nb3O7(OH) — •Wilayat Khan[1], Sophia Betzler[2], Christina Scheu[2], and Jan Minar[1,3] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic — [2]Department of Chemistry, Ludwig-Maximilians-Universität and Center for NanoScience (CeNS), Butenandtstraße 11, 81377 Munich, Germany — [3]Dept. of Chemistry, University of Munich, Germany

Recently, Nb3O7(OH) single crystal has been recommended as a high performing Dye-Sensitized Solar Cell. Theoretical and experimental studies of the Nb3O7(OH) single crystals are performed. The theoretical study were performed by using the full potential linearized augmented plane wave (FP-LAPW) method to calculate the electronic properties The experimental studies were carried out by characterizing this material by EELS [1]. We also performed theoretical calculations using the multiple-scattering Spin-Polarized Relativistic-KKR (SPR-KKR) code to investigate Ok and NbL2,3 egde, in order to support the EELS spectroscopy. The calculated band using the modified Becke Johnson approximation (mBJ) is 2.32 eV which is in comparison to the experimental band gap. The electronic density of states around the Fermi level is dominated by the H-1s and Nb-4p states (VB) and Nb-5d states (CB), which play an important role in optical transition resulting in maximum peaks in the imaginary part of dielectric function. [1] Sophia B. Betzler et al., J. Mater. Chem. A, 2014,2, 12005-12013.

DF 3.6 Mon 12:30 ER 164

Modelling of octahedral tilts in NBT by first-principles — •Kai-Christian Meyer, Melanie Gröting, and Karsten Albe — TU Darmstadt, Jovanka-Bontschits-Str 2, 64287 Darmstadt

In this work we deal with the structural configuration of Sodium Bismuth Titanate (NBT) on a atomistic level by first-principles studies and we link our results to the experimentally observed dielectric properties. NBT is a lead-free relaxor ferroelectric with interesting physical properties around the temperature range from 100-200 °C, where it shows a broad frequency dependent peak in the dielectric constant. Around 200°C the tetragonal and rhombohedral (and octahedral) phase are simultaneously present. We believe that a connection between polar nanoregions (PNR) and planar octahedral defects in a rhombohedral matrix exist. We show among other things that certain chemical orders enhance the probability for PNRs to occur.

DF 3.7 Mon 12:45 ER 164

Formation of n-type defect levels in 1.0 eV GaInNAs layers and their influence on GaInNAs solar cell performance — •Fabian Langer, Svenja Perl, Sven Höfling, and Martin Kamp — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, University of Würzburg, Am Hubland, D97074 Würzburg, Germany

The semiconductor material GaInNAs can be grown lattice matched to GaAs/Ge by molecular beam epitaxy (MBE) with a broad degree of freedom in its bandgap. Besides emerging applications like telecommunication light sensing requiring bandgaps below 0.95 eV, GaInNAs material with a 1.0 eV wide bandgap is of increasing interest for the solar cell industry. Up to now the market for space or concentrator photovoltaic (CPV) is dominated by solar cells made of the material combination GaInP/(In)GaAs/Ge. However, this type of solar cell has reached its practical average efficiency limit. But further improvement by the integration of a 1.0 eV GaInN(Sb)As junction could already be shown. In this presentation we report on the investigation of n-type defects formed during the GaInNAs growth and analyze their influence on the performance of 1.0 eV GaInNAs solar cells. Utilizing these defects we achieved very high internal quantum efficiencies above 90 % due to a compensation effect of the background p-doping in the GaInNAs layer. However, this comes along with a strongly increased dark current generated by the defect states within the bandgap and results in reduced open-circuit voltages of about 0.2 V.

DF 4: Focused Session on Ferroic Domain Walls I (DF with MA)

Part of the 3-days focus on ferroic domain walls:

Tutorial, Symposium (SYDW), three Focused Sessions, and Poster Session.

Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Monday 15:00–18:30 Location: EB 107

Topical Talk DF 4.1 Mon 15:00 EB 107

Domain walls and phase boundaries - new nanoscale functional elements in complex oxides — •Jan Seidel — School of Materials Science and Engineering, UNSW Australia, Sydney, Australia

Interfaces and topological boundaries in complex oxide materials, such as domain walls and morphotropic phase boundaries, have recently received increasing attention due to the fact that their properties, which are linked to the inherent order parameters of the material, its structure and symmetry, can be completely different from that of the bulk material [1]. I will present an overview of recent results on electronic and optical properties of ferroelectric phase boundaries, domain walls, and topological defects in multiferroic materials [2, 3, 4, 5, 6]. The origin and nature of the observed confined nanoscale properties is probed using a combination of nanoscale transport measurements based on scanning probe methods, high resolution transmission electron microscopy and first-principles density functional computations. I will also give an outlook on how these special properties can be found in other material systems and discuss possible future applications [7].
1. J. Seidel, et al., Nature Materials 8, 229 (2009) 2. J. Seidel, et al., J. Phys. Chem. Lett. 3, 2905 (2012) 3. J. Seidel, et al., Phase Trans. 86, 53 (2013) 4. J. Seidel, et al., Adv. Mater., 26, 4376 (2014) 5. Y. Heo, et al., Adv. Mater., DOI: 10.1002/adma.201401958 (2014) 6. K.-E. Kim, NPG Asia Mater. 6, e81 (2014) 7. G. Catalan, J. Seidel, R. Ramesh, and J. Scott, Rev. Mod. Phys. 84, 119 (2012)

DF 4.2 Mon 15:30 EB 107

Dielectric properties of multiferroic hexagonal manganites — •Stephan Krohns[1], Eugen Ruff[1], Peter Lunkenheimer[1], Martin Lilienblum[2], Dennis Meier[2], Manfred Fiebig[2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Multifunctional Ferroics, Department of Materials, ETH Zurich, Switzerland

Hexagonal manganites exhibit a broad variety of highly interesting features as, e.g., domain-wall structure, geometric improper ferroelectricity and antiferromagnetic ordering. The exact mechanism for ferro-

electricity is still under debate as well as the impact of the domain-wall structure to macroscopic quantities (e.g., the dielectric constant). A technique to determine the multiferroic, ferroelectric and domain-wall polarisation phenomena is the measurement of the dielectric response to ac and dc electric fields. Here we thoroughly analyse the dielectric response of $YMnO_3$ single crystals in a broad temperature and frequency range. The crystals were subjected to precisely defined cooling rates from above the ferroelectric transition to vary their domain-wall densities. Two relaxation processes occur at temperatures below 350 K. The major one points to an extrinsic so-called Maxwell-Wagner relaxation, based on a thin insulating layer at the surface of the sample. The second, smaller relaxation seems to be of intrinsic origin. We address the question if the macroscopic dielectric properties are influenced by the ferroelectric domain-wall structure.

DF 4.3 Mon 15:50 EB 107

Domain wall motion in proper and improper ferroelastic materials — •Wilfried Schranz — University of Vienna, Faculty of Physics, Boltzmanngasse 5, Vienna, Austria

Many proper and improper ferroelastic materials display (at low measurement frequncies) a huge elastic softening below Tc. This giant elastic softening is caused by domain wall motion and can be supressed with uniaxial stress. Here we review our results on frequency and temperature dependent elastic measurements of $SrTiO_3$ [1], $KMnF_3$ and $KMn_{1-x}Ca_xF_3$ [2], $PbZrO_3$, $NH_4HC_2O_4 \cdot \frac{1}{2}H_2O$ [3] and $BaFe_2As_2$ [4] and put them into context with data from literature. We also present a model [5] based on Landau-Ginzburg theory to describe superelastic softening observed in some of the perovskite systems (improper ferroelastic) as well as in iron based superconductors (pseudo-proper ferroelastic) and show, how the theory can be extended to describe the effects of domain miniaturization (e.g. near morphotropic phase boundaries) on the macroscopic porperties of materials.

Supported by the Austrian FWF (P23982-N20).

[1] A.V. Kityk, W. Schranz, P.Sondergeld, D. Havlik, E.K.H. Salje and J.F. Scott, Phys. Rev. B 61, 946 (2000) [2] W. Schranz, P. Sondergeld, A.V. Kityk and E.K.H. Salje, Phys. Rev. B 80, 094110 (2009) [3] W. Schranz, H. Kabelka, A. Sarras and M. Burock, Appl. Phys. Lett. 101, 141913 (2012) [4] A.E. Böhmer, P.Burger, F. Hardy, T. Wolf, T. P. Schweiss, R. Fromknecht, M. Reinecker, W. Schranz and C. Meingast, Phys. Rev. Lett. 112, 047001 (2014) [5] W. Schranz, Phys. Rev. B 83, 094120 (2011)

Topical Talk DF 4.4 Mon 16:10 EB 107

Field-induced hysteresis of chiral vortices in ferroelectric $SrTiO_3$ twin walls. — •Ekhard Salje — University of Cambridge, Cambridge, UK

Resonant piezoelectric spectroscopy shows polar resonances in paraelectric $SrTiO_3$ at temperatures below 80 K. These resonances become strong at $T < 40$ K. This piezoelectric response does not exist in paraelastic $SrTiO_3$ nor at temperatures just below the ferroelastic phase transition. The interpretation of the resonances is related to ferroelastic twin walls which become polar at low temperatures in close analogy with the known behavior of $CaTiO_3$. $SrTiO_3$ is different from $CaTiO_3$, however, because the wall polarity is thermally induced; i.e., there exists a small temperature range well below the ferroelastic transition point at 105 K where polarity appears on cooling. As the walls are atomistically thin, this transition has the hallmarks of a two-dimensional phase transition restrained to the twin boundaries rather than a classic bulk phase transition. Simulations of polar twin walls in $SrTiO_3$ show nanoscopic vortices, which can be switched in orientation under an external electric field. The hysteresis of the vortex polarization inside the twin boundary leads to direct applications in non-volatile memory devices. E.K.H. Salje et al. Domains within Domains and Walls within Walls: Evidence for Polar Domains in Cryogenic $SrTiO_3$, Phys. Rev. Lett. 111, 24, 247603 (2014), Zykova-Timan T and Salje E.K.H. Highly mobile vortex structures inside polar twin boundaries in SrTiO3, APL 104, 082907 (2014).

10 min break

Topical Talk DF 4.5 Mon 16:50 EB 107

Spintronic functionality of $BiFeO_3$ domain walls — Ji Hye Lee[1,3], Ignasi Fina[1,2], Dietrich Hesse[1], and •Marin Alexe[1,2] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — [2]University of Warwick, Department of Physics, Coventry CV4 7AL, UK — [3]Division of Quantum Phase and Device, Department of Physics, Konkuk University, Seoul 143-701, Korea

Here we show that the FE domain walls (DWs) in the multiferroic material $BiFeO_3$ (BFO), which are intrinsically two dimensional nanoobjects, are not only conductive, but are also ferromagnetic, showing spin-dependent transport. We will show that the electronic transport across the * FM and FE * domain walls in BFO is modulated by an external magnetic field, resembling the anisotropic magnetoresistance (AMR) in archetypical metallic ferromagnets. The found AMR is accompanied by a visible hysteresis, which is ascribed to the coupling of the FM domain walls to the antiferromagnetic properties of the BFO domains, similar to those found in magnetically coupled FM/AFM structures. Since BFO preserves two switchable electric polarization states, one can manipulate the FE DWs and thus magnetization via an electric field. The electronic transport occurring through the FE DWs in common metal-ferroelectric-metal capacitors has been discriminated from the contribution occurring from the bulk, and the intrinsic conduction mechanism at the DWs is identified.

DF 4.6 Mon 17:20 EB 107

3D-mapping of ferroelectric domain walls by Cherenkov second-harmonic generation — •Thomas Kämpfe[1], Philipp Reichenbach[1], Mathias Schröder[1], Alexander Haussmann[1], Theo Woike[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany — [2]Institut für Strukturphysik, Technische Universität Dresden, Zellescher Weg 16, 01069 Dresden, Germany

Ferroelectric domain walls (DWs) are a novel approach towards nanoelectronic circuitry since providing localized conduction within a fully insulating host matrix. The key factor is the DW inclination angle α with respect to the crystallographic axes determining the amount of polarization charge at the head-to-head DWs. Hence, the conductivity can be considerably tuned via doping concentration and poling conditions. We apply Cherenkov second-harmonic generation (C-SHG) to map such charged DWs in three dimensions throughout a mm-thick Mg:$LiNbO_3$ single crystal [1]. We will present domain wall topologies for different cases, also including surface domains, which are created upon external UV illumination and exhibiting also tail-to-tail DWs. We investigated the domain wall protrusion upon different illumination strengths. Moreover, we will also introduce into an extended version of C-SHG based on interferometric SHG (I-SHG). I-SHG provides several advantages as compared to C-SHG, such as an increased vertical resolution, a larger vertical imaging range, as well as easier imaging conditions.

[1] T. Kämpfe et al., Phys. Rev. B, 89, 035314 (2014).

DF 4.7 Mon 17:40 EB 107

UV-induced AC transport along conductive domain walls in $LiNbO_3$ single crystals — Mathias Schröder[1], Xi Chen[2], •Alexander Haussmann[1], Andreas Thiessen[1], Jan Poppe[3], Dawn A. Bonnell[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, D-01069 Dresden, Germany — [2]Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA — [3]Physikalische Chemie, Technische Universität Dresden, Bergstrasse 66 b, D-01062 Dresden, Germany

The impedance properties of UV-illuminated ($\lambda = 310$ nm) conductive domain walls (CDWs) in 5% Mg-doped $LiNbO_3$ single crystals (sc) are investigated both on the nm length scale using nanoimpedance microscopy (NIM), as well as macroscopically by comparing the transport properties of multi- and single domain samples. Similar to the DC transport, we find the CDWs to be highly conductive for AC currents as well, mostly pronounced for $f < 200$ Hz due to the strong influence of the bulk capacitance at higher frequencies. Moreover, simultaneously applying both an AC and DC voltage results in an increased real part of the AC CDW current. Equivalent circuits accurately describing both the domain and CDW contributions hence were developed; as a result we are able to analyze and quantify the complex dielectric conductive behavior of both bulk and CDWs in sc-$LiNbO_3$ within the framework of the mixed conduction model: Hopping of excited charge carriers along the CDWs was identified as the dominant charge transport process.

Topical Talk DF 4.8 Mon 18:00 EB 107

Functional ferroic domain walls - AC & DC transport — •Lukas M. Eng — Institute of Applied Physics, TU Dresden, 01062 Dresden, Germany

Wide band-gap ferroic oxides exhibit both ferroelectric and ferromagnetic properties that promise a novelty of tunable and spectac-

ular applications such as magneto-electric storage devices [1] or metamaterial-based superlensing [2]. We focus here on the domain wall functionality which is clue in order to engineer devices as the ones mentioned above for modern-type applications. Surprisingly, we find such domain walls in $LiNbO_3$ and other single crystals to exhibit a metallic-like conductivity [3] that can even be tuned or switched on and off. Consequently, such charged domain walls allow for both AC [4] and DC [3] electron transport within a nanometer-wide discontinuity that is embedded in a fully insulating matrix. We investigated these novel topologies with a variety of scanning probe techniques, through transport measurements as well as with nonlinear optical methods [5], Since these metallic-like nanocontacts can be engineered on will, they provide a novel and elegant way for exploring nanoscale 2-dimensional transport properties.

[1] R. Streubel et al., Phys. Rev. B 87, 054410 (2013). [2] S.C. Kehr et al., Nature Comm. 2, 249 (2011). [3] M. Schröder et al., Adv. Funct. Mater. 22, 3936 (2012). [4] M. Schröder et al., Mater. Res. Express 1, 035012 (2014). [5] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014).

DF 5: Poster Session on Ferroic Domain Walls - Multiferroics (DF with KR/MA/TT)

Sponsored by NT-MDT

Part of the 3-days focus on ferroic domain walls:
Tutorial, Symposium (SYDW), and three Focused Sessions.

The goal of the poster session is to present the state of the art of the research on magnetic, ferroelectric, and multiferroic domain walls bringing interested scientist together in a stimulating environment in order to stimulate vivid topical discussions.

Time: Monday 19:00–21:00 Location: Poster C

DF 5.1 Mon 19:00 Poster C

Superdomains in $K_{0.9}Na_{0.1}NbO_3$ thin films on $NdScO_3$ substrates — •Jutta Schwarzkopf[1], Martin Schmidbauer[1], Dorothee Braun[1], Albert Kwasniewski[1], Jan Sellmann[1], and Michael Hanke[2] — [1]Leibniz Institute for Crystal Growth, Berlin, Germany — [2]Paul- Drude-Institut für Festkörperelektronik, Berlin, Germany

Incorporation of lattice strain in thin films gives rise to the creation of controlled arrays of domains and can lead to very complex domain structures. Understanding of strain induced domain formation will open the possibility to selectively influence film properties. Due to its orthorhombic symmetry (K,Na)NbO_3 films offer a large variety of ferroelectric and ferroelastic domain types. In this study $K_{0.9}Na_{0.1}NbO_3$ thin films were grown under slight compressive lattice strain on $NdScO_3$ substrates by MOCVD. Lateral PFM images of the (100) oriented films reveal bundles of ferroelectric domains along the [001] substrate direction and a width of 100-200 nm which are superimposed by ferroelastic domains forming regularly arranged herringbone patterns with a periodicity of 30 nm. The domain walls within the domain bundles are tilted alternatingly by +15° and -15° with respect to the [110] orientation of the substrate. Grazing incidence x-ray diffraction experiments have shown that adjacent superdomain bands exhibit an in-plane monoclinic lattice distortion of 0.12°. We conclude that the hierarchical structure leads to a domain formation on two scales, which effectively release the misfit strain in the film induced by the substrate.

DF 5.2 Mon 19:00 Poster C

Advanced characterization of functional ferroelectric domain walls by X-ray photoelectron emission microscopy — •Jakob Schaab[1], Ingo P. Krug[2,3], Zewu Yan[4], Edith Bourret[4], Claus M. Schneider[3], Ramamoorthy Ramesh[4,5], Manfred Fiebig[1], and Dennis Meier[1] — [1]Department of Materials, ETH Zürich — [2]Institut für Optik und Atomare Physik, TU Berlin — [3]Forschungszentrum Jülich, PGI-6 — [4]Materials Science Division, LBNL Berkeley — [5]Department of Materials Science and Engineering, UC Berkeley

The observation of anomalous electronic transport at ferroelectric domain walls and its significance for nano-electronics triggered tremendous scientific interest. To date, the transport behavior and potential barriers at domain walls have been predominantly scrutinized by scanning probes. This, however, convolutes the intrinsic electronic properties with contact resistance and inhomogeneous probe fields, so that the detailed origin of the behavior remains obscured.

Here, we report on the capability of high-resolution X-ray photoemission electron microscopy (X-PEEM) to image and characterize ferroelectric domain walls contact-free and with nanometer resolution. In the ferroelectric semiconductor ErMnO3, we visualize ferroelectric domain walls by exploiting photo-induced charging effects and generate an electronic conduction map by analyzing the kinetic energy of photoelectrons. With this we open a pathway for non-destructive and element-specific studies of electronic and chemical domain-wall structures bypassing previous experimental limitations and significantly expanding the accessible parameter space.

DF 5.3 Mon 19:00 Poster C

Strain-induced defect-polarization coupling in $SrMnO_3$ films — •Carsten Becher[1], Laura Maurel[2], Ulrich Aschauer[1], Martin Lilienblum[1], Cesar Magen[2], Dennis Meier[1], Eric Langenberg[2], Morgan Trassin[1], Javier Blasco[3], Ingo Krug[4], Pedro Algarabel[3], Nicola Spaldin[1], Jose Pardo[2], and Manfred Fiebig[1] — [1]ETH Zürich, Zürich, Switzerland — [2]Instituto de Nanoscienciencia de Aragon, Zaragoza, Spain — [3]Departemento der Fisica de la Materia Condensada, Zaragoza, Spain — [4]Institut für Optik und Atomare Physik, Berlin, Germany

Epitaxial strain can stabilize new matter phases in thin films and is thus a degree of freedom to increase functionality. Here we demonstrate a novel polar phase in 20 nm $SrMnO_3$ films that are epitaxially grown under tensile strains by pulsed laser deposition. High resolution X-Ray diffraction and transmission electron microscopy confirm the crystalline quality of the tetragonal films. We use nonlinear optics to proof that strain induces polarity, and density functional theory to show that it simultaneously increases the concentration of oxygen vacancies. These vacancies accumulate at the polar domain walls where they establish an electrostatic barrier to electron migration. As a consequence, scanning probe microscopy shows that the electrical conductance is structured into isolated "nanocapacitors" which can be charged individually.

DF 5.4 Mon 19:00 Poster C

Raman spectroscopy for the characterization of ferroelectric materials: An Overview — •Michael Rüsing[1], Peter Mackwitz[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center of Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Nonlinear ferroelectrics are a key material class for application in integrated optics from the high power to the single photon level. The exploitable properties range from the electro-optic effect, to large nonlinear susceptibilities and the possibility to achieve quasi-phase matching by periodic poling. But design and fabrication of devices requires an extensive knowledge on the limiting factors, such as intrinsic and extrinsic defects. Here Raman spectroscopy offers a versatile tool for characterization of material properties due to its sensitivity to a wide range of effects. This work provides an overview on performed Raman studies in various ferroelectrics, including Lithium-Niobate-Tantalate mixed crystals and KTP. Determined properties include the relative scattering tensor strengths, material composition in mixed crystals and dielectric properties. Of particular interest is the study of ferroelectric domain structures, whose behavior influenced by the presence of defects.

DF 5.5 Mon 19:00 Poster C

Laser induced poling inhibition of $LiNbO_3$ using an amorphous Si absorber — Grigoris Zisis[1], Gregorio Martinez-Jimenez[1], Yohann Franz[1], Noel Helay[1], David Grech[2], Harold Chong[2], Elisabeth Soergel[3], Anna Peacock[1], and •Sakellaris Mailis[1] — [1]Optoelectronics Research Centre, University of Southampton, Highfield, Southampton, SO17 1BJ, U.K. — [2]School of Electronic and Computer Science, University of Southampton, Highfield, Southampton SO17 1BJ, U.K. — [3]Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

Here we demonstrate laser-induced inhibition of poling in lithium niobate by irradiating a thin absorbing layer of amorphous Si, deposited on the surface of the crystal. The absorption of a-Si in the visible range is sufficiently high to produce significant temperature gradients in the substrate causing a local change in the stoichiometry of the crystal, which in turn modifies the coercive field locally.

This arrangement enables domain engineering using readily available visible laser sources instead of costly and power limiting UV lasers which were previously used to obtain inhibition of poling in this material.

Examination of the topography and piezoresponse of the PI domains, which are formed using this laser assisted method shown a "soft" domain boundary where the domain wall is not sharp but rather consists of isolated nano-domains whose density and size is a function of the distance from the centre of the laser irradiated track.

DF 5.6 Mon 19:00 Poster C

Raman Spectroscopy and Spin-Phonon-Coupling of Multiferroic $Eu_{1-x}Ho_xMnO_3$ — •Sebastian Elsässer[1], Jean Geurts[1], Vladimir V. Glushkov[2], and Anatoly M. Balbashov[2] — [1]Exp. Phys. III, University of Würzburg, Germany — [2]Prokhorov GPI, Russian Academy of Sciences, Moscow, Russia

The revival of studies on magneto-electric (ME) effects has led to rich insights in the physics of charge and spin degrees of freedom and their mutual interaction via ME coupling [1]. One of the most extensively studied effects is the inverse Dzyaloshinskii-Moriya interaction. Hereby, the ordering of the magnetic moments leads to a lattice distortion which, in turn, can induce in a permanent electric polarization. This manifests itself in the perovskite-like rare-earth manganites $RMnO_3$. Here, the average size of the rare-earth ions R^{3+} directly influences the octahedron tilting angle. This can be used to tune the coupling between the magnetic Mn sites yielding model system for the interplay of crystalline distortion, magnetic frustration and electric polarization. In this study, R= Eu^{3+} ions are partially replaced with Ho^{3+} (<30%) to achieve the multiferroic phase. Spin-phonon-coupling (SPC) is probed by temperature-dependent Raman spectroscopy. We identify the elusive peak at 650cm^{-1} to be the $B_{3g}(1)$ mode. Upon cooling renormalisation of phonon energies due to SPC-effects starts already well above T_N. We observe that the SPC-shift is mode-specific, being strongest (up to 1%) for the $B_{2g}(1)$ and $B_{3g}(1)$, which are both octahedron breathing modes.

[1] M. Fiebig, Journal of Physics D-Applied Physics **38**, 8 (2005)

DF 5.7 Mon 19:00 Poster C

Domain walls in lithium niobate investigated by Raman spectroscopy and density functional theory — •Sergej Neufeld[1], Michael Rüsing[2], Gerhard Berth[2], Artur Zrenner[2], Wolf Gero Schmidt[1], and Simone Sanna[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn — [2]Department Physik, Universität Paderborn

The intensity of the Raman signal associated to different phonon modes of $LiNbO_3$ is strongly modified by the presence of ferroelectric domain boundaries [1]. The intensity modulation can be exploited to map domain structures, thus using Raman spectroscopy as a non-destructive imaging tool for the investigation of polarization-domains and domain walls [2]. Unfortunately, the origin of the modifications in the Raman signal is currently unknown. In an attempt to understand the mechanisms leading to the modification of the measured intensity, we have modeled Raman scattering efficiencies from first-principles. Thereby the Raman susceptibility tensor is calculated within the density functional theory following the approach proposed by Ghosez and co-workers [3]. The approach is validated with the TO bulk phonon modes of A_1 and E symmetry and then applied to domain boundaries. The bulk Raman intensities calculated for all possible combinations of the polarization of incoming and scattered photons are in good agreement with the measured spectra. Results for simplified domain wall models are presented and discussed. [1]P. S. Zelenovskiy et. al., Appl. Phys. A 99, 741 (2010). [2]G. Berth et al., Ferroelectrics 420, 44 (2011). [3]M. Veithen et al., Phys. Rev. B 71, 125107 (2005).

DF 5.8 Mon 19:00 Poster C

Evolution of ferroelectric domain patterns in $BaTiO_3$ at the orthorhombic ↔ tetragonal phase transition — •Thorsten Limböck and Elisabeth Soergel — Institute of Physics, University of Bonn, Nussallèe 12, 53115 Bonn, Germany

Domain patterns in barium titanate (BTO) were investigated by piezoresponse force microscopy (PFM) using a variable-temperature scanning force microscope. By analyzing the vertical and the lateral PFM images, the directions of polarization of the individual domains, i. e. 6 directions for the tetragonal and 12 for the orthorhombic phase, could be identified. The change of a domain pattern when submitting the crystal to a temperature ramp between $+20°$ and $-20°$ synchronized to the PFM scanning process, was directly monitored. Finally, the possible conversions between specific domain orientations upon heating/cooling the crystal across the phase transition were experimentally confirmed.

DF 5.9 Mon 19:00 Poster C

Domain wall conductivity in gold-patterned single-crystal bulk samples using c-AFM — •Thorsten Adolphs and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Wegelerstrasse 8, 53115 Bonn

Domain wall conductivity is generally measured by c-AFM, thereby applying moderate voltages between the tip and a large-area back electrode. This technique being very attractive because of its ease of use it has, however, a couple of drawbacks: (i) the voltage applied to the tip leads to electric fields at the tip apex locally exceeding E_c. Since the displacement of a domain wall is energetically favorable (when compared to the creation of new domains), local poling predominantly takes place at the domain walls, leading to a local poling current which is also seen by c-AFM; (ii) the electrical connection between the tip and the domain wall is not reliable; and (iii) different materials of the tip and the back electrode might lead to Schottky-barrier behavior of the domain-wall current. In order to overcome these drawbacks, we propose the use of small, some μm^2-sized gold-patterns evaporated on top of the sample surface, partially connecting to the domain walls. We will present first experimental results obtained with bulk, single crystalline samples prepared for c-AFM in such a way.

DF 5.10 Mon 19:00 Poster C

Local poling at domain walls in $LiNbO_3$ crystals in connection with c-AFM measurements — •Jakob Frohnhaus and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Wegelerstrasse 8, 53115 Bonn

An electrical current localized at ferroelectric domain walls recorded by means of conductive atomic force microscopy (c-AFM) can basically have two origins: electrical conductivity of the domain wall or local poling. We show that also local poling leads to c-AFM images which cannot straightforwardly be distinguished from those c-AFM images displaying the electrical conductivity of the domain wall.

DF 5.11 Mon 19:00 Poster C

Signature of domain walls in PFM measurements — •Tim Flatten and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn

Piezoresponse force microscopy (PFM) is at present the technique the most used for mapping ferroelectric domain patterns. However, the unambiguous determination of the direction of polarization of the individual domains based on PFM-images is generally not straightforward. Not only the careful analysis of a set of vertical- and lateral-PFM images are required, but possibly also a set of images after the rotation of the sample by $90°$ are necessary for fully determining the domain pattern. In addition to the PFM-signal obtained on top of the domain faces, on might, however, also make use of the signature of the domain walls (DW) in the PFM-signal. For ↑↓ domain walls the PFM-signal shows a symmetric, tangent-like transition between the two domains. This transition, however, should exhibit different features depending on the direction of polarization of the domains adjacent to the DW and the inclination angle of the DW relative to the sample surface. Using this additional information, the full determination of the domain pattern should be facilitated.

DF 5.12 Mon 19:00 Poster C

Measurement system for the magnetoelectric effect — •Ulrich Straube and Kathrin Doerr — Martin-Luther-University Halle, Institute of Physics, FoG, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Magnetoelectric materials have different and frequency-dependent magnetoelectric effects. The correct determination of these effects is difficult because of various problems including electric and magnetic shielding, sample preparation and pretreatment. A simple measurement arrangement containing a Helmholtz coil, a pair of NdFeB permanent magnets and a special preamplifier is presented. Some results obtained from magnetoelectric ceramic materials are shown.

DF 5.13 Mon 19:00 Poster C

The magnetoelectric effect across scales — •Doru C. Lupascu[1], Heiko Wende[2], Jörg Schröder[3], Matthias Labusch[3], Morad Etier[1], Ahmadshah Nazrabi[1], Irina Anusca[1], Harsh Trivedi[1], Yanling Gao[1], Marianela Escobar[1], Vladimir V. Shvartsman[1], Joachim Landers[2], Soma Salamon[2], and Carolin Schmitz-Antoniak[4] — [1]Materials Science & Center for Nanointegration Duisburg-Essen (CENIDE) — [2]Faculty of Physics & CENIDE — [3]Institute of Mechanics, all at University of Duisburg-Essen — [4]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich

Magnetoelectric coupling can arise in intrinsic multiferroics as well as composites. We will outline how for intrinsic BiFeO3 nanoparticles yield different magnetoelectric properties at room temperature than larger grains or bulk material. Magnetoelectric nanoscale composites of $BaTiO_3$ and $CoFe_2O_4$ display rather poor magnetoelectric coupling macroscopically. Their micron scale counterparts on the other hand yield nice macroscopic response. The mechanical, electrical, and magnetic effects are analyzed using techniques including Mössbauer spectroscopy, magnetic force microscopy, piezoforce microscopy, and macroscopic techniques. It will be shown that microscopic coupling is strong also for (partly) conducting magnetic inclusions and nanosystems while macroscopic properties are highly dependent on good insulation of the samples. Experimental asymmetries in determining the magnetoelectric coupling coefficient are discussed.

Support via FP7 Marie Curie Initial Training Network *Nanomotion* (grant n° 290158) & Forschergruppe 1509 are acknowledged.

DF 5.14 Mon 19:00 Poster C

Insitu X-ray studies of mechanical coupling at piezoelectric/magnetostrictive interfaces — •Philipp Jordt[1], Stjepan Hrkac[1], Olaf M. Magnussen[1,2], and Bridget M. Murphy[1,2] — [1]Institut für Experimentelle und Angewandte Physik, ChristianAlbrechts-Universität zu Kiel, Germany — [2]Ruprecht Haensel Laboratory, Christian-Albrechts-Universität zu Kiel, Germany

To optimize magnetoelectric composites for magnetic sensor applications it is necessary to understand the coupling at the interface between a piezoelectric and a magnetostrictive material. To study the coupling at the interface, we measure the lattice deformation of the piezoelectric substrate *insitu* by grazing incidence X-ray diffraction in an external magnetic field and for different thicknesses of the magnetostrictive layer grown by magnetron sputtering, using the high resolution and high intensity X-ray beam provided by Petra III (P08). We investigate the magnetic field induced strain of $(Fe_{90}Co_{10})_{78}Si_{12}B_{10}$ on ZnO and InP substrates. From the Bragg peak positions we determined the interplanar spacings in the substrates and the corresponding strain as a function of the applied magnetic field. We measure the strain for different thicknesses and get a critical thickness for the magnetostrictive layer. We thanks the DPG for funding through PAK 902.

DF 5.15 Mon 19:00 Poster C

Influence of piezoelectric induced strain on the Raman spectra of $BiFeO_3$ films — •Cameliu Himcinschi[1], Andreas Talkenberger[1], Jens Kortus[1], Alexander Schmid[2], Er-Jia Guo[3,4], and Kathrin Dörr[3,4] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Applied Physics, D-09596 Freiberg, Germany — [3]Institute for Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany — [4]Institute for Metallic Materials, IFW Dresden, 01069 Dresden, Germany

$BiFeO_3$ epitaxial thin films were deposited on piezoelectric $0.72Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.28PbTiO_3$ (PMN-PT) substrates with a conductive buffer layer ($La_{0.7}Sr_{0.3}MnO_3$, or $SrRuO_3$) using pulsed laser deposition. The calibration of the strain values induced by the applied voltage on the piezoelectric PMN-PT substrates was realised using X-Ray Diffraction measurements. Raman spectra monitoring as a function of the applied voltage (and hence strain) was performed in resonant conditions, using the 442 nm line of a HeCd laser. The piezoelectric induced strain in the $BiFeO_3$ films causes shifts in the phonon position. The method of piezoelectrically induced strain allows to obtain a quantitative correlation between strain and the shift of the Raman-active phonons, ruling out the influence of extrinsic factors, as growth conditions, crystalline quality of substrates, or film thickness.

This work is supported by the German Research Foundation DFG HI 1534/1-2.

DF 5.16 Mon 19:00 Poster C

Control of the magnetic properties of magnetostrictive thin films by crossing the phase transition on a Mott insulator — S. Finizio[1], A. Fantini[1,2], •T. Lenz[1], M.V. Khanjani[1], S. Altendorf[2,3], D. Passarello[2], S.S.P. Parkin[2], and M. Kläui[1] — [1]Institut für Physik, Universität Mainz, Mainz, Germany — [2]IBM Almaden Research Center, San Jose, CA, USA — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The study of strongly correlated materials such as the Mott insulator VO_2 has recently attracted interest, due to the possibility of manipulating materials properties on ultrafast timescales. VO_2, in particular, has been object of attention as a metal-insulator-transition (MIT) from an insulating monoclinic phase to a conducting rutile phase occurs at accessible temperatures just above RT. These changes in crystalline order within the MIT induce strain at the interface. Combined with magnetostrictive materials such as Ni, the MIT of VO_2 is exploited to study the dynamics of the magneto-elastic coupling. Here, we present MOKE and SQUID magnetometry studies of the influence of the MIT of VO_2 on the magnetic properties of a Ni thin film. VO_2 thin films were heteroepitaxially deposited by pulsed-laser-deposition on (100) TiO_2 substrates, onto which Ni film were deposited by thermal evaporation. The magnetic properties of the Ni thin films were then determined upon thermally crossing the MIT. Our results show that strong changes in the magnetic anisotropy of the Ni films occur upon crossing the MIT leading to changes in the switching fields and characteristics as needed for ultra-fast strain-induced switching.

DF 5.17 Mon 19:00 Poster C

Structural investigation of erythrosiderites by single crystal X-ray diffraction — •Tobias Fröhlich[1], Ladislav Bohatý[2], Petra Becker[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Erythrosiderites $A_2[FeX_5(H_2O)]$, where A stands for an alkali metal or ammonium ion and X for a halide ion, are antiferromagnets with Néel-temperatures ranging from 6 to 23 K [1]. This family of compounds allows to investigate the impact of structural parameters on the magnetoelectric properties by comparing their closely related structures. The compound $(NH_4)_2[FeCl_5(H_2O)]$ was found to be multiferroic with strong magnetoelectric coupling [2]. While most structures of erythrosiderites crystallize in the space group Pnma, $Cs_2[FeCl_5(H_2O)]$ structurally deviates from the other erythrosiderides and crystallizes in space group Cmcm [3]. The structures of $(NH_4)_2[FeCl_5(H_2O)]$ and $Cs_2[FeCl_5(H_2O)]$ are investigated by single-crystal X-ray diffraction. Additionally, the non-magnetic compound $(NH_4)_2[InCl_5(H_2O)]$ is structurally investigated. Irrespective the absence of magnetism, its crystal structure is very similar to that of $(NH_4)_2[FeCl_5(H_2O)]$, therefore it can be used as a reference material to separate magnetoelectric effects.

[1] J. Luzón et al., Physical Review B, **78**, 054414 (2008). [2] M. Ackermann, D. Brüning, T. Lorenz, P. Becker, L. Bohatý, New Journal of Physics **15**, 123001 (2013). [3] M. Ackermann, T. Lorenz, P. Becker, L. Bohatý, J. Phys.: Condens. Matter **26**, 206002 (2014).

DF 5.18 Mon 19:00 Poster C

Multiferroic magnonics: quantum interference, dissipationless energy transport, and Majorana fermions — •Wei Chen[1], Manfred Sigrist[2], Andreas P. Schnyder[1], Peter Horsch[1], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]ETH-Zurich, Zurich, Switzerland

We demonstrate the broad applications of multiferroic materials based on their noncollinear magnetic order and magnetoelectric effect. Upon mapping the noncollinear magnetic order into a spin superfluid, the magnetoelectric effect enables the electrically controlled quantum in-

terference of spin superfluid, indicating the possibility of a room temperature SQUID-like quantum interferometer that manifests the flux quantization of electric field. Because the magnetoelectric effect enables changing the noncollinear magnetic order by electric field, we propose that applying an oscillating electric field with frequency as low as household frequency can generate a fast, coherent rotation of the magnetic order that is free from energy loss due to Gilbert damping, and can be used to deliver electricity up to the distance of long range order. At a superconductor/multiferroic interface, the noncollinear magnetic order imprints into the superconductor via $s-d$ coupling, which can produce Majorana fermions at the edge of the superconductor without the need to adjust chemical potential.

DF 5.19 Mon 19:00 Poster C

Optical properties of Sm-doped $BiFeO_3$ close to the morphotropic phase boundary — •Florian Burkert[1], Michaela Janowski[1], Xiaohang Zhang[2], Ichiro Takeuchi[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA

The perovskite $BiFeO_3$ is a rare example for a magnetoelectric multiferroic above room temperature. It has been demonstrated on $Bi_{1-x}Sm_xFeO_3$ thin films that Sm-doping drives $BiFeO_3$ towards a morphotropic phase boundary with enhanced piezoelectric properties, concomitant with a rhombohedral to pseudo-orthorhombic structural phase transition [1]. We studied the reflectance of a similar, Sm-doped $BiFeO_3$ thin film in the far-infrared range at room temperature and ambient pressure by means of FTIR spectroscopy. With increasing Sm doping, we observe changes in the phonon spectrum, especially at Sm content around $x = 0.14$, indicating the occurrence of a structural phase transition in agreement with earlier studies.

[1] I. Takeuchi et al., Appl. Phys. Lett. **92**, 202904 (2008).

DF 5.20 Mon 19:00 Poster C

Inelastic neutron scattering studies on $LuFe_2O_4$ — •Hailey Williamson[1], Petr Čermák[3], Jörg Voigt[1], Ryoichi Kajimoto[4], Geetha Balakrishnan[2], and Manuel Angst[1] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Germany. — [2]Department of Physics, The University of Warwick, UK. — [3]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Germany. — [4]Neutron Science Section, MLF Division, J-PARC Centre, Japan

Multiferroic oxides, which exhibit a coupling between magnetism and charge order (CO), constitute a strong and competitive avenue of research. The well-known $LuFe_2O_4$, the first proclaimed multiferroic through CO due to mixed valence $Fe^{2+/3+}$ bilayers separated by Lu monolayers, was initially thought to produce ferroelectricity through polarization, from the specific CO configuration within the bilayers. This fuelled intense investigation, leading to the conclusion through XMCD, bond valence sum analysis of data and macroscopic characterization, that the bilayers are charged and not polar. With much of the static crystallographic and magnetic properties uncovered, it is now essential to elucidate the dynamic properties to understand how the spin and charge are coupled. Here we present quasi-elastic magnetic scattering with a profound temperature dependence, as well as phonon dispersions at higher energies. Finally, we show an indication of a spin gap opening, on cooling through the magnetic ordering temperature.

DF 5.21 Mon 19:00 Poster C

Investigation of low-frequency Raman modes in $BiFeO_3$ epitaxial thin films with respect to azimuthal orientation — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Christian Röder[1], Ionela Vrejoiu[2,3], Florian Johann[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle — [3]Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart

In this work we present results of highly accurate Raman spectroscopic experiments applied in azimuthal rotation measurements on epitaxial $BiFeO_3$ thin films grown on different scandate substrates. We observe periodic changes in Raman position, full width at half maximum and intensity for some phonon modes as a function of the azimuthal angle Φ. Further analysis revealed the possibility of the so far controversial assignment of Raman modes at low frequencies (< 250 cm^{-1}) through rotational Raman measurements, that show high sensitivity towards the mentioned parameters. We successfully simulated the azimuthal behaviour of Raman intensity and position of selected modes offering a symmetry assignment for them. In addition our results support the domain character of the BFO/DSO thin film identified by piezoresponse-force microscopy measurements.

This work is supported by the German Research Foundation DFG HI 1534/1-2.

DF 5.22 Mon 19:00 Poster C

X-ray diffraction on stoichiometric YFe_2O_4 single crystals. — •Thomas Müller and Manuel Angst — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany.

$LuFe_2O_{4-\delta}$ was long considered to be the primary example for a charge order multiferroic. $YFe_2O_{4-\delta}$ is isostructural, but the ionic radius of Y is much larger compared to Lu, leading to completely different ordering phenomena. We have grown highly stoichiometric single crystals of $YFe_2O_{4-\delta}$ by the optical floating zone method, showing for the first time 3D charge ordering in x-ray diffraction at low temperature. The phase at 200 K can be indexed using a propagation vector of $(\frac{1}{7}\,\frac{1}{7}\,\frac{9}{7})$ considering 6 twin components and second order. Likewise the 160 K phase can be index with $q = (\frac{1}{4}\,\frac{1}{4}\,\frac{3}{4})$. While cooling not only the threefold symmetry but in contrast to $LuFe_2O_4$ also the mirror plane of the room temperature $R\bar{3}m$ structure of $YFe_2O_{4-\delta}$ are lost according to symmetry-analysis.

DF 5.23 Mon 19:00 Poster C

Photoemission electron microscopy study of two-phase Fe/$BaTiO_3$ multiferroic system — •Ashima Arora, Matteo Cialone, Akin Ünal, Sergio Valencia, and Florian Kronast — Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The phenomenon of magneto-electric coupling is of great technological importance in devices such as data storage due to possible electric field control of magnetic properties. However, a single material possessing different ferroic orders which can be exploited practically is difficult to find. Therefore we study a two-phase ferroic system made up of Fe wedge on top of a $BaTiO_3$ single crystal. Here, we study the magnetization of the ferroelectric film by Photoemission Electron Microscopy (PEEM). The capability of PEEM to be element selective and sensitive to magnetic structure of the sample using the tool of X-Ray Magnetic Circular Dichroism (XMCD) makes it possible to get laterally resolved images of magnetic state for individual element in the sample. We have visualized the magnetic domains on the Fe wedge and observed that they are influenced by the BTO substrate at the bottom. In addition, the spectroscopic information using X-ray Absorption Spectroscopy (XAS) provides a deeper insight on the interplay between the ferroelectric and ferromagnetic properties at the interface of Fe and $BaTiO_3$ in the multi-ferroic system.

DF 5.24 Mon 19:00 Poster C

Towards an experimental evidence of the linear magnetoelectric coupling — •Alexander Sukhov[1], Levan Chotorlishvili[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Centro de Investigacion en Materiales Avanzados (CIMAV S.C.), Chihuahua/Monterrey, 31109 Chihuahua, Mexico — [3]Key Laboratory for Magnetism and Magnetic Materials of the MOE, Lanzhou University, Lanzhou 730000, China

We present a theoretical study combining simulations of ferromagnetic resonance (FMR) for interfacesof Co/$BaTiO_3$ and Fe/$BaTiO_3$ [1] and calculations of the mean first passage times for a system of single-domain Fe-nanoparticles deposited on a ferroelectric $BaTiO_3$-substrate [2]. The study is focused on the consequences of the magnetoelectric coupling - which is considered to be linear in polarization and magnetization due to a screening mechanism - on the spectra of absorbed power [1] and the mean switching times of the Fe-nanoparticles [2]. In particular, we demonstrate and discuss how to extract an information on the symmetry and the strength of the magnetoelectric coupling from FMR-experiments, which was recently evidenced in the experiments of Ref. [3] or from eventual telegraph-noise-like experiments.

[1] A. Sukhov, P.P. Horley, C.-L. Jia, J. Berakdar, J. Appl. Phys. **113**, 013908 (2013). [2] A. Sukhov, L. Chotorlishvili, P.P. Horley, C.-L. Jia, S. Mishra, J. Berakdar, J. Phys. D: Appl. Phys. **47**, 155302 (2014). [3] N. Jedrecy *at al.*, Phys. Rev. B **88**, 121409(R) (2013).

DF 5.25 Mon 19:00 Poster C

Optical investigation of ferroic domains beyond the resolution

limit — •Christoph Wetli, Viktor Wegmayr, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

In recent years optical second harmonic generation (SHG) has been shown to be a versatile, non-destructive tool to investigate the often complex domain structures of ferroic and multiferroic materials. Ferroic domains vary broadly in structure and size, depending on the nature of the ferroic ordering. So far, however SHG was restricted to domains larger than the optical resolution limit of 1 μm. Here we present a method by applying a numerical model and simulation to overcome this limitation and to analyze ferroic domain structures some orders of magnitude smaller than the optical resolution limit.

The method is based on the relation between the orientation of the ferroic order parameter and the phase of the nonlinear optical signal. It gives a relation between domain size and density, optical resolution and the intensity of the SHG signal. To show the reliability of the model, we applied it to several simulated domain structures. The simulation of the domain structures is based on an iterative geometrical algorithm, which allows us to generate complex domain patterns like the ferroelectric vortex structures or the irregular bubble like antiferromagnetic domains in hexagonal $YMnO_3$. The numerical calculations were compared with experimental data and found to be in excellent agreement.

DF 5.26 Mon 19:00 Poster C

Emergence of ferroelectricity in multiferroic h-$YMnO_3$ — •Martin Lilienblum[1], Thomas Lottermoser[1], Sebastian Manz[1], Sverre M. Selbach[2], Andres Cano[3], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [2]Department of Material Science and Engineering, NTNU, N-7491 Trondheim, Norway — [3]CNRS, Université de Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

Universal scaling laws, interfacial nano-electronics, and topological defects are currently studied using hexagonal manganites $R$$MnO_3$ (R= Sc, Y, Dy-Lu) as model system. In spite of the remarkably broad interest in the system, surprisingly little is known about the origin of the ferroelectric state. Here we solve the controversy about the emergence of the spontaneous polarization and its coupling to the underlying structural distortion by applying scanning probe microscopy (SPM) and optical second harmonic generation (SHG). We trace the spontaneous polarization by SHG from 100 K to 1450 K directly and contact-free. We find that only a single transition exists in which the polarization arises slower than expected as by-product of the structural distortion. By thermal treatments close to the structural transition and subsequent SPM scans, we show that the exceptionally robust ferroelectric domain pattern is determined only by the structural distortion. In summary we reveal that the ferroelectric order results from an interplay of electric polarization, topological effects, and temperature.

DF 5.27 Mon 19:00 Poster C

Strain-induced defect-polarization coupling in $SrMnO_3$ films — •Carsten Becher[1], Laura Maurel[2], Ulrich Aschauer[1], Martin Lilienblum[1], Cesar Magen[2], Dennis Meier[1], Eric Langenberg[2], Morgan Trassin[1], Javier Blasco[3], Ingo Krug[4], Pedro Algarabel[3], Nicola Spaldin[1], Jose Pardo[2], and Manfred Fiebig[1] — [1]ETH Zürich, Zürich, Switzerland — [2]Instituto de Nanoscienciencia de Aragon, Zaragoza, Spain — [3]Departemento der Fisica de la Materia Condensada, Zaragoza, Spain — [4]Institut für Optik und Atomare Physik, Berlin, Germany

Epitaxial strain can stabilize new matter phases in thin films and is thus a degree of freedom to increase functionality. Here we demonstrate a novel polar phase in 20 nm $SrMnO_3$ films that are epitaxially grown under tensile strains by pulsed laser deposition. High resolution X-Ray diffraction and transmission electron microscopy confirm the crystalline quality of the tetragonal films. We use nonlinear optics to proof that strain induces polarity, and density functional theory to show that it simultaneously increases the concentration of oxygen vacancies. These vacancies accumulate at the polar domain walls where they establish an electrostatic barrier to electron migration. As a consequence, scanning probe microscopy shows that the electrical conductance is structured into isolated "nanocapacitors" which can be charged individually.

DF 5.28 Mon 19:00 Poster C

Magnetoelectric domain control in multiferroic $TbMnO_3$ — •Sebastian Manz[1], Masakazu Matsubara[1,2], Masahito Mochizuki[3,4], Teresa Kubacka[1], Ayato Iyama[5], Nadir Aliouane[6], Tsuyoshi Kimura[5], Steven Johnson[1], Dennis Meier[1], and Manfred Fiebig[1] — [1]ETH Zürich — [2]Tohoku University — [3]Aoyama Gakuin University — [4]Japan Science and Technology Agency — [5]Osaka University — [6]Paul Scherrer Institute

Spin-spiral multiferroics exhibit a strong coupling between the electric and magnetic subsystems which is of potential interest for technological applications. Although these systems have been investigated for more than a decade, the magnetoelectric domain evolution under external fields is still largely unknown. Using optical second harmonic generation we resolve how electric and magnetic fields affect the multiferroic domains in the archetypal spin-spiral multiferroic $TbMnO_3$. In consecutive electric switching cycles, varying multi-domain patterns emerge before a single-domain state is obtained. This observation reflects that the domain walls can easily move without being pinned by, e.g., structural defects. In striking contrast to the electric-field response, multi-domain patterns persist when the polarization direction is flopped by applied magnetic fields. Here, a uniform polarization rotation is observed within all domains, which incorporates a transformation of neutral into nominally charged domain walls. Our results are explained based on numerical Landau-Lifshitz-Gilbert simulations and provide first evidence for the scalability of macroscopic magnetoelectric properties onto the level of domains.

DF 5.29 Mon 19:00 Poster C

Ab initio expression of magneto-electric coupling coefficients in terms of current response function — •Ronald Starke[1] and Giulio Schober[2] — [1]Institut f. Theo. Physik, Bergakademie Freiberg — [2]Institut f. Theo. Physik, Uni Heidelberg

Based on the Functional Approach to electrodynamics of media, we show that the Maxwell equations imply closed, analytical expressions of the magneto-electric coupling coefficients in terms of the current response functions. On the linear level, these expressions include all effects of inhomogeneity, anisotropy and relativistic retardation. Moreover, we relate the 36 component functions of the constitutive tensor used in the context of bi-anisotropic media to only 9 causal response functions which specify the current response to an external vector potential.

DF 5.30 Mon 19:00 Poster C

First-principles study of magnetic properties of $BaFeO_{3-\delta}$ — •Igor Maznichenko[1], Sergey Ostanin[2], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Oxides with a perovskite atomic structure are ideally suited to grow two-component multiferroics, in which a ferroelectric oxide barrier is sandwiched between magnetic electrodes. For example, the perovskites $ATiO_3$ (A = Ba, Pb) can be used as ferroelectric barrier, while ferromagnetic perovskites (La,Sr)MnO_3 or $SrRuO_3$ can serve as ferromagnetic electrodes. Oxide materials are preferable in such a tunnel junction because of their compatibility and growth. Since the number of ferromagnetic conducting oxides is restricted, a search of new suitable oxide electrodes is highly desirable. Recently, the perovskite $BaFeO_3$ was reported to be ferromagnetic in bulk and as thin film [1]. Here, using a first-principles Green function method within the density functional theory, we present a study on magnetic and electronic properties of bulk $BaFeO_3$ especially focusing on the impact of structural deformations and intrinsic defects.

[1] S. Chakraverty et al., Applied Physics Letters 103, 142416 (2013).

DF 6: Poster Session DF

Time: Monday 19:00–21:00 Location: Poster C

DF 6.1 Mon 19:00 Poster C

Analysis of immittance spectra: unambiguous electrical equivalent circuits representing the underlying physics — •Julian Alexander Amani, Tristan Koppe, Hans Hofsäss, and Ulrich Vetter — II. Physikalisches Institut der Georg-August-Universität Göttingen, Deutschland

We propose an approach of analysing immittance spectra with electrical equivalent circuits, which not only eliminates circuit ambiguity but also directly extracts the parameters of the selected physical models.

Analysis of immitance spectra is usually performed by optimising the values of idealised, lumped components in an electrical equivalent circuit to fit the measured data. Those circuits consisting only of idealised components are known to be ambiguous, i. e. different arrangements of components fit the measured data equally well. Hence, definite association of circuit components with physical parts of the system is not possible.

To find the arrangement representing the underlying physics correctly, we derived a fundamental electrical equivalent circuit from Maxwell's equations, describing a homogeneous piece of material, that allows non-linear components dependent on external parameters. In the resulting Voigt circuit, actual physical models are used as resistive and a complex capacitive components. Using measurements of a heterostructure as example we show how, with variation of external parameters (e. g. bias voltage), the unambiguous circuit can be used to extract parameters of the model (e. g. Schottky barrier height) instead of single values of resistance and capacitance.

DF 6.2 Mon 19:00 Poster C

Water-Lithiumniobate Interface from Ab initio Molecular Dynamics — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — Universität Paderborn

$LiNbO_3$ (LN) has been intensively used since decades for various optical and acoustic applications due to its pronounced piezoelectric, pyroelectric, and photorefractive properties and optical nonlinearities. More recently, the possibility to manipulate locally the surface reactivity and surfaces properties by means of polarization reversal of ferroelectric domains has stimulated interest in novel applications from the areas of e.g. nanochemistry or molecular detectors[1].

In order to effectively exploit the phenomena related to the strong and switchable electric fields at ferroelectric surfaces, a detailed microscopic understanding is indispensable. Previous studies [2,3] indicate a highly specific adsorption behaviour of water molecules depending on the surface polarization for water thin films of monolayer thickness. Here we extend the study to the interface between bulk water and LN and perform ab initio molecular dynamics at a wide temperature range. The result show a layered water structure below and slightly above the freezing temperature.

At higher temperatures the molecular water clusters dissolve and the water double layer cannot be recognized anymore.

[1] D. Li, M. H. Zhao, et al., Nat. Mat. 7, 473 (2008)
[2] S. Sanna, R. Hölscher, W.G. Schmidt, PRB 86, 205407 (2012)
[3] S. Rode, R. Hölscher, et al., PRB 86, 075568 (2012)

DF 6.3 Mon 19:00 Poster C

Dielectric, ferroelectric, and energy density properties of barium titanate based ceramics — •Tino Band and Martin Diestelhorst — Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany

Barium titanate ($BaTiO_3$) has been investigated extensively as a dielectric for energy storage due to its high dielectric constant. To achieve higher energy densities a large dielectric breakdown strength (BDS) should be reached by adding a glass or polymer. As is generally known the matrix influences also the dielectric response of the final capacitor. We performed impedance spectroscopy, hysteresis and DC measurements on the ceramics to characterize them. As a result we present the influence of sample properties, like thickness, fraction of the additive or sintering temperature, and external factors, such as frequency or amplitude. Additional we discuss possible effects e.g. interfacial polarization or porosity.

DF 6.4 Mon 19:00 Poster C

AC eletrical measurement on amorphous phase change materials — •Chao Chen[1], Volker Hanno[1], Peter Jost[1], and Wuttig Matthias[1,2] — [1]I. Institute of Physics (IA) of the RWTH Aachen, Germany — [2]JARA-FIT, RWTH Aachen, Germany

Phase-change materials (PCMs) have already been employed in rewritable optical data storage (eg. Blue-ray disc). In the near future, PCM-based electrical memories, phase-change random access memories (PCRAM), could become a competitor for both Flash and DRAM [1,2]. Therefore it is necessary to understand the electronic transport properties of phase change materials for electrical storage.

There is a tremendous difference between crystalline and amorphous PCMs in terms of optical and electrical properties, which is attributed to the presence of resonant bonding in crystalline PCMs [3]. The crystal structure and electrical properties of crystalline PCMs have already been intensively studied. However, the phenomena of resistance drift and threshold switching in amorphous PCMs are not yet well understood. Here we present AC conductivity and impedance spectroscopy data which have been measured in order to investigate the electrical and dielectric properties of the amorphous phase. We expect these data to provide valuable insight into the structural and bonding properties which are supposed to be responsible for the aforementioned phenomena.

DF 6.5 Mon 19:00 Poster C

Dynamics of Oxygen Vacancies in TiO2 — •Michael Wehlau, Jan M. Knaup, and Thomas Frauenheim — BCCMS Universität Bremen, Germany

Resistive switching materials like titania (TiO2) are potentially capable for applications in next-generation semiconductor devices or as components of artificial neurons. Resistive switching effect of metal oxides is based on phase-change mechanisms induced by accumulation of oxygen vacancy defects (VO) and following transformation of insulating TiO2 into substoichiometric conductive phases. For this reason the VO migration is a crucial mechanism for resistive switching. In this work we investigate the dynamics of oxygen vacancies in two ways. We involve thermodynamics in calculations of the free energy surface by metadynamics and obtain accurate minimum energy paths (MEP) for rutile and anatase. We calculate free energy profiles for the VO diffusion using metadynamics, employing a modified version of the PLUMED code, coupled to DFTB+, which implements a permutation invariant vacancy tracking (PIVOT) collective variable. This method provides a technique for rare event sampling without specifying reaction paths. Furthermore, we also perform nudged elastic band calculations to find the MEP for essential VO transitions using the ab-initio DFT method provided by the vasp code. We find free energy barriers and MEP in good agreement. We also find a strong dependency of the activation energy on the crystallographic direction, the crystal structure and the material density.

DF 6.6 Mon 19:00 Poster C

Müller-Matrix-ellipsometry analysis of blazed gratings produced by reactive ion beam etching — Lennart Fricke[1], Carsten Bundesmann[2], Renate Fechner[2], Matthias Burkhardt[3], Michael Helgert[3], Alexandre Gatto[3], Frank Frost[2], •Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universität Leipzig, Inst. für Experimentelle Physik II, Halbleiterphysik, Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V, Leipzig, Germany — [3]Carl Zeiss Jena GmbH, Jena, Germany

We have modeled the optical response of balzed gratings in fused silica using the topography profiles measured by atomic force microscopy for the real space geometry. The obtained spectra are in reasonable agreement with spectra measured by Mueller-Matrix ellipsometry at angles of incidence greater 65° and different azimuthal orientations.

For the simulation of the Mueller-Matrix spectra we employed the rigorous coupled wave approach. The dielectric function of fused silica was taken from a database, thus our modelling procedure is free of any adjustable parameters.

The gratings were produced using interference lithography and reactive ion etching to transfer the pattern defined by lithography into the fused silica substrate. To characterize the sample geometry evolution during etching we investigated a series of samples with different etching times by this modelling technique.

DF 6.7 Mon 19:00 Poster C

Phonon modes in thin-film lithium niobate: A basic study — •Sebastian Krehs[1], Kai Spychala[1], Michael Rüsing[1], Hui Hu[3,4], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics (CeOPP), 33098 Paderborn, Germany — [3]School of Physics, Shandong University, Jinan 250100, China — [4]Nanoln Co. Ltd., Shunhua Road 750, Jinan 250100, China

In the recent years ferroelectric thin films have attracted much attention due to the large quantity of possible applications like infrared detectors and optical filters. For further advancement a better understanding of its physical properties will be inevitable. Therefore the vibrational fingerprints of thin-film lithium niobate ($LiNbO_3$) were studied via μ-Raman spectroscopy. The main focus of the work was concentrated on classification of the occurring vibrational modes in thin-film $LiNbO_3$ with respect to the crystallographic orientation. Here we found a congruent phonon-mode signature to bulk crystal which permits us to conclude that the realized thin-films are of good crystalline quality. Due to the specific fabrication process of thin-film layers, the realized thin-films were attached to different kinds of interface layers. In this context we studied in a further step the influence of different interface layers (e.g. Si- or Cr-layer) on the vibrational properties of thin-film $LiNbO_3$. Furthermore an angle-dispersive characterization was utilized for a defined classification of emerging vibrational modes and a verification of mode-coupling respectively. Here differences could be found which might be linked to surface related effects.

DF 6.8 Mon 19:00 Poster C

Influence of charging temperature on the hysteresis behavior of tubular-channel fluoroethylenepropylene (FEP) ferroelectrets — •Markus Steffen, Xunlin Qiu, Werner Wirges, and Reimund Gerhard — Applied Condensed-Matter Physics,University of Potsdam

Ferroelectrets are internally charged polymer foams or polymer systems with internal cavities which exhibit strong piezoelectricity after bipolar charging (poling) [1].The gas-filled cavities can be charged via a series of dielectric barrier discharges (DBDs). During the DBDs, charges of both polarities are separated, and then deposited onto the internal top and bottom surfaces of the cavities, respectively. The internally charged cavities can be regarded as macroscopic dipoles, whose direction can be switched by reversing the applied electric field. Thus, DBDs inside the cavities lead to a phenomenological hysteresis behavior similar to that of other ferroic materials [2]. In the present study, the influence of the charging temperature on the hysteresis loops of tubular-channel fluoroethylenepropylene (FEP) ferroelectrets is systematically studied over a wide temperature range from -100 to $150°C$. The coercive field and the remanent polarization of the ferroelectret samples are determined as functions of the charging temperature. The results are discussed in the light of Paschen's law for electric breakdown by taking into account the respective gas temperature.

[1] S. Bauer, R. Gerhard(-Multhaupt) and G. M. Sessler, Phys. Today 57(2), 37 (2004).
[2] X. Qiu, *et al.*, J. Appl. Phys. 113, 224106 (2013).

DF 7: Focused Session on Ferroic Domain Walls II (DF with MA)

Part of the 3-days focus on ferroic domain walls:
Tutorial, Symposium (SYDW), three Focused Sessions, and Poster Session.
Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Tuesday 9:30–13:00 Location: EB 107

Topical Talk DF 7.1 Tue 9:30 EB 107

Polarization charge as a reconfigurable dopant in wide-bandgap ferroelectrics — •Tomas Sluka — Ceramics Laboratory, EPFL Swiss Federal Institute of Technology, Lausanne, CH-1015 Switzerland — DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland

Tuning the charge carrier density in semiconductors by spatially fixed chemical impurities has been the cornerstone of electronics for over 50 years. As the miniaturization of CMOS technology approaches critical limits, efforts are turned to conceptually new devices based on emerging electronic properties of materials and interfaces. Recently it has been shown that the effect of chemical doping in semiconductors can be also induced by the polarization charge at Charged Domain Walls (CDWs) in wide-bandgap ferroelectrics. The polarization-charge doping, unlike the chemical doping, implies the intriguing possibility to write, displace, erase and re-create channels having a metallic-type conductivity inside an excellent insulator. This suggests the possible use of CDWs as real-time doping switches in hardware reconfigurable electronics. The talk will introduce methods of CDW engineering in ferroelectric crystals and thin films, the intrinsic properties of individual CDWs, their nanoscale manipulation and implementation into submicron device structures. Nanometers thick CDWs ranging from millimeters to tens of nanometers sizes and having metallic-type conductivity which exceeds 10^3 - 10^9 times the thermally activated conductivity of the bulk and neutral domain walls will be discussed.

DF 7.2 Tue 10:00 EB 107

Nonlinear characteristic of ferroelectric domains: From single domain wall to the periodic structure — •Kai Spychala[1], Moritz Grothe[1], Alex Widhalm[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

On the way to smaller periods of periodically poled structures in ferroelectrica a comprehensive acknowledgement of the domain wall's nonlinear response is necessary. In this approach the analysis of the ferroelectric domain structures have been realized by means of second harmonic (SH) microscopy. In our study the nonlinear characteristic of an isolated transition between two contrarily poled ferroelectric domains has been determined. Here for the nonlinear sequence in the region of a single domain wall, a symmetric trend transverse to the domain transition was initially detected. A detailed depth-resolved and polarization-dependent study hints at a SH-signature conditioned by the orientation of the crystals. Additionally a functional dependence on depth of such sequences was observed. Here an influence of surface charge and inner electric field distribution can be assumed. Furthermore specific nonlinear signatures which are directly connected to the period of the do-main grating were detected in the system's nonlinear response. Due to the long-range character of the correlation between the domain boundaries, an assumed direct link with the inner electric field distribution is suggested.

DF 7.3 Tue 10:20 EB 107

Ferroelectric 180° domain wall motion controlled by biaxial strain — •Robert Roth[1], Er-Jia Guo[1,2], Andreas Herklotz[1,2], Dietrich Hesse[3], and Kathrin Dörr[1,2] — [1]MLU Halle-Wittenberg, Institute for Physics, 06099 Halle, Germany — [2]Institute for Metallic Materials, IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Switching polarization in a ferroelectric proceeds by nucleating reversed domains which subsequently expand. Therefore, wall velocity (v) limits the speed of switching. In thin films, measured values of v are many orders below sound velocity [1], whereas bulk crystals showed larger v. Why are domain walls in films so slow? New insights can be derived from local studies of domain wall velocity by piezoresponse force microscopy in in-situ controlled elastic strain states of the sample. In c-oriented epitaxial $PbZr_{0.2}Ti_{0.8}O_3$ films on piezoelectric substrates, the velocity of non-ferroelastic 180° walls has been investigated employing the approach of Tybell et al. [2]. Remanent circular domains showed strong strain dependences of both, domain relaxation / shrinking in zero electric field and field-driven velocity. We discuss results in the light of known physical mechanisms, identify a strain-induced change of the driving field arising from built-in Schottky junctions at electrodes and suggest a new mechanism of strain-induced charging of tilted domain walls (wall sections).

[1] A. Grigoriev et al., Phys. Rev. Lett. 96, 187601 (2006)

[2] T. Tybell et al., Phys. Rev. Lett. 89, 097601 (2002)

Topical Talk DF 7.4 Tue 10:40 EB 107

Influence of defects on domain wall mobility in ferroelectrics — •Susan Trolier-McKinstry[1], Daniel Marincel[1], Stephen Jesse[2], Sergei Kalinin[2], Huiaruo Zhang[3], and Ian Reaney[3] — [1]Penn State University, University Park, PA, USA — [2]ORNL — [3]University of Sheffield

The dielectric and piezoelectric properties of ferroelectric thin films depend both on the intrinsic response of the material, as well as the motion of domain walls. There are a host of factors that can affect domain wall motion, including grain boundaries, other ferroelectric or ferroelastic domain walls, phase boundaries, dislocations, point defects, some electrode/dielectric interfaces, and core-shell microstructures. One of the challenges that faces the field is the difficulty in isolating the role played by a single type of pinning center or domain wall in controlling the response of an electroded ferroelectric. Instead the amalgamated response of millions of domains and domain walls is probed. This paper will describe the use of scanning probe microscopy and transmission electron microscopy to characterize the motion of domain walls in ferroelectric films, with a concentration on how mechanical stresses at the film * substrate interface and grain boundaries influence the correlated motion of domain walls. Measurements were made on 3 compositions of PZT with a variety of different grain boundary angles. It was found that the domain structure at the grain boundary controlled the width of influence on the domain wall motion. Depending on the angle this width ranged from 0 to hundreds of nm from the boundary.

10 min break

Topical Talk DF 7.5 Tue 11:20 EB 107

The electronic structure of longitudinal domain walls: a DFT perspective — •Gustav Bihlmayer, Kourosh Rahmanizadeh, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Whenever ferroelectric domains meet "head-on", a local accumulation of charge and/or defects compensating this charge can arise. As there is no general atomistic picture of these charged domain walls (DWs), ab-initio studies are still rather scarce. Motivated by detailed transmission electron microscopy images of transversal and longitudinal DWs in PZT [1,2], we studied these walls in $PbTiO_3$ using density functional theory (DFT). We explore the possibility of introducing defects acting as electron-acceptors or -donors at the DWs, as well as the localization of electrons due to correlation effects at the Ti site and compare the DW profiles with experimental data. Our calculations allow to investigate the distribution of defects in the DWs as well as the electronic structure of the bands hosting the accumulated charges. We find that states with magnetic- charge- and orbital order allow to realize an insulating (or semiconducting) behavior even in charged DWs [3]. We further discuss spin-polarization effects in the electron gas forming at the DWs due to relativistic phenomena in charged 90° walls.
[1] C. L. Jia et al., Nature Mater. **7**, 57 (2008). [2] Y. L. Tang et al., Sci. Rep. **4**, 4115 (2014). [3] K. Rahmanizadeh et al., Phys. Rev. B **90**, 115104 (2014). *Financial support of the EU grant NMP3-LA-2010-246102 (IFOX) is gratefully acknowledged.*

DF 7.6 Tue 11:50 EB 107

***Ab initio* investigation of ferroelectric domain walls in barium fluorides** — •Maribel Núñez Valdez and Nicola Spaldin — Materials Theory, ETH Zürich, Wolfgang-Pauli-Strasse 27, CH-8093 Zürich, Switzerland

We present results of first-principles calculations of the ferroelectric domain walls in the layered perovskite-related barium fluorides, $BaMF_4$ (M = Mg, Zn).

The ferroelectricity in the barium fluorides is driven by the softening of a single polar phonon mode consisting of both rotations of the MF_6 octahedra and polar displacements of Ba cations. This so-called "geometric ferroelectricity" is a strikingly different mechanism from that in conventional ferroelectrics [C. Ederer and N.A. Spaldin Phys. Rev. B **74**, 024102,2006].

Using density functional theory (DFT) within the general gradient approximation (GGA) we perform detailed structural relaxations of neutral domain walls (parallel to the polar *c* axis) and calculate the corresponding energies.

Based on comparisons of the total energies, we determine which domain wall orientations and configurations are most likely to form, and we compare their structural and electronic properties to those of domain walls in conventional ferroelectrics.

Finally we explore the strain dependence of the ferroelectric polarization, again comparing to that of conventional ferroelectrics.

DF 7.7 Tue 12:10 EB 107

Advanced characterization of functional ferroelectric domain walls by X-ray photoelectron emission microscopy — •Jakob Schaab[1], Ingo P. Krug[2,3], Zewu Yan[4], Edith Bourret[4], Claus M. Schneider[3], Ramamoorthy Ramesh[4,5], Manfred Fiebig[1], and Dennis Meier[1] — [1]Department of Materials, ETH Zürich — [2]Institut für Optik und Atomare Physik, TU Berlin — [3]Forschungszentrum Jülich, PGI-6 — [4]Materials Science Division, LBNL Berkeley — [5]Department of Materials Science and Engineering, UC Berkeley

The observation of anomalous electronic transport at ferroelectric domain walls and its significance for nano-electronics triggered tremendous scientific interest. To date, the transport behavior and potential barriers at domain walls have been predominantly scrutinized by scanning probes. This, however, convolutes the intrinsic electronic properties with contact resistance and inhomogeneous probe fields, so that the detailed origin of the behavior remains obscured.

Here, we report on the capability of high-resolution X-ray photoemission electron microscopy (X-PEEM) to image and characterize ferroelectric domain walls contact-free and with nanometer resolution. In the ferroelectric semiconductor $ErMnO_3$, we visualize ferroelectric domain walls by exploiting photo-induced charging effects and generate an electronic conduction map by analyzing the kinetic energy of photoelectrons. With this we open a pathway for non-destructive and element-specific studies of electronic and chemical domain-wall structures bypassing previous experimental limitations and significantly expanding the accessible parameter space.

Topical Talk DF 7.8 Tue 12:30 EB 107

Electronic reconstruction and transport at ferroelectric domain walls — •Dennis Meier — ETH Zürich, Switzerland

Unusual electronic properties arise at ferroelectric domain walls due to the low local symmetry and hypersensitivity of these natural oxide interfaces to electrostatics and strain. Such domain walls can, for instance, be highly conducting even when the host material is rather insulating. A major challenge is to understand the complex domain wall physics at the nanoscale and gain control of their properties with the ultimate goal to exploit them for designing domain-wall-based next-generation devices. In my talk I will discuss the case of domain walls in so-called improper ferroelectrics, i.e., systems in which the ferroelectric domain formation is determined by a primary order parameter other than the polarization. Due to the secondary nature of the polarization unusual domain wall configurations are stabilized, which leads to novel degrees of freedom and functionalities. Here, the multiferroic hexagonal manganites are a striking example. I will show that both positively and negatively charged ferroelectric domain walls naturally form in the as-grown state. Driven by the polarity mismatch at these walls, a variety of exotic interface effects emerge giving rise to, e.g., orientation-dependent conduction properties as well as local variations in the electrochemical interface structure. Results gained by electron microscopy, scanning-probe microscopy, and nonlinear optics will be shown, providing novel insight to the domain-wall physics across all relevant length scales from the nanometer to the millimeter regime.

DF 8: High-k and Low-k Dielectrics (DS with DF)

Time: Tuesday 11:15–12:15 Location: H 0111

DF 8.1 Tue 11:15 H 0111

Broadband dielectric response of doped rutile: intrinsic or extrinsic colossal dielectric constants? — •Martin Wohlauer, Stephan Krohns, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg (Germany)

Materials exhibiting so-called colossal effects have an enormous potential for future use in correlated electronics, including capacitors for energy storage and integrated circuits. The search for functional ceramics showing colossal dielectric constants (CDC) is still an active field of research[1]. Different phenomena, e.g., charge-order or internal as well as external electrical heterogeneities can lead to CDCs[2]. For the most prominent ceramic, $CaCu_3Ti_4O_{12}$, the mechanism giving rise to a dielectric permittivity of up to 10^5 is of extrinsic nature, e.g. interface polarisation. The discovery of CDCs in indium- and niobium-doped rutile at room temperatures recently also attracted high scientific interest[3]. In this talk, broadband dielectric measurements on various doped rutile ceramics will be presented. The results will be thoroughly discussed, especially emphasizing the contributions of external and internal interface effects influencing the permittivity. We demonstrate, that extrinsic interface effects are responsible for the CDCs in doped rutile.

[1]S. Krohns *et al.*, *Nat. Mat.*, **10**:899 (2011).
[2]P. Lunkenheimer *et al.*, *Eur. Phys. J. Special Topics*, **180**:61 (2010).
[3]W. Hu *et al.*, *Nat. Mat.*, **12**:821 (2013).

DF 8.2 Tue 11:30 H 0111

Structuring and interface manipulation of ultra-thin silicate films on a $Si(001)$ surface — •Shariful Islam[1], Karl Hofmann[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik (ATMOS), Leibniz Universität Hannover — [2]Inst. f. Bauelemente der Mikroelektronik, Leibniz Universität Hannover

The dielectric-substrate interface plays a very important role on the growth condition and on the chemical, structural and kinetic properties of dielectric layers. Some very important properties like the sharpness of the interface, trap densities and band alignment also influenced by the cleanliness of substrate surface. We found the crystalline high-k silicate $(Ba_{0.8}Sr_{0.2})_2SiO_4$ and Ba_2SiO_4 to have dielectric constants ~ 18 and ~ 20 respectively. We studied the silicates elaborately both on structured and unstructured $Si(001)$ surface after depositing both at room and at high temperature ($650°C$). In addition to the spectroscopic measurements (XPS, SPA-LEED, EELS, AFM and TEM) we performed electrical measurements (C-V & I-V) of the silicate as an alternate gate dielectric in a MOS diode to study the dielectric-substrate interface in detail. The crystalline orthorhombic Ba_2SiO_4 grown here has a band gap of $E_G = 5.7$eV, an interface trap density $D_{it} \sim 10^{12}eV^{-1}cm^{-2}$, very low hysteresis < 0.5mV, band offset > 2eV, leakage current $< 6\ mA/cm^2$ at +1V; additional structural and electrical properties will be discussed.

DF 8.3 Tue 11:45 H 0111

k-restore Process with Plasma Enhanced Fragmentation for Damaged ULK Materials — A DFT and MD Study — •Anja Förster[1,5], Christian Wagner[2], Jörg Schuster[1], Sibylle Gemming[3,4], and Stefan Schulz[1,2] — [1]Fraunhofer ENAS, Chemnitz — [2]Center for Microtechnologies, TU Chemnitz, Chemnitz — [3]Institute of Physics, TU Chemnitz, Chemnitz — [4]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [5]cfaed, TU Dresden, Dresden

Because of their low dielectric constant (k-value) ultra-low-k (ULK) materials are used for isolating the interconnects in integrated circuits. However, during the manufacturing process the k-value lowering methyl groups are replaced by hydroxyl groups and hydrogen atoms. This process is called OH- and H-damage.

In our simulation study we use fragmented silyation molecules (OMCTS, DMADMS) to repair the OH-and H-damages and restore the k-value of the ULK material by reinserting lost methyl groups. The fragmentation of DMADMS and OMCTS is investigated as a function of the reaction temperature using DFT on the PBE/DNP-level.

The repair behavior of the so obtained fragments are studied with two model systems: an assortment of small ULK-fragments and a silica cluster. We show that larger repair fragments with two and three methyl groups are energetically favorable.

DF 8.4 Tue 12:00 H 0111

Dissipative hydrogen two-level systems in Al_2O_3 — •Hazem Abu-Farsakh[1,2], Luke Gordon[1], Anderson Janotti[1], and Chris G. Van de Walle[1] — [1]Materials Department, University of California, Santa Barbara — [2]Prince Sultan University, Riyadh, Saudi Arabia

Superconducting qubits based on Josephson tunnel junctions are promising candidates for quantum computing. A limiting factor for their performance is the resonant absorption by two-level systems (TLSs) in the dielectric material. However, the microscopic nature of these TLSs has not been identified. In this work we propose that hydrogen interstitial atoms are the main source of TLSs in Al_2O_3. Using *ab-initio* calculations employing hybrid functionals we identify H binding sites and show that a hydrogen atom forms a H-bond in Al_2O_3 and feels a double potential well, resulting in a tunneling effect. We map the three-dimensional potential energy of an interstitial H atom and calculate its tunneling frequency by solving the corresponding Schrödinger equation. Our results show that the tunneling of H atoms gives rise to a resonant absorption in the 10 GHz region, in agreement with experimental observations. This work was supported by IARPA.

DF 9: Focused Session on Ferroic Domain Walls III (DF with MA)

Part of the 3-days focus on ferroic domain walls:

Tutorial, Symposium (SYDW), three Focused Sessions, and Poster Session.

Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Tuesday 14:00–16:00 Location: EB 107

DF 9.1 Tue 14:00 EB 107

STM imaging of ferroelectric domains of strained $BaTiO_3$ films at the thickness limit — •Maik Christl[1], Klaus Meinel[1], Stefan Förster[1,2], and Wolf Widdra[1,3] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Department of Physics, University of Zurich, Zurich, Switzerland — [3]Max Planck Institute of Microstructure Physics, Halle, Germany

Ultrathin ferroelectric films are of increasing interest due to novel oxide based applications. In particular, the domain structure as well as the critical thickness are essential key aspects for ferroelectricity in thin films [1].

In this work, we report on in-situ STM and STS studies to image ferroelectric out-of-plane and in-plane nanodomain structures. $BaTiO_3$(100) ultrathin films have been grown pseudomorphically on Pt(100) and Au(100), which corresponds to 2% lateral compression and 2% expansion, respectively [2]. Films with a thickness of 2 unit cells (uc) show already ferroelectricity at room temperature as verified by reversible domain writing and reading using STM. On Pt(100), an irregular c^+/c^- nanodomain configuration is visible in dI/vV maps that are taken at domain sensitive voltages. With film thickness, the domain width increases from 2 nm for 2 uc to 6 nm for 25 uc. In contrast, for expanded $BaTiO_3$ films on Au(100) a regular structure with domain walls proceeding along [100] directions is observed which evidences an in-plane domain arrangement.

[1] Y. Wang *et al.*, *Materials 7*, 103390 **2014**
[2] S. Förster *et al.*, *J. Chem. Phys. 135*, 104701 **2011**

DF 9.2 Tue 14:20 EB 107

Microscopic perspective of magnetoelectric effect in multiferroic composites — •Harsh Trivedi[1], Vladimir V. Shvartsman[1], Doru C. Lupascu[1], Robert C. Pullar[2], Marcos S. A. Medeiros[2], Andrei L. Kholkin[2], Pavel Zelanovskiy[3], and Vladimir Ya. Shur[3] — [1]Institute for Materials Science and Centre for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, 45141 Essen, Germany — [2]Department of Materials and Ceramic Engineering & CICECO, University of Aveiro, 3810193 Aveiro, Portugal — [3]Institute of Natural Sciences, Ural Federal University, 620002 Ekaterinburg, Russia

An extensive analysis of microscopic studies on bulk multiferroic composites is presented. Piezoresponse force microscopy (PFM) is used as a tool to study magnetoelectric effect in composites at local scale. Indirect influence of the stress, that mediates the ME effect, on the PFM response and local switching parameters is evaluated. Principal component analysis is utilized to extract the valuable data buried under noise and statistical inhomogeneity in order to create a spatial visualization of the effect. The spatial distribution of the intensity of the magnetoelectric coupling reveals interesting phenomena at the interface suggesting a resemblance to Eshelby's solution for elliptical inclusion in a matrix. Spatially resolved Raman spectroscopy mapping reveals a similar dominance of the stress at the interfaces corroborating the PFM findings. Finally, a simplified FEM based theoretical model simulating the realistic polycrystalline microstructure is presented, in order to compare the experimental findings.

DF 9.3 Tue 14:40 EB 107

Domain structure in anisotropically strained $K_{0.75}Na_{0.25}NbO_3$ thin films on $TbScO_3$ — •Dorothee Braun[1], Albert Kwasniewski[1], Philipp Müller[1], Martin Schmidbauer[1], Jan Sellmann[1], Michael Hanke[2], and Jutta Schwarzkopf[1] — [1]Leibniz-Institute for Crystal Growth, Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Understanding and controlling of domain formation in ferroelectric thin films at the nanoscale is essential for fundamental research as well as for potential applications. The incorporation of anisotropic in-plane lattice strain has a decisive impact on the stability of ferroelectric phases and is achieved by the deposition on lattice mismatched substrates. In this study 30 nm thick $K_{0.75}Na_{0.25}NbO_3$ films were epitaxially grown on $TbScO_3$ substrates by metal-organic chemical vapor deposition. They experience in average a slight compressive lattice strain of 0.47% and are $(100)_c$ oriented. Our PFM measurement revealed both a lateral and a vertical component of the polarization vector whereby the latter one is less pronounced. The lateral PFM shows regularly arranged 90° domains in two directions with domain walls running along <110> and a periodicity of 50 nm has been observed. According to x-ray measurements, the films are grown fully strained on the substrate. The film unit cell is monoclinically distorted in the vertical direction, but no in-plane monoclinic distortion has been detected. These results indicate the occurrence of monoclinic M_C domains which were not observed in (K,Na)NbO_3 thin films before.

DF 9.4 Tue 15:00 EB 107

Ferroelectric Domains of partially relaxed $NaNbO_3$ films under tensile strain — •Jan Sellmann, Dorothee Braun, Albert Kwasniewski, Martin Schmidbauer, and Jutta Schwarzkopf — Leibniz-Institute for Crystal Growth, Max-Born-Str. 12489, Berlin

Lead-free alkaline niobates have recently attracted much attention due to their promising piezoelectric properties like high Curie temperatures. In thin film form they exhibit large densities of ferroelectric domains so that the domain walls are expected to contribute significantly to electrical and electromechanical responses of the material. In the present work, epitaxial $NaNbO_3$ films have been grown by Pulsed Laser Deposition under optimized growth conditions yielding 2D growth and nearly stoichiometric films. Tensile lattice strain was induced by the use of $TbScO_3$ substrates. Increasing the film thickness above the critical thickness the formation of misfit dislocations resulted in partial plastic lattice relaxation and thus a reduction of the effective in plane strain. Concurrently, the ferroelectric domain pattern changes at the critical thickness from lateral 1D a1/a2/a1/a2 stripes domains with exclusive in-plane polarization to a periodic stripe domain pattern with both vertical and lateral polarization components. The latter can be described as a1c/a2c domains with head-to-head configuration in some cases possibly resulting in charged domain walls. Similar results with regard to the domain structure have been found for $NaNbO_3$ thin films on $DyScO_3$ substrates. However, it is in contrast to NaNbO3 thin films grown on DyScO3 and $TbScO_3$ by MOCVD where in-plane domains are exclusively found well beyond the onset of plastic strain relaxation.

DF 9.5 Tue 15:20 EB 107

Investigation of second order nonlinear susceptibility tensor elements at the transition of ferroelectric domains — •Alex Widhalm[1], Kai Spychala[1], Moritz Grothe[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Second harmonic (SH) microscopy is an established method for characterizing periodically poled ferroelectric materials. This work focusses on mapping the second order susceptibility tensor elements in ferroelectric domain structures using spatially resolved second harmonic analysis with respect to a focused laser beam. Our novel nondestructive technique allows for a nonlinear confocal scanning probe microscopy as well as for a basic analysis of occurring point spread functions with respect to a fixed excitation point. The resulting complex distribution of polarization states of excitation and generated SH light, allows a prediction about the detectable nonlinear response of the whole system. Here the experimental results obtained by this method are in good agreement with the expected theoretical occurrence of the nonlinear field distributions. In our spatially resolved experiments we found, that in the transition region of contrarily poled domains and its immediate environment some susceptibility tensor elements disappear whereas other elements appear. This results strongly contribute to a deeper understanding of the occurring physics at domain walls and corresponding contrast mechanisms in ferroelectric domains respectively.

DF 9.6 Tue 15:40 EB 107

Visualization of ferroelectric domain structures in KTP by confocal Raman imaging — •Peter Mackwitz[1], Michael Rüsing[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

The nonlinear optical material Potassium titanyl phosphate (KTP) unifies several outstanding material properties. Its distinguished features contain a high damage threshold compared with the considerable well known further ferroelectrics, exalted electro-optical coefficients and especially high nonlinear coefficients. The achieving of periodically poled structures in this material represents one of the significant deployments of KTP in integrated optics. Within the common effects of nonlinear implementation frequency conversion is one of the central uses. In order to achieve a highly efficient frequency conversion it is required to supply a nearly ideal surrounding for quasi-phasematching. Periodically poled materials like PPKTP provide this condition. Confocal Raman imaging depicts a noninvasive technique for visualizations of poled structures which is the premise for a characterization. In this work the confocal Raman imaging was achieved in due consideration of different incident polarizations. The measurements were performed as well in y-cut geometry as in z-cut samples. For this purpose numerous phonon modes have been identified as a continuation of previous work. The fundamental result of this work can be outlined as the designation of PPKTP as a proper candidate for domain imaging.

DF 10: Multiferroics I (DF with DS/KR/MA/TT)

Time: Wednesday 9:30–13:00 Location: EB 107

DF 10.1 Wed 9:30 EB 107

Magnetoelectric domain control in multiferroic $TbMnO_3$ — •Sebastian Manz[1], Masakazu Matsubara[1,2], Masahito Mochizuki[3,4], Teresa Kubacka[1], Ayato Iyama[5], Nadir Aliouane[6], Tsuyoshi Kimura[5], Steven Johnson[1], Dennis Meier[1], and Manfred Fiebig[1] — [1]ETH Zürich — [2]Tohoku University — [3]Aoyama Gakuin University — [4]Japan Science and Technology Agency — [5]Osaka University — [6]Paul Scherrer Institute

Spin-spiral multiferroics exhibit a strong coupling between the electric and magnetic subsystems which is of potential interest for technological applications. Although these systems have been investigated for more than a decade, the magnetoelectric domain evolution under external fields is still largely unknown. Using optical second harmonic generation we resolve how electric and magnetic fields affect the multiferroic domains in the archetypal spin-spiral multiferroic $TbMnO_3$. In consecutive electric switching cycles, varying multi-domain patterns emerge before a single-domain state is obtained. This observation reflects that the domain walls can easily move without being pinned by, e.g., structural defects. In striking contrast to the electric-field response, multi-domain patterns persist when the polarization direction is flopped by applied magnetic fields. Here, a uniform polarization rotation is observed within all domains, which incorporates a transformation of neutral into nominally charged domain walls. Our results are explained based on numerical Landau-Lifshitz-Gilbert simulations and provide first evidence for the scalability of macroscopic magnetoelectric properties onto the level of domains.

DF 10.2 Wed 9:45 EB 107

Critical behavior at the order-disorder transition in multiferroic $DyMnO_3$ — •Markus Schiebl, Alexey Shuvaev, Anna Pimenov, Graeme Eoin Johnstone, Uladzislau Dziom, and Andrei Pimenov — Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna Austria

We present the results of detailed dielectric investigations of the relaxation dynamics in $DyMnO_3$ multiferroic manganite. In addition to known domain wall relaxation a second strong mode is observed at low frequencies. We provide an experimental evidence that the new relaxation mode is coupled to the chirality switching of the spin cycloid.

We demonstrate that the relaxation dynamics in $DyMnO_3$ is typical for an order-disorder phase transition. Therefore, $DyMnO_3$ follows an order-disorder transition scenario implicating that a short range cycloidal order of Mn-spins exists above T_C. The results suggest that the paramagnetic sinusoidal phase should be explained as a dynamic equilibrium between the clockwise and counterclockwise cycloidal magnetic orders. The short range order in the paraelectric phase is transformed to a long range cycloid at the ferroelectric transition temperature.

DF 10.3 Wed 10:00 EB 107

Biquadratic and four-spin ring interactions in orthorhombic perovskite manganites — •Natalya Fedorova, Andrea Scaramucci, Claude Ederer, and Nicola A. Spaldin — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093, Zurich, Switzerland

We use *ab initio* electronic structure calculations, based on DFT within the GGA+U approximation, to estimate the microscopic exchange interactions in the series of orthorhombic perovskite manganites (o-RMnO$_3$), in order to find a model Hamiltonian which can provide an accurate description of the magnetism in these materials. At low temperatures o-RMnO$_3$ with small radii of R cations (therefore, large octahedral tiltings) demonstrate a spiral or E-type antiferromagnetic orderings (E-AFM), which drive their multiferroic properties. Usually the establishment of such magnetic orderings is explained within the framework of a Heisenberg model with competing nearest-neighboring (NN) and next-nearest-neighboring exchange interactions. However, we find that the mapping the results of *ab initio* calculations onto the Heisenberg Hamiltonian for o-RMnO$_3$ show a clear deviation from the Heisenberg-like behavior. We demonstrate that this deviation can be explained only by the presence of biquadratic and four-spin ring exchange couplings and show that they have the strongest effect in compounds where NN exchange interactions are weakened, for example, due to large octahedral tiltings.

DF 10.4 Wed 10:15 EB 107

Time resolved polarized neutron scattering and dielectric spectroscopy reveal multiferroic domain dynamics in $MnWO_4$ and $TbMnO_3$ — •Jonas Stein[1], Daniel Niermann[1], Christoph Grams[1], Max Baum[1], Tobias Cronert[1], Jeannis Leist[2], Karin Schmalzl[3], A Agung Nugroho[4], Alexander C Komarek[5], Götz Eckold[2], Petra Becker[6], Ladislav Bohatý[6], Joachim Hemberger[1], and Markus Braden[1] — [1]II. Physikalisches Institut, Uni Köln — [2]Institut für Phys. Chemie, Uni Göttingen — [3]JCNS at ILL, France — [4]Institut Teknologi Bandung, Indonesia — [5]MPI Dresden — [6]Institut für Kristallographie, Uni Köln

Multiferroic materials are promising for future memory devices with low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spin spiral multiferroics $TbMnO_3$ and $MnWO_4$. Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an electric field. Using the stroboscopic technique we follow the reversion of chiral domains in the timescale of a few hundred microseconds to hours. In $TbMnO_3$ we find a simple logarithmic relation between the rise time and temperature that is fulfilled over 5 decades. Broadband linear and nonlinear dielectric spectroscopy revealed the domain dynamics in the MF phase of $MnWO_4$. The rise time reaches values in the minute range in the middle of the multiferroic temperature regime at T≈10 K but unexpectedly decays again on approaching the lower, first-order phase boundary at T_{N1}≈7.6 K.

[1] Niermann et al. **PRB 89**,134412 [2] Baum et al. **PRB 89**,144406

DF 10.5 Wed 10:30 EB 107

Polarization control at spin-driven ferroelectric domain walls — •Naëmi Leo[1], Anders Bergmann[2], Andres Cano[3], Narayan Poudel[4], Bernd Lorenz[4], Manfred Fiebig[1], and Dennis Meier[1] — [1]ETH Zurich, Switzerland — [2]Uppsala University, Sweden — [3]University Bordeaux, France — [4]University of Houston, USA

As was recently demonstrated, domain walls in ferroelectric materials show emergent electronic properties, like enhanced conductivity tunable by the relative orientation of the polarisation in the adjacent domains. Here, multiferroic materials with a coexistence of magnetic and electric order offer a new route for the control of such localised functionalities at domain boundaries.

Using spatially-resolved optical second harmonic generation we demonstrate the magneto-electric-field control of the multiferroic domains in Co-doped $MnWO_4$. In particular, the obtained domain distribution remains unchanged upon the magnetic-field-induced continuous 90°-rotation of the ferroelectric polarization.

This stability implies that multiferroic domain walls can accommodate for varying local polarisation configurations leading to local charging and discharging. We discuss the microscopic structure of the domain walls using micro-magnetic simulations.

DF 10.6 Wed 10:45 EB 107

Tuning order-by-disorder multiferroicity in CuO by doping — •Johan Hellsvik[1,2], Marcello Balestieri[1], Tomoyasu Usui[3], Alessandro Stroppa[2], Anders Bergman[4], Lars Bergqvist[5], Dharmalingam Prabhakaran[6], Olle Eriksson[4], Silvia Picozzi[2], Tsuyoshi Kimura[3], and José Lorenzana[1,2] — [1]ISC-CNR, Rome, Italy — [2]CNR-SPIN, L'Aquila, Italy — [3]Osaka University, Osaka, Japan — [4]Uppsala University, Uppsala, Sweden — [5]KTH, Stockholm, Sweden — [6]University of Oxford, Oxford, United Kingdom

The high Curie temperature multiferroic compound CuO has a quasidegenerate magnetic ground state that makes it prone to manipulation by the so-called "order-by-disorder" mechanism. First principle computations supplemented with Monte Carlo simulations and experiments show that isovalent doping allows us to stabilize the multiferroic phase in nonferroelectric regions of the pristine material phase diagram with experiments reaching a 250% widening of the ferroelectric temperature window with 5% of Zn doping. Our results allow us to validate the importance of a quasidegenerate ground state on promoting multiferroicity on CuO at high temperatures and open a path to the material engineering of multiferroic materials. In addition we present a complete explanation of the CuO phase diagram and a computation on the incommensurability in excellent agreement with experiment without free parameters.

[1] J. Hellsvik et al., Phys. Rev. B 90, 014437 (2014) [2] T. Kimura et al., Nature Mat. 7, 291 (2008) [3] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011)

DF 10.7 Wed 11:00 EB 107

Dielectric properties and electrical switching behavior of the spin-driven multiferroic $LiCuVO_4$ — •Alexander Ruff[1], Stephan Krohns[1], Peter Lunkenheimer[1], Andrey Prokofiev[2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Solid State Physics, Vienna University of Technology, Austria

The spin-1/2 chain cuprate $LiCuVO_4$ exhibits both ferroelectric and magnetic order at low temperatures. This so-called multiferroic behavior is of great scientific interest due to the underlying complex physical mechanisms, especially in the case of strong magnetoelectric coupling. Here we thoroughly discuss the multiferroic properties of the prototypical spin-driven ferroelectric material $LiCuVO_4$. At temperatures below about 2.5 K, it exhibits a three dimensional helical spiral spin order, with propagation in the *b* direction and a spin helix in the *ab* plane, which induces via an inverse Dzyaloshinskii-Moriya interaction a ferroelectric polarization in the *a* direction. In an external magnetic field, the direction of the spin spiral and thus the direction of the electrical polarization can be switched. This switching behavior of the polarization was demonstrated via dielectric spectroscopy on a single crystalline sample oriented in two different directions in magnetic fields up to 9 T. Detailed magnetic-field and temperature-dependent ferroelectric hysteresis-loop measurements imply the electric control of the spin helicity [1]. This rarely documented feature indicates the close coupling of electric and magnetic order of $LiCuVO_4$.
[1] A. Ruff *et al.*, *J. Phys.: Condens. Matter*, **26**:485901 (2014).

15 min coffee break

DF 10.8 Wed 11:30 EB 107

Emergence of ferroelectricity in multiferroic h-$YMnO_3$ — •Martin Lilienblum[1], Thomas Lottermoser[1], Sebastian Manz[1], Sverre M. Selbach[2], Andres Cano[3] und Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [2]Department of Material Science and Engineering, NTNU, N-7491 Trondheim, Norway — [3]CNRS, Université de Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

Universal scaling laws, interfacial nano-electronics, and topological defects are currently studied using hexagonal manganites $R\mathrm{MnO_3}$ (R= Sc, Y, Dy-Lu) as model system. In spite of the remarkably broad interest in the system, surprisingly little is known about the origin of the ferroelectric state. Here we solve the controversy about the emergence of the spontaneous polarization and its coupling to the underlying structural distortion by applying scanning probe microscopy (SPM) and optical second harmonic generation (SHG). We trace the spontaneous polarization by SHG from 100 K to 1450 K directly and contact-free. We find that only a single transition exists in which the polarization arises slower than expected as by-product of the structural distortion. By thermal treatments close to the structural transition and subsequent SPM scans, we show that the exceptionally robust ferroelectric domain pattern is determined only by the structural distortion. In summary we reveal that the ferroelectric order results from an interplay of electric polarization, topological effects, and temperature.

DF 10.9 Wed 11:45 EB 107

Monte Carlo approach to the ferroelectric phase transition in hexagonal manganites — •Thomas Lottermoser[1], Martin Lilienblum[1], Andres Cano[2], and Manfred Fiebig[1] — [1]ETH Zurich, Zurich, Switzerland — [2]Université de Bordeaux, Pessac, France

Despite several experimental and theoretical efforts in recent years the nature of the structural high temperature phase transition in the hexagonal manganites and its relation to the occurrence of a ferroelectric polarization in this materials is still not fully understood. Experimental data give two contradicting answers to this problem. Some experiments indicate a simultaneous appearance of the polarization in a single structural phase transition while others hint to a second phase transition several hundred Kelvin below the structural transition. In order to clarify these contradictions we performed Monte Carlo simulations based on the so-called clock model. In this model the six trimerization states of the manganite crystal structure are represented by six clock vectors in the complex plane. From the simulation data we calculated the temperature dependence of the complex structural order parameter and the induced ferroelectric polarization. The results point to a single phase transition with a strongly suppressed polarization contribution at high temperatures. This is experimentally confirmed by direct measurements of the ferroelectric polarization using optical second harmonic generation. Contradictions with other experimental data can be explained as finite size effects depending on the length scale of the experimental probe.

DF 10.10 Wed 12:00 EB 107

Magon-phonon interactions in hexagonal multiferroic $YMnO_3$ — •Andreas Kreisel[1], Shantanu Mukherjee[1], Brian M. Andersen[1], Turi Schäffer[1], Sonja Holm[1], Kim Lefmann[1], Niels C.R. Momsen[1], Jacob Larsen[2], Amy Fennell[3], Uwe Stuhr[3], and Zahra Yamani[4] — [1]Niels Bohr Institute, University of Copenhagen, Denmark — [2]Institute of Physics, Technical University of Denmark — [3]Laboratory of Neutron Scattering, Paul Scherrer Institute, Switzerland — [4]Chalk River National Laboratory, Canada

The multiferroic material $YMnO_3$ is known to show a large spin lattice coupling such that the spin and lattice degrees of freedom influence various properties, as for example the thermal conductivity that is found to have an anomalous contribution. The magnetoelastic modes have been measured recently in neutron diffraction experiments and linked to certain spectral features in Raman signals. Starting from a Heisenberg model on a triangular lattice with single ion anisotropies, we investigate the spin-phonon coupling via the magnetostriction mechanism and derive a coupled magnon-phonon model valid in the entire Brillouin zone. Within a spin-wave approach, where the coupling yields a hybrid magnon-phonon mode, we calculate the dynamic structure factor and compare to recent experimental neutron results.

DF 10.11 Wed 12:15 EB 107

Stability of magnetic and electric domains against chemical doping in hexagonal manganites — •Ehsan Hassanpour Yesaghi, Viktor Wegmayr, Jakob Schaab, Dennis Meier, and Manfred Fiebig — Department of Materials, ETH Zürich, Zürich, Switzerland

The unique properties of magnetoelectric multiferroics are, to a large extent, determined by the coexistence and interaction of magnetic and electric domains. A major challenge towards future applications is to optimize the properties of these domains, such as their transport, without weakening or even losing the existing multiferroic order. Here, we present our study of ferroelectric and antiferromagnetic domains in chemically doped hexagonal manganites. We show that the electronic conductance of $ErMnO_3$ can be enhanced or suppressed by introducing either divalent (Ca^{2+}) or tetravalent (Zr^{4+}, Ti^{4+}) ions into the system. Using piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG) we monitor the corresponding changes on the level of domains. We find that the $RMnO_3$-characteristic domain topography, as well as the multiferroic transition temperature, are robust against the applied ionic alteration, which demonstrates the usability of chemical doping for non-perturbative property-engineering of multiferroic domains.

DF 10.12 Wed 12:30 EB 107

Anisotropy study of multiferroicity in the pyroxene $NaFeGe_2O_6$ — •Lionel Andersen[1], Thomas Lorenz[1], Matthias Ackermann[2], Ladislav Bohatý[2], and Petra Becker[2] — [1]II. Physikalisches Institut - Universität zu Köln, Germany — [2]Institut für Kristallographie - Universität zu Köln, Germany

Since the mineral aegirine was found to be the first multiferroic member of the pyroxenes an intensive search for further related multiferroics was initiated [1]. In this contribution, we present a detailed study of the dielectric, magnetic and magnetoelastic properties of the pyroxene $NaFeGe_2O_6$ with special respect to the anisotropy. Unlike other investigations on $NaFeGe_2O_6$ [2] large single crystals where synthesized to examine pyroelectric currents, dielectric constants and magnetic susceptibilities as well as the thermal expansion and the magnetostriction. The spontaneous electric polarization detected below $T_C \simeq 11.6$ K in an antiferromagnetically ordered state ($T_N \simeq 13$ K) is mainly lying within the *ac* plane with a small component along *b*, indicating a triclinic symmetry of the multiferroic phase of $NaFeGe_2O_6$. The electric polarization can be strongly modified by applying magnetic fields along different directions. We derive detailed magnetic-field versus temperature phase diagrams and identify three multiferroic low-temperature phases, which are separated by a non-ferroelectric, antiferromagnetically ordered state from the paramagnetic high-temperature phase [3].

[1] S. Jodlauk *et al.* J. Phys.: Condens. Matter **19** (2007)
[2] I. Kim *et al.* J. Phys.: Condens. Matter **24** (2012)
[3] M. Ackermann *et al.* New J. Phys. (submitted, arXiv:1408.6772)

DF 10.13 Wed 12:45 EB 107

***Ab Initio* analysis of ferroelectric and magnetic properties of potentially multiferroic aurivillius phases** — •Axiel Yael Birenbaum, Jan van den Broek, and Claude Ederer — Materials Theory, ETH Zürich

A promising class of high temperature polar magnetic multiferroic materials are the Aurivillius family of layered-perovskites related compounds. They combine high temperature ferroelectric properties with a layered structure that allows for systematic introduction of magnetic ions. The simplest of such cases to have been studied is $Bi_5FeTi_3O_{15}$. However, no well-established value exists for its spontaneous electric polarization, and contradictory reports as to its magnetic states.

We perform Density Functional Theory calculations on $Bi_5FeTi_3O_{15}$, and conclude on a high spontaneous electric polarization. To better understand the mechanism for ferroelectricity, we examine 9 systems, based on $SrBi_2Ta_2O_9$ as reference. We find a high spontaneous polarization even in the case of with no nominally ferroelectrically-active cations. We discuss these results in light of the tri-linear coupling between soft and hard modes demonstrated for $SrBi_2Ta_2O_9$ and the general concept of "hybrid improper ferroelectricity". To clarify the range of temperatures expected for magnetic long range order despite a low concentration of magnetic ions and the short range of superexchange interactions, we perform Monte Carlo simulations. We discuss possible strategies to increase magnetic ordering temperatures.

DF 11: Small Polarons in $LiNbO_3$

Small polarons determine a variety of optical and electrical features of lithiumniobate, $LiNbO_3$, and can be used, e.g., to interprete the bulk photovoltaic effect on a microscopic level. In this session, excitation, lattice deformation, phonon-coupling, transport and recombination mechanisms of small free and bound polarons are discussed considering results of a broad range of modern experimental techniques as well as theoretical calculations and numerical modeling.

Organizer: Mirco Imlau (Universität Osnabrück)

Time: Wednesday 9:30–13:00 Location: EB 133C

DF 11.1 Wed 9:30 EB 133C

Two-photon absorption in presence of small polaron formation in lithiumniobate — •Mirco Imlau, Holger Badorreck, Stefan Nolte, Felix Freytag, and Javid Shirdel — Department of Physics, Osnabrueck University, D-49069 Osnabrueck

Two-photon absorption (TPA) appears in nominally undoped lithiumniobate with photon energies below the band gap energy of 3.8 eV and intensities of a few PW/m^2; it is commonly studied by means of the z-scan technique. However, using ultrashort laser pulses with durations below 100 fs, the transmission signal is additionally affected by optically excited free carriers (FCA) and subsequently formed small polarons that have rise times of 50-100 fs (Nb_{Nb}^{4+} [Qiu et al. phys. stat. sol. c **2**, 232 (2005)]) and below 400 fs (Nb_{Li}^{4+} [Beyer et al. Appl. Phys. B **83**, 527 (2006)]). We applied the z-scan technique with 100 fs laser pulses at 2.5 eV to study the composed transmission loss that is given by TPA, FCA, and small polaron absorption. For data analysis, the well-known theory of Sheik-Bahae (IEEE J. Quantum Electron. **26**, 760 (1990)) is modified by contributions from absorption centers within the band gap [Shanmugavelu, J. Appl. Phys. **114**, 243103 (2013)]. The results of our analysis is experimentally verified by systematic z-scan studies using stretched pulses with durations up to 1.000 fs. We discuss the possibility to determine risetime and absorption cross section of optically excited hot carriers and present a refined model for the small polaron formation path in lithiumniobate. Financial support by the DFG (IM37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

DF 11.2 Wed 9:50 EB 133C

Density functional theory investigation of iron small bound polarons — •Simone Sanna and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn

Iron doped lithium niobate is one of the most prominent photorefractive materials and is vastly employed, among others, for holographic data storage and optical filters. The dominant charge transport mechanism initiating photorefractive effect is the bulk photovoltaic effect, which is currently interpreted on the basis of $Fe^{2+/3+}$ small bound polarons [1]. In this work, we present a quantitative microscopic description of $Fe^{2+/3+}$ polaronic centers. Spin-polarized density functional theory with Hubbard corrections is employed to investigate the atomic structure around Fe_{Li} centers. The theoretical models are compared with available experimental results [2,3], providing clear evidence for the polaronic distortion upon $Fe^{2+/3+}$ charge transition. The calculated atomic and electronic structures allow for a detailed consideration of the microscopic processes leading to the optical absorption, as well as the extrapolation of data that can be employed in the classic polaronic theory.

[1] O. F. Schirmer et al., Phys. Rev. B 83, 165106 (2011)
[2] T. Vitova et al., J. Appl. Phys. 105, 013524 (2009)
[3] A. Sanson et al., Submitted to Phys. Rev. B (2014)

DF 11.3 Wed 10:10 EB 133C

Direct measurement of the Fe-polaron deformation in Fe:$LiNbO_3$ — •Marco Bazzan, Andrea Sanson, Annamaria Zaltron, Nicola Argiolas, and Cinzia Sada — Università di Padova, Padova, Italy

In this talk some recent experimental results on the structural characterization of the Fe small polarons in iron doped lithium niobate will be discussed.

On one hand, High Resolution X-rays Diffraction shows a bulk average strain appearing in the crystal as a consequence of the reduction process $Fe^{3+} + e \rightarrow Fe^{2+}$. It will be shown that this effect has to be attributed to strain dipoles located at the Fe centers, with a magnitude dependent on the charge state of the Fe ion.

These findings are definitely confirmed using X-Ray Absorption Fine Structure Spectroscopy at the Fe edge: upon oxidation or reduction the oxygen cage surrounding the Fe impurity is more or less compressed with respect to the regular $LiNbO_3$ structure.

Those results give a quantitative picture of the polaronic lattice deformation associated to the localization of an electronic charge at the Fe impurity.

DF 11.4 Wed 10:30 EB 133C

Polarons trapped at Ti centres in $LiNbO_3$ — •Gábor Corradi — Wigner Research Centre for Physics, Budapest, Hungary

Ti in $LiNbO_3$ is a well known dopant on Li-site changing the refractive index which can be used e.g. for producing waveguiding surface layers by Ti in-diffusion. The index change can be attributed to the existence of 3d-type $Ti^{4+/3+}$ donor polaron states in the gap which are similar to antisite $Nb^{5+/4+}$ polaron states with homologous 4d-type electron structure, the Ti level being only 0.11 eV deeper than the $Nb^{5+/4+}$ one. Mg co-doping can be used, similarly to the case of Nb(Li) antisites, also for the elimination of Ti(Li) centres, resulting in the appearance of Ti on Nb site. All four trapped-polaron d1 centres $Ti(Li)^{3+}$, $Ti(Nb)^{3+}$, $Nb(Li)^{4+}$, and $Nb(Nb)^{4+}$ show absorption bands due to charge transfer to states inside the conduction band with slightly stronger local admixture for Ti than for Nb. As shown by the analysis of the EPR spectra, all four centres are subjected to Jahn-Teller distortion with increasing JT energy as one goes from Nb^{4+} to Ti^{3+} centres, or from Li to Nb substitution. The systematically shifted properties can be used for fine tuning polaronic effects by Ti and Mg doping and appropriate levels of reduction treatments.

30 min break with Posters (DF 1.5)

DF 11.5 Wed 11:20 EB 133C

Polar niobate-nanocrystals: Synthesis and nonlinear optical analysis — •Anke Düttmann[1], Christian Kijatkin[1], Karsten Kömpe[2], Javid Shirdel[1], and Mirco Imlau[1] — [1]Dept. of Physics, Osnabrueck University, D-49069 Osnabrueck — [2]Instit. of Chemistry, Osnabrueck University, D-49076 Osnabrueck

Niobate-nanocrystals can be used as light emitters on the nanoscale by means of second harmonic generation (SHG). They are of interest as markers in high-resolution nonlinear optical microscopes for cell biology and tumor visualization as they offer a tremendeous contrast in comparison to fluorescent markers. Although, however, the growth of $KNbO_3$ or $LiNbO_3$ single crystals is well established, almost nothing is known about respective nanocrystals synthesis with homogeneous size distribution and diameters in the range from 5-50 nm. In this contribution, we present our results on size-controlled synthesis of niobate-nanocrystals and their nonlinear optical analysis by means of SHG-microscopy. By choosing suitable oxidic precursors and their stabilization, we succeeded in a targeted synthesis of $KNbO_3$ and $NaNbO_3$ (20 - 80 nm). The dispersion properties of the SHG signal verify the polar nature of the nanocrystals and the possibility to induce a polarization wave in crystals with diameters smaller than the wavelength. Studies as a function of nanocrystal diameter follow the behavior expected from coupled wave theory such that signals detection of particles below 10 nm becomes possible. Financial support by the DFG (INST 190/165-1 FUGG) is gratefully acknowledged.

DF 11.6 Wed 11:20 EB 133C

Light-induced polaron transport in 1, 2, and 3-dimensional systems — •Christoph Merschjann[1,2] and Stefan Lochbrunner[1] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Freie Universität Berlin, D-14195 Berlin, Germany

Transient optical spectroscopy of functional materials is frequently used to extract important electronic quantities, such as the nature of the photoexcitations (e.g., excitons or separated charge carriers, polarons, etc.), their concentrations, and mobilities. This is especially helpful for powders or microcrystalline samples which do not allow for macroscopic investigations like, e.g., standard conductivity measurements. The most prominent experimental techniques are pump-probe transient-absorption measurements and time-resolved fluorescence investigations. Very often, non-exponential decays of the transient spectra are observed, which are too frequently left unexplained or misinterpreted.

We apply a random-walk approach to model diffusion-type transports of light-induced charge carriers (e.g., small polarons). The obtained set of rate equations reveals distinct power-law behaviors for the decays of transient absorption and fluorescence. Typical phenomena like geminate and bimolecular recombination are clearly distinguishable. From the characteristics, one is able to directly deduce not only the dimensionality of the transport, but also mobilities and concentrations of the involved carriers.

DF 11.7 Wed 11:40 EB 133C

Temperature dependence of polaron relaxation in iron-doped congruent lithium niobate: a Monte-Carlo simulation — •Laurent Guilbert and Imed Mhaouech — Laboratoire Matériaux Optiques, Photonique et Systèmes, Université de Lorraine et Supélec, 2, Rue E. Belin 57070 Metz (France)

The three elementary processes involved in the relaxation of bound polarons $NbLi^{4+}$ in iron-doped lithium niobate (trapping at Fe^{3+} ions, hopping on Nb antisites and spontaneous conversion to the free polaron state $NbNb^{4+}$) are simulated in a Monte-Carlo loop. Simulated decays match more or less the Kohlrausch-William-Watts law, $\exp[-(t/\tau)^b]$, similarly to experimental decays recorded by light-induced absorption (LIA) and reported in the literature. We focus here on the temperature dependence of the decays. As expected, the Arrhenius plots $\log(\tau)$ or $\log(<\tau>)$ (average lifetime) versus $1/T$ evidence three regimes. Their activation energies reflect, but are however not strictly equal to, the energy barriers of the elementary processes. As far as b is concerned, a low-T limit is found. It corresponds to the trapping regime in which most of the bound polarons are trapped in a single hop. The limit value of b depends mainly on the Fe^{3+} trap concentration and on the orbital parameter c involved in the distance dependence of the trapping time in $\exp(r/c)$. The sharp increase of $b(T)$ above 300 K, experimentally evidenced but poorly explained in previous models, now appears as a natural consequence of a trap size effect.

DF 11.8 Wed 12:00 EB 133C

Temperature dependence of small polaron transport in Fe-doped lithium niobate — •Simon Messerschmidt, Felix Freytag, Holger Badorreck, and Mirco Imlau — Department of Physics, Barbarastraße 7, 49069 Osnabrück

Small bound Nb_{Nb}^{4+}, Nb_{Li}^{4+} electron and O^- hole polarons are generated by single ns-laser pulses (2.5 eV) in Fe-doped lithiumniobate, $LiNbO_3$ (source: Univ. Padova, Italy), thus, inducing a pronounced change of the macroscopic absorption $\alpha_{\rm li}$. Inspection of the temporal decay $\alpha_{\rm li}(t)$ at photon energies characteristic for the specific polaron species allows to get insight to small polaron transport features and mutual recombination processes. Although, however, comprehensive studies on hopping processes at room and elevated temperature are available ($270 - 400$ K, Merschjann et al.. Phys. Rev. Lett. **96**, 186404 (2006) and Refs. therein), studies of $\alpha_{\rm li}(t)$ at low temperatures are missing. The temperature range between $20 - 300$ K particularly is of interest for transport studies as freezing of small polaron hopping accompanied by a predominance of tunneling is to be expected. We here present our systematic study in this temperature range by means of transient absorption spectroscopy and discuss our findings, i.e. pronounced changes in the recombination lifetime as well as of the shape of $\alpha_{\rm li}(t)$, using the Holstein model, Emin's polaron theory and established recombination models in presence of Fe-doping (Herth et al., Phys. Rev. B **71**, 125128 (2005)). Financial support by the DFG (IM37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

DF 11.9 Wed 12:20 EB 133C

Protons in doped $LiNbO_3$ crystals resistant to photorefractive damage — •Krisztián Lengyel, László Kovács, Viktor Szalay, and Gábor Corradi — Wigner Research Centre for Physics, Budapest, Hungary

Protons are common impurities in $LiNbO_3$ forming OH^- ions in the lattice. The characteristic spectrum in the 3400–3600 cm^{-1} wavenumber range due to stretching vibrations of O–H is very sensitive to neighbouring defects (e.g. antisite Nb_{Li}, various dopants, polarons, etc). Studying the details of OH^- incorporation is also helpful for understanding the behavior of neighboring defects. Proton dynamics can be investigated by the SIESTA quantum chemical software package as already successfully demonstrated for undoped stoichiometric and congruent $LiNbO_3$. Dopants like Mg, Zn, Sc, In, Hf, Zr or Sn leading to photorefractive optical damage resistance (ODR ions) can change the polaronic behavior of $LiNbO_3$ crystals as well. ODR-doping of $LiNbO_3$ crystals above a threshold concentration also leads to substantially modified OH absorption bands which can be explained by assuming the existence of ODR_{Nb}^{n+}–OH defect complexes. In the present work this model will be discussed using the results of theoretical calculations of OH^- ions incorporated into ODR-doped $LiNbO_3$ crystals. This project has been supported by the Hungarian Scientific Research Fund (OTKA) K83390.

DF 11.10 Wed 12:40 EB 133C

Light induced changes in the OH^--stretching bond by frequency-resolved femtosecond infrared absorption spectroscopy in congruent $LiNbO_3$ — •Felix Freytag, Phillip Booker, and Mirco Imlau — Department of Physics, Osnabrueck University, D-49069 Osnabrueck

The light induced generation of polarons in $LiNbO_3$ is well studied by observing the absorption changes in the VIS/NIR spectral range. However, time-resolved measurements of the generation and relaxation of polarons in the MIR spectral range are missing. $LiNbO_3$ crystals contain defects from OH^--ions with a concentration of $c_{OH^-} \approx 10^{18}\,cm^{-3}$. Due to protons coupling these ions attach to the O^{2-}-ions in the lattice at four different positions [Lengyel et al., Ferroelectrics **257**, 255 (2001)]. Polarons change the enviroment of OH^--Ions an therefore their vibrational resonance. Here we show data of a frequency-resolved femtosecond infrared spectroscopy experiment of the OH^--stretching bond ($\lambda \approx 2870$ nm) in congruent $LiNbO_3$ consisting of four components (due to slightly different positions in the crystal lattice). The transmission of mid-infrared pulses ($\tau \approx 230$ fs) is detected by two multichannel HgCdTe detectors as a function of a variable time delay to an intense VIS pump pulse of $\tau \approx 100$ fs duration. We discuss the light-induced changes in the optical density of the OH^--stretching bond. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUUG) is gratefully acknowledged.

DF 12: Optical and Nonlinear Optical Properties I (DF with CPP)

Time: Wednesday 9:30–11:00 Location: EB 407

Invited Talk DF 12.1 Wed 9:30 EB 407

Holographic microstructuring of liquid-crystalline elastomers — •Irena Drevensek-Olenik[1,2], Martin Čopič[1,2], Martin Fally[3], Valentina Domenici[4], and Antoni Sánchez-Ferrer[5] — [1]Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI1000 Ljubljana, Slovenia — [2]J. Stefan Institute, Jamova 39, SI1000 Ljubljana, Slovenia — [3]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria — [4]Dipartimento di Chimica e Chimica Industriale, Università degli studi di Pisa, via Risorgimento, 35, 56126 Pisa, Italy — [5]Department of Health Sciences and Technology, ETH Zurich, Schmelzbergstrasse 9, 8091 Zurich, Switzerland

Adding a small amount of photoactive component, for instance a photo-isomerizable azobenzene derivative, to the matrix of a liquid-crystalline elastomer (LCE) opens up various possibilities for optical manipulation of mechanical, thermal, electrical and optical properties of the material. Holographic microstructuring in LCEs is based on the coupling between isomerization state of the azobenzene groups and orientational order of the mesogenic side chains. Due to collective nature of this process light-induced spatial modifications of optical refractive index in LCEs are several magnitudes larger than in conventional azobenzene-based holographic media. Holographic patterning of LCEs consequently provides a very convenient method for fabrication of tuneable optical diffraction structures that can easily be manipulated by external stimuli, such as strain, external fields and temperature variations.

DF 12.2 Wed 10:00 EB 407

Random-Cavity Lasing from Electrospun Polymer Fiber Networks — •Sarah Krämmer[1], Christoph Vannahme[2], Cameron L. C. Smith[2], Tobias Grossmann[1], Michael Jenne[1], Stefan Schierle[1], Minh Tran[1], Lars Jørgensen[3], Ioannis S. Chronakis[3], Anders Kristensen[2], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Germany — [2]Department of Micro- and Nanotechnology, Technical University of Denmark (DTU), Denmark — [3]DTU-Food, DTU, Denmark

Electrospinning is a versatile, simple, low-cost and high-throughput technique for the fabrication of fibers and fiber networks with fiber diameters in the micro- and nanometer range. The resulting high surface-to-volume ratio makes the fibers excellent candidates for sensing, tissue-growth and filtering. In the field of photonics they serve as waveguides and light sources when doped with an emitter. We report on the lasing emission from random cavities formed in networks of electrospun dye-doped polymer fibers. Spatially resolved spectroscopy and spectral analysis prove that the observed laser emission originates from individual ring resonators randomly distributed throughout the network. Preliminary measurements show the suitablity of the fiber networks as gas sensors where the spectral position of a lasing mode serves as transducer.

DF 12.3 Wed 10:20 EB 407

Whispering Gallery Modes in Single Copolymer Microspheres — •Daniel Braam[1], Kenichi Tabata[2], Soh Kushida[2], Robert Niemöller[1], Günther M. Prinz[1], Yohei Yamamoto[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Faculty of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan

Copolymers are promising candidates for use in optoelectronic devices due to their low fabrication cost and high emission efficiency. Here we investigate several π-conjugated alternating copolymers, which combine the advantages of being a dye, a dielectric and a self-assembled resonator, as they form nearly perfect spheres when precipitated from solution. Excitation leads to standing waves inside these microspheres, known as whispering gallery modes (WGMs). Their spectral position, number and line width is dependent on the sphere diameter. The measurements, showing both TM- and TE-modes, are in good agreement with model calculations [1]. The relative amplitude of the modes is strongly dependent on the sphere's excitation spot, revealing leakage of polar modes to the substrate, while equatorial modes sustain. During continuous illumination we observe lifting of degeneracy of the WGMs, followed by slow deterioration. Covering the spheres with a thin layer of titanium leads to an improved resistance against irradiation damage.

[1] Tabata, K., Braam, D. *et al.* Self-assembled conjugated polymer spheres as fluorescent microresonators. Sci. Rep. **4**, 5902; DOI:10.1038/srep05902 (2014).

DF 12.4 Wed 10:40 EB 407

TiO_2 coated Whispering Gallery Mode (WGM) Resonators for Label-free Biosensing — •Fabian Ruf[1], Sarah Krämmer[1], Christoph Vannahme[2], Antonina Vigovskaya[3], Ljiljana Fruk[3], Anders Kristensen[2], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Germany — [2]Department of Micro- and Nanotechnology, Technical University of Denmark (DTU), Denmark — [3]DFG-Centre for Functional Nanostructures CFN, Karlsruhe Institute of Technology (KIT), Germany

Biosensors for label-free detection offer a huge variety of applications in life sciences and medicine since they facilitate point-of-care diagnostics. We use goblet-shaped polymeric high-Q WGM microresonators fabricated within a low-cost manufacturing process also suitable for mass production. After fabrication the polymeric resonators are coated with titanium dioxide using sputter deposition techniques. The sensitivity as figure of merit is given here by the size of the shift of a resonant mode when the surrounding of the resonator changes. Finite element simulations predict a significantly increased sensitivity for resonators coated with TiO_2. Moreover, titanium dioxide is a well-suited platform for functionalization with dopamine derivates. The use of antibody-protein binding processes is expected to enable the specific detection of proteins and antibodies interesting for medical analysis.

DF 13: Ceramics and Applications (DF with KR)

Time: Wednesday 11:20–13:00 Location: EB 407

Invited Talk DF 13.1 Wed 11:20 EB 407

Twisting the anionic-electronic transport kinetics to trigger memristance for resistive switching non-volatile memories: new materials, structering and methods — •Jennifer Rupp, Felix Messerschmitt, Sebastian Schweiger, Rafael Schmitt, and Markus Kubicek — ETH Zürich, Elektrochemische Materialien

Resistive switches are a new class of non-volatile memories which switch between low- and high-resistance values by application of voltage pulses. Despite their promises oxide-based resistive switches are rarely connected in their oxide diffusion kinetics to the memristive device performance under bias. Models to describe the mixed anionic-electronic defect contributions for two-carrier systems are missing. We review methods to probe carrier diffusion and memristance for mixed anionic-electronic resistive switches. Secondly, we use chronoamperometry to analyze via the Memristor-based Cottrell analysis diffusion constants and kinetics for mixed anionic-electronic Pt|$SrTiO_{3-\delta}$|Pt switches. Thirdly, material engineering of oxides is discussed to control device properties like retention, R_{on}/R_{off} ratios and power consumption by "interfacial strain engineering of mixed conducting oxide". Both examples implicate new material design and selection routes to tune the anionic-electronic transport in resistive switches by either knowledge on their diffusion kinetics and novel analyses or new interfacial strain engineering routes to alter electro-chemo-mechanics and transport.

DF 13.2 Wed 11:50 EB 407

Effects of heavy-ion irradiation in crystals studied by SAXS/SANS — •Daniel Schauries[1], Maik Lang[2], Christina Trautmann[3], and Patrick Kluth[1] — [1]Australian National Univer-

sity, Canberra — [2]University of Tennessee, Knoxville, USA — [3]GSI Darmstadt, Germany

Insulators and semiconductors exposed to swift heavy ions can form ion tracks as a result of the ion-electron interaction. These tracks are narrow, cylindrical-shaped amorphous regions embedded within the crystalline host matrix. In materials engineering they are utilized to modify (opto-)electronic properties, create nanowires and membranes as well as nuclear detectors. Typically, ion tracks are enlarged via chemical etching to make them accessible to microscopy.

Here, we present an experimental investigation into the formation and recovery mechanisms of un-etched tracks. Tracks were created at the high-energy heavy ion accelerator at GSI Darmstadt. Small angle x-ray and neutron scattering (SAXS/SANS) at the Australian Synchrotron and Oak Ridge National Lab [1] was used to investigate parameters such as temperature and pressure on the track size. Elevated temperatures during track formation yielded larger tracks, due to a reduction of the necessary melting energy. For existing tracks however, higher temperatures increases their recovery rate and makes the damaged lattice recrystallizing faster [2].

Work supported by the Australian Research Council and US-DOE.
[1] P. Kluth et al., Phys. Rev. Lett. 101 (2008) 175503.
[2] D. Schauries et al., J. Appl. Cryst 46 (2013) 155.

DF 13.3 Wed 12:10 EB 407

Tuning structure in epitaxial $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ thin films for ferroelectric applications by using miscut substrates — •Michael Mietschke[1,2], Max Hössler[1,3], Stefan Engelhardt[1,2], Sebastian Fähler[1,2], Ludwig Schultz[1,2], and Ruben Hühne[1] — [1]IFW Dresden — [2]TU Dresden — [3]TU Chemnitz

Ferroelectric materials like lead magnesium niobate - lead titanate (PMN-PT) show a large electrocaloric effect induced by an electrical field during a diffusionless phase transition, which can be used for novel solid state cooling devices. However, the interplay between the microstructure and the ferroelectric properties is not completely understood so far.

Therefore, epitaxial 1-x $Pb(Mg_{1/3}Nb_{2/3})O_3$- $xPbTiO_3$ films were grown by pulsed laser deposition on (001)-oriented single crystalline $SrTiO_3$ (STO) substrates with a miscut angle between 0 and 15 degrees towards the [100] direction. The structural properties in dependence from the miscut angle and the deposition parameters are studied by detailed x-ray diffraction, atomic force microscopy and transmission electron microscopy. Temperature dependent ferroelectric characterization was performed by using $La_{0.7}Sr_{0.3}Co_3$ buffer layers and additional Pt top electrodes on the surface of the PMN-PT layer. Normal ferroelectric as well as relaxor ferroelectric behavior was found in dependence of the PT content. First attempt were made to determine the electrocaloric properties from the temperature dependent polarization curves.

Invited Talk DF 13.4 Wed 12:30 EB 407

Investigation of dielectrics under electron irradiation — •Hans-Joachim Fitting — Institute of Physics, University of Rostock, D-18059 Rostock, Germany

Electron beam induced conductivity (EBIC) in insulating materials has been described by a flight-drift model of electrons and holes,[1] and then extended by an intrinsic field conductivity to a flight-drift-conduction model,[2], describing now the selfconsistent charge transport and storage in full insulating materials (c=0), as well as in semi-insulators and wide-gap semiconductors up to intrinsic conductivities of c = 10-6 S/m. This model reflects a more realistic simulation of electron spectroscopic processes in context with electrical charching and/or their prevention, [3]. Moreover, we found the mean relaxation time of ballistically excited electrons with 75 fs, [4]. The experimentally accessable quantities of field assisted total secondary electron emission $\sigma(t)$ as well as the resulting surface potential V0(t) due to internal currents j(x,t), charges $\rho(x,t)$, field F(x,t), and potential V(x,t) distributions are obtained. Thus a given Al2O3 ceramic sample series approaches an intrinsic electrical conductivity of c = (E-10 - E-8) S/m. [1] X. Meyza, D. Goeuriot, C. Guerret-Piécourt, D. Tréheux, and H.-J. Fitting, J. Appl. Phys. 94, 5384 (2003). [2] H.-J. Fitting, M. Touzin, J.A.P. 110, 044111 (2011) [3] M. Touzin, D. Goeuriot, C. Guerret-Piécourt, D. Juvé, D. Tréheux, and H.-J. Fitting, J.A.P, 99, 114110 (2006). [4] H.-J. Fitting and M. Touzin, J.A.P, 108, 033711 (2010)

DF 14: Multiferroics II (DF with DS/KR/MA/TT)

Time: Wednesday 15:00–18:50 Location: EB 107

Invited Talk DF 14.1 Wed 15:00 EB 107

Low energy consumption spintronics using multiferroic heterostructures — •Morgan Trassin — ETH Zurich, Zurich, Switzerland

Magnetization reversal in spintronics applications requires either an externally applied magnetic field or a large current density, which is accompanied by significant energy dissipation. A reversal of magnetization induced only by the application of an electric field would lead to low-power devices. Using multiferroics, previous approaches have seen limited success by only achieving rotations of the magnetization or a change in anisotropy by applying an electric field. To pave the way to new low-power devices, the more desirable electric-field driven magnetization reversal must be achieved and read out with a small current. In multiferroic heterostructures, ferromagnetic domains can be moved and switched using different charge states, strain configurations or magnetoelectric coupling. Ferroelectric domain engineering using epitaxial strain is critical towards the achievement of deterministic switchings. A combination of scanning probe microscopy and optical second harmonic generation were used to characterize multiferroic thin films strain state. Using electron microscopy and transport based techniques, a room temperature magnetization reversal of a CoFe thin layer solely induced by the application of a few volts to the heterostructure will be described.

DF 14.2 Wed 15:30 EB 107

Probing ferroic order in thin film heterostructures with optical second harmonic generation — •Gabriele De Luca, Manfred Fiebig, and Morgan Trassin — ETH Zurich, Switzerland

The evidence of the electric field control on the antiferromagnetic ordering in multiferroic bismuth ferrite ($BiFeO_3$) [1] increased interest in low energy consumption logic and memory devices. However, to exploit such functionality for devices it is essential to attain deterministic control of ferromagnetism at the single domain scale. Therefore a ferromagnet/multiferroic heterostructure has been designed based on the combination of magnetoelectric coupling in $BiFeO_3$ (BFO) and exchange coupling between magnetic materials thus offering a new pathway for the electrical control of magnetism [2,3]. Here we show that second harmonic generation (SHG), can detect the distribution of ferroelectric domains in BFO thin films non-invasively and unimpeded by transport properties. We use epitaxial strain for engineering different types of BFO domain patterns that are characterized by SHG, showing a unique relation between the domain distribution and the film symmetry. We then manipulate the BFO film by voltage poling and demonstrate the sensitivity of the SHG process to this manipulation. The concept applied to BFO is transferable to other multiferroics compounds thus indicating the general feasibility of SHG as a characterization technique for heterostructures in which buried ferroelectricity plays a key role in the emergence of magnetoelectric coupling. 1.Zhao et al., Nat. Mat. 5, 823 (2006) 2.Heron et al., Phys. Rev. Lett. 107, 217202 (2011) 3.Trassin et al., Phys. Rev. B 87, 134426 (2013)

DF 14.3 Wed 15:45 EB 107

Investigation of the antiferromagnetic coupling at $SrRuO_3$ / $La_{0.7}Sr_{0.3}MnO_3$ interfaces — •Sujit Das[1,2], Diana Rata[1], Andreas Herklotz[3], Er Jia Guo[4], Robert Roth[1], and Kathrin Dörr[1,2] — [1]Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany — [2]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [3]Oak Ridge National Lab., Oak Ridge, 37830 TN, USA — [4]Affiliation: Institute for Physics, Johannes-Gutenberg University Mainz, 55128 Mainz, Germany

$La_{0.7}Sr_{0.3}MnO_3/SrRuO_3$ superlattices grown on piezoelectric substrates show large antiferromagnetic coupling of the two ferromagnetic components and a significant strain effect on interfacial coupling [1]. Here we present a systematic investigation of the antiferromagnetic

interface coupling in bilayers of $SrRuO_3$ (SRO) and $La_{0.7}Sr_{0.3}MnO_3$ (LSMO), grown by pulsed laser deposition (PLD) on (100)- oriented $SrTiO_3$ substrates. Epitaxial and coherent growth of the bilayers was confirmed by in-situ RHEED and ex-situ x-ray diffraction (XRD). Magnetic characterization was performed by SQUID magnetometry. We observed a strong dependence of the AFM coupling on the layer sequence and the thickness of the individual layers. The bilayers exhibit exchange bias, with the magnitude and sign of the exchange field strongly dependent on cooling field. Results of this study and ongoing work will be discussed. [1] Sujit Das et al, arXiv:1411.0411

DF 14.4 Wed 16:00 EB 107

Massive magnetoelectric modulation of the magnetic anisotropy in an epitaxial $La_{0.7}Sr_{0.3}MnO_3$/PMN-PT heterostructure — •Martin Wahler[1], Sujit Das[1], Kathrin Dörr[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We use ferromagnetic resonance (FMR) to investigate the strain induced change of the in-plane magnetic anisotropy of an epitaxial ferromagnetic oxide layer on a piezoelectric substrate. The samples consist of 20 nm thick $La_{0.7}Sr_{0.3}MnO_3$ layers on two different substrates, namely $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (PMN-PT) (001) and (110) single crystals. The two substrates induce either isotropic or anisotropic in-plane strain, respectively. For $La_{0.7}Sr_{0.3}MnO_3$ on (001) PMN-PT substrate, it has already been demonstrated by SQUID magnetometry that the Curie-temperature and saturation magnetization can be changed by applying an electric field normal to the sample plane [1]. Here we show that for the same substrate orientation there is a small but significant change in FMR resonance fields along the directions of the magnetic easy axes. For the (110) substrate, however, a massive shift of the resonance fields is observed, resulting in a change of the uniaxial anisotropy of more than 0.5 kOe for an applied electric field of 12 kV cm^{-1}. All measurements are carried out at a temperature of 120 K.

[1] C. Thiele et al., Phys. Rev. B, **75** 054408 (2007)

DF 14.5 Wed 16:15 EB 107

Inverse TMR effect in multiferroic tunnel junctions studied from first principles — •Vladislav Borisov[1,2], Sergey Ostanin[2], and Ingrid Mertig[1,2] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg — [2]Max Planck Institute of Microstructure Physics

The spin-polarized electronic transport in multiferroic tunnel junctions (MTJ): Co/PTO/Co and LSMO/PTO/Co was computed from first principles. We confirm that the so-called four-state tunnelling magnetoresistance (TMR) may be detected for each MTJ when its TMR and TER are controlled by the reversible barrier polarization as well as reversible magnetization of the leads. The *ab initio* based results are directly compared to the experimental features of the inverse TMR recently reported for LSMO/PZT/Co [1]. We show how the observed effect originates from the magnetoelectric coupling seen at both interfaces of the MTJ [2]. The role of half-metallic LSMO as well as the effect of Zr substitutes in PTO are analysed in the context of the inversion of the TMR signal [1]. Another important issue of TMR discussed here concerns the functional (insulating) barrier thickness, which is always less than the nominal thickness and which depends on the polarization direction. We found that the functional barrier thickness is systematically reduced when the polarization is directed toward the Co electrode due to charge transfer at the Co/PTO interface.

[1] D. Pantel *et al.*, *Nat. Mater.* **11**, 289 (2012).
[2] V. S. Borisov *et al.*, *Phys. Rev. B* **89**, 054436 (2014).

DF 14.6 Wed 16:30 EB 107

Origin of superstructures in (double) perovskite thin films — •Vikas Shabadi, Marton Major, Philipp Komissinskiy, Aldin Radetinac, Mehran Vafaee, Wolfgang Donner, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Strasse 2, 64287 Darmstadt, Germany

We have investigated the origin of superstructure peaks as observed by X-ray diffraction of multiferroic $Bi(Fe_{0.5}Cr_{0.5})O_3$ thin films grown by pulsed laser deposition on single crystal $SrTiO_3$ substrates. The photon energy dependence of the contrast between the atomic scattering factors of Fe and Cr is used to rule out a chemically ordered double perovskite Bi_2FeCrO_6 (BFCO). Structural calculations suggest that the experimentally observed superstructure occurs due to unequal cation displacements along the pseudo-cubic [111] direction that mimic the unit cell of the chemically ordered compound [1]. This result helps to clarify discrepancies in the correlations of structural and magnetic order reported for Bi_2FeCrO_6. The observation of a superstructure in itself is not a sufficient proof of chemical order in double perovskites.

[1] V. Shabadi, M. Major, P. Komissinskiy, M. Vafaee, A. Radetinac, M. Baghaie Yazdi, W. Donner, and L. Alff, J. Appl. Phys. **116**, 114901 (2014).

DF 14.7 Wed 16:45 EB 107

Using multiferroic systems as a spin filter - an ab initio study — •Stephan Borek[1], Jürgen Braun[1], Hubert Ebert[1], Angelika Chassé[2], Gerd Schönhense[3], Hans-Joachim Elmers[3], Dmytro Kutnyakhov[3], and Ján Minár[1,4] — [1]Ludwig-Maximilians-Universität München — [2]Martin-Luther-Universität Halle-Wittenberg — [3]Johannes-Gutenberg-Universität Mainz — [4]University of West Bohemia, Pilsen

Multiferroic heterostructures such as ultrathin $Fe/BaTiO_3(001)$ films are of high interest for technical applications giving the opportunity to control the ferromagnetic state with an electric field or vice versa. In our theoretical study we investigated the effect of changing the electric polarization of the ferroelectric substrate $BaTiO_3$ on the ferromagnetic state of Fe and Co thin films using the method of Spin Polarized Low Energy Electron Diffraction (SPLEED). This method has been shown to be an effective tool for the investigation of surface properties like the determination of surface magnetic moments and the local crystal structure. The possibility of an application of the multiferroic heterostructures Fe/BTO(001) and Co/BTO(001) as a spin filter is discussed. It will be shown that a change of the polarisation of the $BaTiO_3$ results in a significant change of the exchange asymmetry giving the possibility to control the diffraction of electrons using the exchange interaction at the Fe (Co) surface. We focus on the systems of 1 ML, 2 ML and 3 ML Fe (Co) on $BaTiO_3$ because their electronic and magnetic structure as well as the coupling mechanism between the ferroic phases have been intensively discussed in the literature.

20 min coffee break

DF 14.8 Wed 17:20 EB 107

Optical investigation of ferroic domains beyond the resolution limit — •Christoph Wetli, Viktor Wegmayr, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

In recent years optical second harmonic generation (SHG) has been shown to be a versatile, non-destructive tool to investigate the often complex domain structures of ferroic and multiferroic materials. Ferroic domains vary broadly in structure and size, depending on the nature of the ferroic ordering. So far, however SHG was restricted to domains larger than the optical resolution limit of 1 μm. Here we present a method by applying a numerical model and simulation to overcome this limitation and to analyze ferroic domain structures some orders of magnitude smaller than the optical resolution limit. The method is based on the relation between the orientation of the ferroic order parameter and the phase of the nonlinear optical signal. It gives a relation between domain size and density, optical resolution and the intensity of the SHG signal. To show the reliability of the model, we applied it to several simulated domain structures. The simulation of the domain structures is based on an iterative geometrical algorithm, which allows us to generate complex domain patterns like the ferroelectric vortex structures or the irregular bubble like antiferromagnetic domains in hexagonal $YMnO_3$. The numerical calculations were compared with experimental data and found to be in excellent agreement.

DF 14.9 Wed 17:35 EB 107

Multiferroicity in $DyMnO_3$ thin films — •Chengliang Lu[1,2], Hakan Deniz[2], and Jun-Ming Liu[3] — [1]School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle(Saale), Germany — [3]Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

The mutual control of ferroelectricity and magnetism is stepping towards practical applications proposed for quite a few promising devices in which multiferroic thin films are involved. Although ferroelectricity stemming from specific spiral spin ordering has been reported in highly distorted bulk perovskite manganites, the existence of magneti-

cally induced ferroelectricity in the corresponding thin films remains an unresolved issue, which unfortunately halts this step. Here we report magnetically induced electric polarization and its gigantic response to magnetic field (an enhancement of 800% upon a field of 2 Tesla at 2 K) in $DyMnO_3$ thin films grown on Nb-$SrTiO_3$ substrates. Interestingly, we found a consecutive control of the polarization under a rotating magnetic field by detailed multiferroic response measurements. This is distinct to the standard polarization-flop process which results in a sudden change in polarization in multiferroics with spiral-spin-ordering state. The cooperative action of dual multiferroic mechanisms (the inverse Dzyaloshinskii-Moriya interaction among Mn moments and the exchange striction working between Dy and Mn moments) and phase coexistence associated with a twin-like structure was proposed as the origin of this phenomenon.

DF 14.10 Wed 17:50 EB 107

Observation of direct and converse local magnetoelectric switching at room-temperature in modified single-phase bismuth ferrite — •Leonard Frederic Henrichs[1], Oscar Cespedes[1], James Bennett[1], Joachim Landers[2], Wolfgang Kleemann[2], Heiko Wende[2], Doru Lupascu[2], and Andrew Bell[1] — [1]University of Leeds, Leeds, GB — [2]Universität Duisburg/Essen, Duisburd/Essen, Germany

Multiferroics are promising for applications in sensors and memory. However, no single-phase material with both ferroelectric and ferro- or ferrimagnetic order at room-temperature has been reported to date. Here, we observe very large local magnetoelectric coupling in the novel single-phase multiferroic $(BiFeCo_{0.1}O_3)_{0.4}$-$(K_{1/2}Bi_{1/2}TiO_3)_{0.6}$ at room-temperature. On ceramic samples, both direct and converse magnetoelectric switching was observed using piezoresponse force-microscopy and magnetic force-microscopy respectively. Areas where converse switching occurred, incorporate both a ferroelectric and magnetic domain-like cluster and thus appear to be (relaxor) ferroelectric and ferrimagnetic at room-temperature. The direct coupling-coefficient estimated from the experiments is 1.0×10^{-5} s/m, and thus extremely large. The locally observed converse meangetoelectric effect has a similar of magnitude. we propose that the material can be interpreted as a pseudo-nanocomposite with an ideal strain-mediated coupling due to congruent polar and magnetic nanoregions which are related to the relaxor ferroelectric and superparamagnetic nature of the material.

DF 14.11 Wed 18:05 EB 107

Tiny cause with large effects: the origin of the large magnetoelectric and magnetoelastic effect in $EuTiO_3$ — •Annette Bussmann-Holder — MPI-FKF, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The magnetoelectric coupling in the perovskite $EuTiO_3$ is analyzed within a spin-phonon coupled Hamiltonian. It is shown that the tiny magnetostriction which accompanies the onset of antiferromagnetic order at $T_N = 5.7$ K induces a substantial hardening in the soft optic mode and a drop in the dielectric constant. The reduction of magnetostriction with increasing magnetic field reverses this behavior. While for small fields ferromagnetic order rapidly sets in accompanied by a volume expansion, this is destroyed with increasing fields and a strange paramagnetic state obtained. This exotic observation can be understood as stemming from the interplay between the enhanced oxygen p Ti d dynamical covalency which alters the crystal field at the Eu site and inhibits the virtual transition from $4f7$ to $4f65d$ responsible for ferromagnetic order.

DF 14.12 Wed 18:20 EB 107

First principles calculations on the effect of inner cationic site disorder, single and multiple cation and anion doping on the magnetic properties of $GaFeO_3$ — •Jacqueline Atanelov, Wernfried Mayr-Schmölzer, and Peter Mohn — Institute of Applied Physics - Computational Materials Science, Vienna University of Technology, Austria

$GaFeO_3$ is a promising multiferroic suitable for a wide range of applications in electronic devices. Motivated by that we investigate the influence of single and multiple cation and anion doping on the electronic and magnetic properties of gallium ferrite. Further we consider the well known fact of innner cation site disorder in $GaFeO_3$. In terms of cation doping we replace Ga atoms by Fe atoms and vice versa so that in total a concentration range of $0.9 \leq x \leq 2.0$ in $Ga_2 - xFe_xO_3$ is investigated. In addtion to that we substitute oxygen by B, C, N and S atoms. GFO is also known to show magnetic anisotropy for different cristallographic directions and sublattices. Beside changes in the total net magnetic moment induced by cation and anion doping, the magnetic anisotropy energy (MAE) can be affected as well. Doping therefore can lead to an enhancement or reduction of the MAE. First principles density functional theory (DFT) calculations performed by the Vienna ab Initio Simulation Package (VASP) are used to predict and analyze the ground state electronic structure of the investigated systems.

DF 14.13 Wed 18:35 EB 107

Mechanism of interfacial magnetoelectric coupling in composite multiferroics — Chenglong Jia[1], Tongli Wei[1], Changjun Jiang[1], Desheng Xue[1], •Alexander Sukhov[2], and Jamal Berakdar[2] — [1]Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou 730000, China — [2]Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, 06099 Halle (Saale), Germany

We present a mechanism for the magnetoelectric coupling at ferroelectric/ferromagnetic interfaces based on screening via interfacial spin-rearrangement [1]. We find an electric-polarization-driven, non-collinear spin region extending over the spin-diffusion length in the ferromagnet. The orbital motion of the carriers in the ferromagnet is affected by the gauge field associated with the non-collinear spin order and hence indirectly by the electric polarization. Changing the latter, e.g., via an electric field influences the interfacial magnetic order and hence the spin-orbital coupled motion of the carriers. This allows for tuning the interfacial spin-dependent transport via electric fields. The resulting coupling is robust at room temperature and can be well approximated by a linear polarization- magnetization coupling, whose strength estimate for the composite Co(40 nm)/(tetragonal)$BaTiO_3$ is in line with recent experiments [2].

[1] C.-L. Jia, T.-L. Wei, C.-J. Jiang, D.-S. Xue, A. Sukhov, J. Berakdar, Phys. Rev. B **90**, 054423 (2014). [2] N. Jedrecy, H.J. von Bardeleben, V. Badjeck, D. Demaille, D. Stanescu, H. Magnan, A. Barbier, Phys. Rev. B **88**, 121409(R) (2013).

DF 15: Optical and Nonlinear Optical Properties II (DF with KR)

Time: Wednesday 15:00–17:40 Location: EB 407

DF 15.1 Wed 15:00 EB 407

Local defect structure and dielectric relaxation in $LiNbO_3$ single crystals — Guillaume F. Nataf, Nadège Meyer, and •Torsten Granzow — Luxembourg Institute of Science and Technology (LIST), Belvaux, Luxembourg

The defect structure of $LiNbO_3$ (LN) has been studied more extensively than that of most other oxide ferroelectrics for several reasons. First, congruently melting LN is already rich in defects: it is strongly Li-deficient and contains a high concentration of Nb_{Li} antisite defects. Second, the possibility to adjust the optical properties by doping with a wide range of ions has increased the usefulness of LN for optical applications. Third, due to the high mobility of Li at moderate temperatures, the poling procedure can have a profound influence on the local defect structure. However, few studies have considered the effect of this local structure on the dielectric properties of LN. In this presentation, the temperature dependence of the real and imaginary part of the electrical permittivity of differently doped LN single crystals is investigated in the frequency range from 1 Hz to 1 MHz. Different relaxation phenomena are caused by thermal and electrical treatment and traced to differences in the local defect structure. Ferroelectric domain walls stabilize the local defect structure. These assumptions are supported by measurements of the temperature dependence of electrical conductivity and the thermally stimulated depolarization current.

DF 15.2 Wed 15:20 EB 407

Influence of defects on the ferroelectric and electrocaloric properties of $BaTiO_3$ — •Anna Grünebohm[1] and Takeshi

Nishimatsu[2] — [1]Fakultät für Physik, Uni Due, Germany — [2]IMR, Tohoku University and Faculty of Physics, Japan

The electrocaloric effect is an adiabatic temperature change of a material upon applying an external electrical field. Recently, this effect has been rediscovered as a promising candidate for solid state refrigeration as large temperature changes have been found in experiment and theoretical simulations.[1,2,3] However, the underlying mechanisms for the large caloric response as well as possible obstacles are still not well understood. In addition, the effective temperature range in pure ferroelectric materials is narrow. We thus perform molecular dynamics simulations of an ab initio based effective Hamiltonian as implemented in the *feram* package[3] in order to study the effect of defects, strain, and alloying on the electrocaloric response and its operation range.

[1] A. Mishenko, *et al*, Science **311**, 1270 (2006)
[2] I. Ponomareva *et al*, Phys. Rev. Lett. **108**, 167604 (2012)
[3] T. Nishimatsu *et al*, J. Phys. Soc. Jpn., **82**, 114605 (2013)

DF 15.3 Wed 15:40 EB 407

Probing of local polarization dynamics in uniaxial SrxBa1-xNb2O6 single crystals — •Vladimir Shvartsman[1], Jan Dec[2], Sergei Kalinin[3], Wolfgang Kleemann[4], and Doru Lupascu[1] — [1]Institute for Materials Science, University Duisburg-Essen, Essen, Germany — [2]Institute of Materials Science, University of Silesia, Katowice, Poland — [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA — [4]Faculty of Physics, University Duisburg-Essen, Duisburg, Germany

Unique properties of relaxor ferroelectrics are to a great extent determined by dynamics of the local polarization. In these materials only short range polar order exists inside so called polar nanoregions (PNRs). Being dynamic at high temperatures, PNRs are "frozen" below certain critical temperature forming a glassy-like state.

Here we report on our recent piezoresponse force microscopy (PFM) investigations of local polarization dynamics in SrxBa1-xNb2O6 (SBN100x) single crystals. The temperature dependent PFM studies of relaxors SBN75 and SBN80 revealed appearance of static PNRs already far above the freezing temperature. These static PNRs coexist with still dynamic those in a broad temperature interval. The response from dynamic PNRs was probed by studying the temporal decay of local piezoresponse after excitation by an electric field pulse. A mapping of relaxation parameters has been performed to reveal spatial heterogeneity of the polarization dynamics. The effect of temperature and composition on the local polarization dynamics has been analyzed.

DF 15.4 Wed 16:00 EB 407

Multiphoton-induced luminescence and its domain contrast in Mg-doped $LiNbO_3$ and $LiTaO_3$ — •Philipp Reichenbach[1], Thomas Kämpfe[1], Andreas Thiessen[1], Alexander Haussmann[1], Robin Steudtner[2], Theo Woike[3], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George- Bähr-Str. 1, 01069 Dresden, Germany, 01069 Dresden, Germany — [2]Institut für Ressourcenökologie, Helmholtz-Zentrum Dresden, Bautzner Landstraße 400, 01328 Dresden — [3]Institut für Strukturphysik, Technische Universität Dresden, Zellescher Weg 16, 01069 Dresden, Germany

Mg doped $LiNbO_3$ (LNO) and $LiTaO_3$ (LTO) emit a spectrally broad multiphoton luminescence upon excitation with tightly-focused ultrashort laser pulses centered at 2.5 eV [1,2]. Time-resolved acquisition reveals a stretched exponential decay of the photoluminescence, which confirms the luminescence to stem from recombination of electron and hole polarons. Furthermore, the luminescence also shows a distinct contrast between virgin and single inverted domains of about 3% and 20 - 30% for LNO and LTO, respectively [2]. LNO exhibits the same contrast value when thermally pretreated at 1000°C under oxygen atmosphere before poling. The contrast decays thermally-excited above 100°C with an activation energy around 1 eV for both LNO and LTO. This indicates the contrast and its decay to be strongly connected to the lithium ion concentration and their activation.

[1] P. Reichenbach et al., J. Appl. Phys. 115, 213509 (2014)
[2] P. Reichenbach et al., Appl. Phys. Lett. 105, 122906 (2014)

DF 15.5 Wed 16:20 EB 407

Extended *ab-initio* study of the $LiNbO_3$ band gap — •Arthur Riefer, Simone Sanna, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33098 Paderborn

Lithium niobate ($LiNbO_3$) is one of the most important ferroelectric materials and the most important nonlinear optical material. The electronic and optical properties of $LiNbO_3$ have been studied in recent years with *ab-initio* methods [1-4] within high accuracy indicating good agreement with experimental results. However, measurements by Redfield *et al.* [5] show a temperature dependence of the band gap, which can be traced back to different effects. In order to model the temperature dependence of the electronic band gap, we have extended the approaches described in Refs. [1-4] under two aspects. On the one hand, hybrid functionals are employed to provide improved starting points for many-body perturbation theory, which is applied to study the electronic properties. On the other hand, the influence of the temperature on the $LiNbO_3$ band gap is investigated by means of molecular dynamics simulations. The results are compared with former works and experimental findings.

[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.*, IEEE Trans. on Ultrasonics, Ferroelectrics and Frequency Control **59**, 1929 (2012).
[4] A. Riefer *et al.*, Phys. Rev. B. **87**, 195208 (2013)
[5] Redfield *et al.*, J. Appl. Phys. **45**, 10, (1974)

DF 15.6 Wed 16:40 EB 407

Structural characterization of substituted lanthanum tungstates with X-Ray and Neutron Diffraction — •Andrea Fantin[1], Tobias Scherb[1], Gerhard Schumacher[1], Janka Seeger[2], and Wilhelm A. Meulenberg[2] — [1]Helmholtz-Zentrum Berlin für Materialen und Energie, Hahn-Meitner-Platz 1, D-14109 Germany — [2]Forschungszentrum Jülich, D-52425 Jülich, Germany

Our work on proton conducting materials deals with structural characterization of two different series of substituted lanthanum tungstates: La5.4W(1-x)MxO12-delta with M=Mo,Re and 0<=x<=0.2. The main methods used to understand their crystal structure are Neutron Diffraction (ND) and High-Resolution X-Ray Diffraction (HRXRD). Experiments were carried at ILL (Grenoble, France) and PSI (Villigen, Switzerland). Different elemental contrast is reached with these complementary diffraction techniques.

Our specimens consist of three cations (La, W, Mo or Re) and oxygen anions. In order to distinguish W (Z=74, b=4.86fm) and Re (Z=75, b=9.2fm) neutrons are needed, while for La (Z=57, b=8.2fm), W(Z=74, b=4.86fm) and Mo (Z=42, b=6.7fm) good contrast is also given by X-Rays. Combined refinements to model accurately antisite disorder, position of the substituted elements and oxygen (Z=8, b=5.8fm) positions in this highly disordered material are mandatory.

Measurements in dependence of temperature down to 1.5K confirm the structural model suggested by one of the coauthors without any unmodeled static disorder. Substitution and deuteration/humidification show no relevant structural changes.

DF 15.7 Wed 17:00 EB 407

Structure Solution and Prediction for Complex Modular Materials — •Kathryn Bradley, Matthew Dyer, Christopher Collins, John Claridge, George Darling, and Matthew Rosseinsky — Department of Chemistry, University of Liverpool, Liverpool, L69 7ZD, United Kingdom

Complex functional transition metal oxides can generally be described in terms of layers or modules containing elements in particular chemical environments. This observation has led to the development of the Extended Module Materials Assembly (EMMA) approach for the generation of plausible candidate structures of particular compositions. Combining the modular description with classical lattice dynamics and structure optimization with DFT, the EMMA method has recently been extended to study hexagonal perovskite structures, exploring the family of B-site deficient barium cobalt niobates.[1]

[1] K. Bradley et al., Phys. Chem. Chem. Phys., 2014,16, 21073-21081. DOI: 10.1039/C4CP01542H

DF 15.8 Wed 17:20 EB 407

Perspectives for photorefractive materials in neutron physics — •Romano Rupp[1], Martin Fally[1], Jürgen Klepp[1], Christian Pruner[2], Yasuo Tomita[3], and Irena Drevensek[4] — [1]Univ. Wien, Austria — [2]Univ. Salzburg, Austria — [3]University of Electro-Communications, Tokyo, Japan — [4]Univ. Ljubljana and Josef-Stefan-Institute Ljubljana, Slovenia

The phenomenon where light irradiation changes the refractive index is called a photorefractive effect. There are several mechanisms that may result in neutron photorefraction. For example, all photoconductive isolators have in principle the potential to exhibit neutron photore-

fraction. Particularly strong effects appear in piezoelectric materials, mixed electronic-ionic conductors or materials close to, e.g., a ferroelectric phase transition. We report on neutron diffraction from holographic gratings induced by light irradiation, neutron-induced holographic grating decay, and investigations on light-sensitive dielectrics and nanoparticle composites for applications in neutron physics.

DF 16: Focused Session on GHz Dielectrics: Materials for Mobile Communication I (DF with HL/MM)

The world wide amount of wireless data exchange doubles roughly every year. In addition the individual data rates increase and the efficiency of the data exchange needs improvements. Antenna and filter elements are key components for such a development and are subject to intense research efforts. Impulses for innovation also originate from materials while new antenna and filter concepts influence material development. Two Focused Sessions are addressing the subject.

Organizer: Martin Letz (Schott AG Mainz)

Time: Thursday 9:30–13:00 Location: EB 407

Topical Talk DF 16.1 Thu 9:30 EB 407

New application scenarios for dielectric materials in mobile communication systems of the 5th generation — •Roland Gabriel — Kathrein-Werke KG, Anton-Kathrein-Straße 1-3, D-83004 Rosenheim / Germany

The worldwide data volume in mobile communication systems double nearly every year. To address this challenge, higher frequency bands will be used and broadband and multiband equipment are required. The new standard LTE-A and the standardization process for the 5th generation of the mobile communication systems enforces changes in the technology of antennas and filters. Beside the usage of new and higher frequency bands up to 60 GHz the broadband and multiband approach increase the requirements for the linearity of the components. For the use in FDD (frequency division duplexing) - systems this means an extreme low level of the active and passive intermodulation. In this contribution the extendend requirements for passive intermodulation are discussed. Different available solutions for the filter technology will be compared regarding the usage for different system solutions of the 4th and 5th generation. In addition the use of dielectric radiators in antennas will be reconsidered with respect to the multiband approach and the required inter- and intra-band isolation.

DF 16.2 Thu 10:00 EB 407

Impedance matching for high power transistors based on printed ceramics — •Alex Wiens, Daniel Kienemund, and Rolf Jakoby — Technische Universität Darmstadt, Institut für Mikrowellentechnik und Photonik

The multitude of standards in modern tele-communication systems, such as GSM, UMTS, LTE and WiFi make the hardware of a radio front end face a variety of frequencies and bands. Generally, each element of the front end is optimized to perform best at a certain frequency band and signal type. Power amplifiers can be considered as the most critical components of RF/microwave communication systems, as they dominate the power consumption and hence the efficiency of the whole system. They are therefore consequently the focus of intense research to achieve improved linearity and increased power efficiency. Barium-Strontium-Titanate (BST) varactors offer an alternative to semiconductor and MEMS technologies in the design of tunable matching networks for reconfigurable multi-band RF-power amplifiers, and for load modulation applications, where the varactor tuning is used to maintain high efficiency over a large dynamic range of the input signal. Recent advances in fabrication of high power tunable RF varactors based on BST are presented and discussed. Measurement results of a BST-based tunable matching network, implemented inside a GaN HEM Transistor show promissing performance for telecommuncation frequency range.

DF 16.3 Thu 10:20 EB 407

Enhanced magnetooptic Kerr effect and magnetic properties of Ce:YIG thin films — •Andreas Kehlberger[1], Kornel Richter[1], Gerhard Jakob[1], Mehmet C. Onbasli[2], Gerald F. Dionne[2], Dong Hun Kim[2], Taichi Goto[2], Gerhard Götz[3], Günter Reiss[3], Timo Kuschel[3], Caroline A. Ross[2], and Mathias Kläui[1] — [1]Universität Mainz, Mainz, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]CSMD, Physics Department, Bielefeld University, Germany

Yttrium iron garnet (YIG) is a ferrimagnetic and electrically insulating garnet oxide that has low intrinsic magnetic damping. These properties make YIG a functional layer for spin-wave generation and filtering for telecommunication devices operating at microwave bands. The substitution of Y by Ce allows for an enhancement of the magnetooptic properties and to further influence the magnetic material properties. Our work presents an extensive study of high quality epitaxial Ce:YIG thin films and reveals that not only the magnetooptic properties but also the magnetic anisotropy can be tailored by the Ce substitution. For the first time we show that beside the Faraday rotation also the magnetooptic Kerr effect is enhanced compared to pure YIG, making a broader range of wavelength, including the fibreoptics band, accessible. We present growth methods for polycrystalline Ce:YIG films, which allow the development of integrated on-ship devices.[1,2] Our results show the suitability of Ce:YIG thin film for future magnetooptic and spintronic applications. [1] Lei Bi et al., Nature Photon. 5, 758-762 (2011) [2] Taichi Goto et al., J. Appl. Phys. 113, 17A939 (2013)

DF 16.4 Thu 10:40 EB 407

Design of miniaturized antennas for GNSS applications using a high DK dielectric material — •Stefano Caizzone — Institute of Communications and Navigation, German Aerospace Center (DLR), Wessling, Germany

The use of high dielectric constant (high DK) materials is particularly appealing for a vast number of Radio Frequency (RF) applications, including antenna design. In this field, in fact, high DK low-loss dielectric materials could enable consistent improvements in antenna miniaturization. To the present day, however, common high-DK materials suffer from relatively large manufacturing tolerances, implying remarkable frequency shifts in the antenna radiation and need for retuning. This work, on the other hand, shows the use of a new dielectric material with diminished tolerances for antenna design purposes, both through preliminary tests with a simple antenna structure and through the enhanced design of a miniaturized antenna for GNSS applications. The initial tests were performed in order to validate the usability of the material in the RF area: it was used as a substrate for a microstrip patch antenna. The results show a good behavior of the high DK material and its aptitude for RF antenna design. As a consequence, a Dielectric Resonator Antenna (DRA), fully exploiting the dielectric properties of the material, was designed for use in the lower L-Band of the Global Navigation Systems, allowing for good performance over a wide bandwidth, covering E5, L2 and E6 bands.

Topical Talk DF 16.5 Thu 11:00 EB 407

Dielectric-loaded antennas for circular polarisation: their contribution to the information capacity of wireless terminals — •Oliver Leisten — Maruwa Europe Ltd, UK

Dielectric-loaded multi-filar helix antennas offer solutions as miniature circular polarised antennas in small devices with the advantage that body-loading can suppress reflections from the device: improving circular polarisation discrimination. This is an example of materials-science enabling the design of antennas providing relatively predictable performance in a cluttered and changing near environment. Modern wireless systems typically operate with complex scattering from objects in the indoor environment which can be scaled in frequency to be compared to the Rayleigh scattering of light from the particles of dense smoke.

Indeed modern MIMO devices exploit the low spatial autocorrelation of such fields invoking the principle of spatial multiplexing to multiply the information capacity per unit of spectral bandwidth. Such systems use multiple receiving antennas to receive scattered signals summing by superposition, at those discrete antenna locations, of information streams transmitted from multiple transmitting antennas. The small resonance volume dielectric-loaded antennas, together with platform independent polarisation, enhances statistical independence of signals, improving system data-capacity by reducing interference between data-streams. The use of right and left hand circular polarised antennas to invoke polarisation diversity is interesting as Rayleigh scattering develops spin-turbulent fields.

20 min Coffee Break

DF 16.6 Thu 11:50 EB 407

$Ba_4Al_2Ti_{10}O_{27}$ glass-ceramics as dielectric materials for antenna elements in wireless communications — •Martun Hovhannisyan[1], Hubertus Braun[1], Yuliang Zheng[2], Arshad Mehmood[2], Martin Letz[1], and Rolf Jakoby[2] — [1]Material & Technology Development, SCHOTT AG, Hattenbergstrasse 10, Mainz, 55122, Germany — [2]Technical University of Darmstadt, Darmstadt, D-64283 Darmstadt, Germany

Dielectric glass-ceramics with $Ba_4Al_2Ti_{10}O_{27}$ as the main crystalline phase are obtained by controlled heat-treatment of a non-porous bulk-glass phase. Such a non-porous material has advantages over ceramics with residual porosity wherever metallization steps are applied to the material. Depending on the details of heat-treatment profile the $Ba_4Al_2Ti_{10}O_{27}$ is formed as a main phase with secondary phases $BaTi_4O_9$ or $BaAl_2Si_2O_8$. Microstructural observation using scanning electron microscopy (SEM) shows nanometer-sized crystals (40nm) grown in a true glass phase. The microwave dielectric characterization using Hakki-Coleman setup shows a Qf from 2000 GHz to 10.000 GHz, dielectric constant from 19 to 33 and |tf| of <20 ppm/K. Balancing between different crystalline phases allows to adjust |tf| to zero. To our knowledge the present work is the first one emphasizing the attractiveness of the microwave dielectric properties of the phase $Ba_4Ti_{10}Al_2O_{27}$. Such glass-ceramics are well suited for antenna and filter applications in microwave electronics.

DF 16.7 Thu 12:10 EB 407

Highly conducting $SrMoO_3$ thin films for microwave applications — •Aldin Radetinac[1], Arzhang Mani[1], Sergiy Melnyk[2], Mohammad Nikfalazar[2], Jürgen Ziegler[1], Yuliang Zheng[2], Rolf Jakoby[2], Lambert Alff[1], and Philipp Komissinskiy[1] — [1]Institute for Materials Science, TU Darmstadt, Germany — [2]Institute for Microwave Engineering and Photonics, TU Darmstadt, Germany

We have measured the microwave resistance of highly conducting perovskite oxide $SrMoO_3$ thin film coplanar waveguides. The epitaxial $SrMoO_3$ thin films were grown by pulsed laser deposition and showed low mosaicity and smooth surfaces with a root mean square roughness below 0.3 nm. Layer-by-layer growth could be achieved for film thicknesses up to 400 nm as monitored by reflection high-energy electron diffraction and confirmed by X-ray diffraction. We obtained a constant microwave resistivity of 29 $\mu\Omega$cm between 0.1 and 20 GHz by refining the frequency dependence of the transmission coefficients. Our result shows that $SrMoO_3$ is a viable candidate as a highly conducting electrode material for all-oxide microwave electronic devices. This work was supported by the DFG project KO 4093/1-1.

[1] A. Radetinac, A. Mani, S. Melnyk, M. Nikfalazar, J. Ziegler, Y. Zheng, R. Jakoby, L. Alff, and P. Komissinskiy, Appl. Phys. Lett. **105**, 114108 (2014)

Topical Talk DF 16.8 Thu 12:30 EB 407

Tunable GHz-components with ferroelectric and liquid crystal technologies for mobile terrestrial and satellite-based systems — •Rolf Jakoby — Institute of Microwave Engineering and Photonics, Technische Universität Darmstadt, Merckstr. 25, 64283 Darmstadt, Germany

Recent progress in Liquid Crystal (LC) technology made in Darmstadt is very promising for next-generation reconfigurable/tunable microwave and millimeter wave devices because they exhibit excellent properties at high frequencies above 15 GHz, since LC losses generally decrease with increasing frequency. This opens up new low-cost LC applications beyond optics. In contrast, ferroelectric material, particularly Barium Strontium Titanate (BST), is well suited at frequencies below 15 GHz, using screen and inkjet printing of BST layers. Hence, with these two material classes, we can cover a frequency range from 1 GHz up to 1 THz for tunable components such as varactors, tunable delay and loaded lines, phase shifters, tunable filters, adaptive matching networks, tunable frequency selective surfaces, tunable multiband antennas, polarization-agile antennas, phased-scanning reflect- and phased arrays. This contribution presents an overview of the both technologies, BST and LC, including basic principles, tuning mechanisms, processing technologies, device concepts and design, packaging and integration issues as well as functional tests with focus on frequency-agile multiband antennas and filters as well as electronically beam-steering antennas for mobile terrestrial and satellite-based applications.

DF 17: Focused Session on GHz Dielectrics: Materials for Mobile Communication II (DF with HL/MM)

Organizer: Martin Letz (Schott AG Mainz)

Time: Thursday 15:00–17:00 Location: EB 407

Topical Talk DF 17.1 Thu 15:00 EB 407

Temperature stable low loss ceramics for resonators and filters — •Ian Reaney — Materials Science and Engineering, University of Sheffield, Sheffield, UK

Micro wave (MW) dielectric ceramics are required to be temperature stable and have a low dielectric loss to prevent heating of the sample when operated at or near resonance. They are used in many applications but specifically in this contribution the use of MW dielectric ceramics as resonators, filters and antennas is considered. The relevant technologies for these application are reviewed along with their selective materials parameters. The underpinning crystal chemistry that leads to optimisation of properties is also reviewed and some new materials and novel processing routes to improve device performance are discussed.

DF 17.2 Thu 15:30 EB 407

Titanate-based paraelectric glass-ceramics for applications in GHz electronics — •Hubertus Braun[1,2,3], Martin Letz[2], Martun Hovhannisyan[2], and Hans-Joachim Elmers[1] — [1]Johannes-Gutenberg Universität Mainz — [2]SCHOTT AG, Mainz — [3]Graduate School Materials Science in Mainz

In the current work, titanate-based glass-ceramics (TiO_2 > 45 mol %) in the La_2O_3-TiO_2-SiO_2-B_2O_3 system are developed ($\varepsilon_r \approx$ 20-30, Qf $\approx$ 10.000 GHz, $|\tau_f| <$ 10 ppm/K) which show promising properties as microwave materials and offer numerous advantages in comparison to conventional sintered ceramics. Glass-ceramics which are obtained via a true glassy phase are comparatively new in this field and will be presented as suitable alternative. Glass-ceramics are produced in a two step process: At first, a basic glass is casted in a conventional glass production process. Then the glass undergoes a temperature treatment with a defined temperature profile to initiate a controlled partial crystallization of desired paraelectric phases inside the glassy matrix. Obtaining materials via a homogeneous glassy phase enables intrinsically pore-free materials with comparatively superior surface properties. The effect of solid solution type doping on the dielectric properties and glass stability is investigated. The effect of solid solution type doping on the A(La) and B(Ti) site of the crystalline phases with ions of similar ionic radius is investigated concerning their influence on the dielectric properties and glass stability. Further the materials are analyzed concerning suitability for dielectric loaded antenna

applications.

DF 17.3 Thu 15:50 EB 407

Microwave electric properties of thin-film $Ba_xSr_{1-x}TiO_3$ varactors with highly-conducting epitaxial $SrMoO_3$ oxide electrodes — •Arzhang Mani[1], Aldin Radetinac[1], Mohammad Nikfalazar[2], Sergiy Melnyk[2], Philipp Komissinskiy[1], Yuliang Zheng[2], Rolf Jakoby[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Deutschland — [2]Institut für Mikrowellentechnik und Photonik, Technische Universität Darmstadt, 64283 Darmstadt, Deutschland

We present high-frequency properties of MIM thin-film varactors with dielectric $Ba_xSr_{1-x}TiO_3$ (x = 0.4, 0.5, 0.6). Single crystalline $Ba_xSr_{1-x}TiO_3$ layers were grown epitaxially on highly-conducting oxide $SrMoO_3$ electrodes with room-temperature resistivity of 30 $\mu\Omega\cdot$cm. Au/Pt top electrodes were deposited by magnetron sputtering on top of the $Ba_xSr_{1-x}TiO_3$ / $SrMoO_3$ heterostructures and patterned with photolithography and lift-off. Influence of Ba content (x), thickness of $Ba_xSr_{1-x}TiO_3$ layer, and size of the top electrodes on performance of the varactors were investigated in the frequency range of 100 MHz to 10 GHz. Capacitance of 15 pF, quality factor of 15, and tunability of 40% at 0.3 MV/cm were obtained at 100 MHz. The obtained results suggest a high potential of the oxide perovskite electrode material $SrMoO_3$ [1] for fabrication of highly tunable varactors in microwave applications.

[1] A. Radetinac *et al.*, Appl. Phys. Lett. **105**, 114108 (2014).

DF 17.4 Thu 16:10 EB 407

Continuously tuneable, high performance phase shifters based on liquid crystal for applications in phased array antennas — •Matthias Jost, Christian Weickhmann, and Rolf Jakoby — Institute of Microwave Engineering and Photonics, Technische Universität Darmstadt, Merckstr. 25, 64283 Darmstadt, Germany

During the last decade, calamitic-nematic liquid crystals (LCs), well-known from the LC-display technology (LCD), have become increasingly popular in the field of microwave engineering. Due to their unique property of exhibiting local anisotropy, they offer the possibility of realising passive, continuously tuneable devices, such as phase shifters, tuneable filters, polarisers or matching networks. LC can be oriented continuously between the two extreme states (parallel or perpendicular to an applied RF field), either by applying a magneto-static or an electro-static field. Depending on the orientation of the LC, its permittivity and dielectric loss changes. This work presents the recent progress of our research in the topic of hollow waveguide based LC phase shifters for application in phased array antennas. This kind of phase shifter is suitable for high performance applications due to its high figure of merit (FoM), defined by the ratio of the maximum differential phase shift over the highest insertion loss in all tuning states. Full wave simulation results as well as measurement results of realised phase shifters will be shown and a perspective of a phased array antenna for satellite communication will be given.

Topical Talk DF 17.5 Thu 16:30 EB 407

Low loss flexible and stretchable dielectrics for microwave applications — •Mailadil Sebastian — Department of Electrical Engineering, University of Oulu, 90014 Oulu

Flexible, bendable and stretchable dielectrics which can cover even curved surfaces are important for applications in electronic control systems, consumer electronics, heart pacemakers, body worn antenna etc. The requirements for a material to be used as a flexible dielectric waveguide are mechanical flexibility, high relative permittivity, low dielectric loss, high thermal conductivity, low coefficient of thermal expansion (CTE) etc. It is very difficult to identify a single material which possesses all these properties simultaneously. There are a number of ceramic materials with high relative permittivity and low dielectric loss but are brittle in nature. Butyl and silicone rubbers have low loss with good mechanical flexibility and stretchability but they have low relative permittivity and high CTE. Therefore, the practical applications of a rubber or a ceramic alone is limited. By integrating the flexibility, stretchability and low processing temperature of a rubber with high relative permittivity and low loss of ceramics, a composite may be formed, which can deliver improved performances. In this talk the effect of addition of several ceramics such as SiO_2, Al_2O_3, TiO_2, $Ba(Mg_{1/3},Ta_{2/3})O_3$, $Ba(Zn_{1/3},Ta_{2/3})O_3$, $BaTiO_3$, $Ba_{0.7}Sr_{0.3}TiO_3$, $SrTiO_3$, AlN, $Sr_2Ce_2Ti_5O_{15}$ in butyl and silicone rubbers on the microwave dielectric properties, thermal conductivity, thermal expansion, moisture absorption, mechanical properties etc will be discussed.

DF 18: Glasses and Glass Transition I (DY with DF/CPP)

Time: Thursday 15:00–17:30 Location: BH-N 128

DF 18.1 Thu 15:00 BH-N 128

Binary colloidal mixtures investigated by differential dynamic microscopy — •Tatjana Sentjabrskaja, Marco Laurati, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine University, D-40225 Duesseldorf, Germany

We investigate dynamics of colloids in binary mixtures of hard spheres with large size asymmetry, using confocal differential dynamic microscopy (con-DDM). This technique allows to study wave vector dependent dynamics of particles by analysing time series of confocal microscopy images. Analysis of the Fourier spectra of image differences acquired at different delay times allows to determine the time-dependent density-density correlation functions and, from its shape and decay time, the nature and characteristic times of particles' dynamics. To benchmark con-DDM, we investigate one-component systems of colloidal particles at different volume fractions. Diffusion coefficients of particles as a function of volume fraction obtained from con-DDM measurements are found to be in good agreement with those obtained using dynamic light scattering experiments. We additionally show that con-DDM can be used to separately study the dynamics of single species in multicomponent systems using fluorescent labeling. In particular, we are able to determine the dynamics of sub-resolution tracer particles in binary colloidal mixtures with large size asymmetry, as a function of increasing volume fraction of the large particles. The motion of the tracer, small particles becomes increasingly constrained by the dense matrix of large spheres, resulting in complex, non-diffusive motion of the tracers.

DF 18.2 Thu 15:15 BH-N 128

Critical-like behaviour in non-crystalline solids caused by angular correlations — •Mariya Rasshchupkyna[1,2,3], Volodymyr Bugaev[3,4], Johannes Roth[5], Gerhard Grübel[6,1], and Peter Wochner[3,4] — [1]The Hamburg Centre for Ultrafast Imaging (CUI) — [2]University of Hamburg — [3]Max Planck Institute for Intelligent Systems, Stuttgart — [4]Max Planck Institute for Solid State Research, Stuttgart — [5]Institute for Functional Materials and Quantum Technologies, University of Stuttgart — [6]DESY

Modern experimental techniques on the basis of coherent scattering data, such as X-ray cross-correlation analysis (XCCA) [1] allow the direct determination of angular correlations (and their modes) in molecular disordered systems. We performed molecular dynamics (MD) simulations for model systems with Dzugutov-type [2] interaction adjusted for the creation of glassy-type quasi-equilibrium states. XCCA applied to the simulated coherent scattering patterns of the MD samples reveals a four-point dodecagonal dominant mode responsible for the formation of non-commensurate structures, as found in glasses and quasicrystals. Strikingly, this mode exhibits a pronounced temperature-dependence indicating a critical-type behavior in the vicinity of the glassy-type transition.

References

1. P. Wochner, C. Gutt, T. Autenrieth, T. Demmer, V.N. Bugaev, A. D. Ortiz, A. Duri, F. Zontone, G. Grübel, H. Dosch, Proc. Natl. Acad. Sci. USA 106, 11511 (2009).

2. M. Dzugutov, Phys. Rev. Lett. 70, 2924 (1993).

DF 18.3 Thu 15:30 BH-N 128

Nonaffine deformations, glass transition, and yielding in disordered solids — •Alessio Zaccone — Physics-Department, Technische Universität München

A new approach to the glass transition has been recently developed from the angle of nonaffine elasticity. Due to structural disorder, the

particle motions in glasses under shear do not merely follow the imposed affine pathways prescribed by the strain tensor of standard continuum linear elasticity, but deviate significantly to undergo additional nonaffine displacements. Importantly, these nearest-neighbour forces would exactly cancel out mutually in any ordered lattice with local center-inversion symmetry. The concept of nonaffine free energy of deformation can be applied to molecular and atomic glasses. The resulting scheme has been implemented to predict the T-dependence of the shear modulus of polymer glasses and its vanishing at the glass transition. The main effect leading to vanishing of rigidity can be identified with the decrease of the average effective intermolecular connectivity as the material expands upon increasing T. In turn, this makes the negative nonaffine contribution to free energy become increasingly more important as T rises, until the free energy of deformation vanishes at a critical temperature for mechanical instability, which is very close to the calorimetric glass transition. Besides nonaffinity, an important role is played by anharmonic interactions which control the thermal expansion coefficient of the glass, which in turn controls how connectivity decreases with increasing T.

DF 18.4 Thu 15:45 BH-N 128

The Potential Energy Landscape of microrheologically driven supercooled liquids — •Carsten F. E. Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]NRW Graduate School of Chemistry, Münster, Germany

We perform computer simulations of a fragile model glass-former in which a single particle is driven by an external force through the liquid. Thereby, we track the path the system takes through its underlying Potential Energy Landscape (PEL) and aim for understanding how this is altered by the external field[1,2] and how the altering is related to the nonlinear responses of dynamic quantities.

In the PEL approach, the dynamics of undriven (strong *and* fragile) glass formers have found to be very well described in terms of an improved trap model, the Gaussian Glass Former (GGF)[3]. In this talk we want to demonstrate, how the GGF can be extended to driven supercooled liquids. This enables one to predict typical nonlinear responses like the nonlinear decay of the local friction coefficient as well as highly nontrivial effects like the occurrence of effective temperatures. Within this framework we can quantitatively predict the numerically observed effective temperatures in terms of the kinetics of the force-dependent hopping processes in the PEL. This establishes an intimate relation between the thermodynamics and the kinetics also in the highly non-equilibrium regime.

[1] C. F. E. Schroer, A. Heuer, *J. Chem, Phys* **138**, 12A518 (2013)
[2] C. F. E. Schroer, A. Heuer, *Phys. Rev. Lett* **110**, 067801 (2013)
[3] A. Heuer, *J. Phys.: Condens. Matter* **20**, 373101 (2008)

DF 18.5 Thu 16:00 BH-N 128

Physical mechanisms of nonlinear conductivity: A model analysis — •Andreas Heuer and Lars Lühning — Institute for Physical Chemistry, University of Münster, Germany

Nonlinear effects are omnipresent in thin films of ion conducting materials showing up as a significant increase of the conductivity upon increasing electric field. For a disordered hopping model general physical mechanisms are identified giving rise to the occurrence of positive or negative nonlinear effects, respectively. Analytical results are obtained in the limit of high but finite dimensions [1]. They are compared with the numerical results for 3D up to 6D systems. A very good agreement can be found. The results can also be used to rationalize previous numerical simulations. The implications for the interpretation of nonlinear conductivity experiments on inorganic ion conductors are discussed.

[1] A. Heuer, L. Lühning, J. Chem. Phys. 140, 094508 (2014).

15 min. break

DF 18.6 Thu 16:30 BH-N 128

Where to go in a rough free-energy landscape? — •Stefan Schnabel and Wolfhard Janke — Universität Leipzig

Frustrated spin systems like the Edwards-Anderson spin glass are notorious for disorder-induced frustration. Sampling their rough free-energy landscape is very challenging and only small systems can be investigated. Over the years great efforts have been made to improve both hardware and implementation, yet the basic method for the investigation of 3d spin glasses is and has been parallel tempering [1]. Here, we explore the possibility of using additional information obtained by a local minimization procedure similar to the basin-hopping algorithm [2]. Altering the statistical weight of conformations according to the depth of nearby local minima can reduce autocorrelation time. We investigate whether this improvement outweighs the additional computational cost.

[1] K. Hukushima and K. Nemoto, J. Phys. Soc. Japan 65 (1996) 1604. [2] D. J. Wales, J. Phys. Chem. A 101 (1997) 5111.

DF 18.7 Thu 16:45 BH-N 128

Evidence for a Novel Relaxation Mechanism in Glasses at Very Low Temperatures — •Marius Hempel, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The acoustic and dielectric properties of amorphous solids at low temperatures are governed by two level tunneling systems and can be described in similar ways. One difference is however, that electric fields couple only to tunneling systems carrying an electric dipole moment, whereas acoustic measurements couple to all tunneling systems. Thus, the two methods complement each other and can therefore lead to a better understanding of the underlying processes.

Low frequency measurements of the dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively, have recently shown unexpected behavior, which cannot be understood in terms of the so called standard tunneling model. This behavior has been attributed to the very large nuclear electric quadrupole moments of ^{181}Ta and ^{165}Ho.

We present the first measurements of the acoustic properties of N-KZFS11 and HY-1 in the kHz range down to 10 mK. The results of these measurements underpin the observations seen in dielectric experiments and provide further evidence for a novel relaxation mechanism in such glasses.

DF 18.8 Thu 17:00 BH-N 128

Non-Universal Dielectric Properties of Glasses at Very Low Temperatures — •Annina Luck, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems and described by the standard tunneling model, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause specific material-dependent effects in magnetic fields.

We show measurements of dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively. As ^{181}Ta and ^{165}Ho both carry very large nuclear electric quadrupole moments, these glasses are ideal candidates to determine the influence of these moments on the physical properties of glasses down to very low temperatures.

Our measurements not only show unique dielectric behaviour in both glasses, but also differ significantly from various predictions of the standard tunneling model.

DF 18.9 Thu 17:15 BH-N 128

Thermography on Luminescent Barium Borate Glass for White-LED Applications — •Florian Wagner[1], Peter Nolte[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Mechanics of Materials IWM, Lübecker Ring 2, 59494 Soest

White light-emitting diodes (W-LEDs) represent one of the most promising lighting technologies for the future. Primarily used in many lighting applications is a blue LED combined with a yellow phosphor. The phosphor powder is usually embedded in an organic polymer and coated onto the LED chip. Heat-induced degradation of the organic encapsulate, however, results in an efficiency decrease and color temperature change. Luminescent glasses or glass ceramics are an interesting alternative due to their higher thermal and chemical stability. This work focuses on the thermal behaviour of luminescent barium borate glasses under intense excitation with ultraviolet/blue light. The glasses are doped with rare-earth ions for optical activation. Upon absorbing the ultaviolet/blue light, the rare-earth ions show their typical emission in the visible spectral range. Here, not all of the absorbed light is frequency-downshifted, but a significant part is released in the form of heat. Contact-free infrared thermography enables an analysis

of the heat development in these materials. An algorithm based on the partial differential heat equation is developed to calculate the heat source density of the optical excitation from the surface temperature distribution.

DF 19: Glasses and Glass Transition II (CPP with DF/DY)

Time: Friday 9:30–11:15 Location: C 243

DF 19.1 Fri 9:30 C 243

Stable glasses from strong liquids — •Yeong Zen Chua[1], Mathias Ahrenberg[1], Michael Tylinski[2], Mark D. Ediger[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706 USA

To date, only several materials have been observed to form ultra-stable glasses by vapor deposition. Some authors have suggested that fragility might be a controlling factor in the ability to form stable glasses by vapor deposition, with highly stable glasses only being possible for highly fragile liquids. Glasses of ethylcyclohexane, fragility index 56.5, and 1-pentene, a very small molecule, produced by physical vapor deposition have been characterized by in situ AC chip nanocalorimetry. Since the fragility index of 1-pentene was not available, it was determined as 52 from the calorimetric glass transition temperatures measured in the frequency range from 0.2 Hz to 4 kHz. Ethylcyclohexane and 1-pentene are both strong glass formers, for which possibility of stable glass formation has been questioned. On the contrary, we observed formation of highly stable glasses of ethylcyclohexane and 1-pentene. The results on ethylcyclohexane and 1-pentene will be presented and compared with literature data of other known glass formers.

DF 19.2 Fri 9:45 C 243

Broadband dielectric spectroscopy of ionic liquids — •Pit Sippel[1], Michael Aumüller[1], Stephan Krohns[1,2], Peter Lunkenheimer[1], and Alois Loidl[1,2] — [1]Experimental Physics V, University of Augsburg, Germany — [2]Institute for Materials Resource Management, University of Augsburg, Germany

Due to their high potential for applications, e.g., in energy-storage devices such as supercapacitors or batteries, during recent years ionic liquids have come into the focus of research [1]. Ionic liquids are composed of organic cations and weakly coordinating anions. An essential method for the study of ionic transport is dielectric spectroscopy. Our results on a large variety of ionic liquids cover a broad frequency and temperature range. This allows obtaining valuable information on phenomena like dc charge transport, the glass transition, electrode polarization, and relaxation. We analyze the dielectric spectra using an equivalent-circuit approach [2]. Amongst others, this enables the deduction of the relaxation times of the involved dynamic processes. We conclude that the main reorientational relaxation process of these ionic liquids, the α relaxation, is closely linked to the dc-conductivity. This provides insight into the underlying conductivity mechanisms and, thus, the mobility of the ionic charge carriers. Moreover, a number of secondary relaxation processes is found, including hints at the presence of a Johari-Goldstein relaxation process [3].
[1] M. Armand *et al.*, Nat. Mat. **8**, 621 (2009). [2] S. Emmert *et al.*, Eur. Phy. J. B **83**, 157 (2011). [3] G.P. Johari and M. Goldstein, J. Chem. Phys. **53**, 2372 (1970).

DF 19.3 Fri 10:00 C 243

Dielectric spectroscopy on glycerol and water confined in metal-organic frameworks — •Jonas Fischer[1], Pit Sippel[1], Peter Lunkenheimer[1], Dmytro Denysenko[2], Dirk Volkmer[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg, Germany — [2]Chair of Solid State and Material Chemistry, University of Augsburg, Germany

Approaching the glass transition, the slowing down of molecular dynamics generally proceeds much stronger than expected for thermally activated motions. This can be ascribed to a temperature-dependent activation energy arising from the cooperative motion of increasing numbers of molecules at low temperatures [1]. The number of correlated molecules can be controlled by confining the glass-forming liquid in small pores. Previously, glass formers have been confined in porous glasses, zeolites and other silicates [2]. Recently, metal-organic frameworks (MOFs) have become available. This class of porous coordination polymers consists of metal-containing units and organic linkers. MOFs are tunable in many regards [3], thus allowing confinement in pores of different inner surfaces and varying sizes. Here, we present broadband dielectric spectroscopy data of glycerol and water confined in different MOFs, of the MFU-type [4]. It is shown that MOFs are well-suited for the measurement of confined liquids.
[1] T. Bauer *et al.*, Phys. Rev. Lett. **111**, 225702 (2013).
[2] A. Huwe *et al.*, Phys. Rev. Lett. **82**, 2338-2341 (1999).
[3] H. Furukawa *et al.*, Science **341**, 1230444 (2013).
[4] D. Denysenko *et al.*, Chem Commun. **48**, 1236 (2012).

DF 19.4 Fri 10:15 C 243

Dynamics of the glass transition in confined glycerol under hard and soft confinement, investigated by ^{2}H NMR — •Michael Lannert, Matthias Sattig, Thomas Blochowicz, and Michael Vogel — Hochschulstraße 6-8, 64289 Darmstadt, Germany

^{2}H NMR allows us to access correlation times of molecular rotational dynamics, ranging from τ=10^{-12}s to τ=10^{-1}s, by using longitudinal relaxation, solid echo, and stimulated echo sequences. Findings for confined glycerol, which is subjected to spherical soft confinement (using AOT/toluene micro-emulsions) and cylindrical hard confinement (using microporous silica, namely MCM-41) are compared, and a shift in correlation times to shorter times is observed for the hard confinement, but not for the soft confinement. Various diameters (2nm to 9nm) were used in order to gain a comprehensive understanding of the finite size effect. Investigation of the dynamics of the glycerol in the supercooled regime proved to be a challenging enterprise in soft confinement, because of the onset of rotational diffusion of the whole microemulsion droplet, which exceeds the contribution of molecular rotational dynamics. Therefore droplet size-dependence and viscosity-dependence of the dynamics where investigated additionally, in order to evaluate the impact of these results.

DF 19.5 Fri 10:30 C 243

Structure and Dynamics of Asymmetric Poly(styrene-*b*-1,4-isoprene) Diblock Copolymer under 1D and 2D Nanoconfinement — •Wycliffe K. Kipnusu[1], Mahdy M. Elmahdy[1], Emmanuel U. Mapesa[1], Jiangi Zhang[2], Detlef-M. Smilgies[3], Christine M. Papadakis[4], and Friedrich Kremer[1] — [1]Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — [2]National Center for Nanoscience and Technology (NCNST), No.11 ZhongGuanCun BeiYiTiao, 100190 Beijing, P.R. China. — [3]Cornell High Energy Synchrotron Source (CHESS), Wilson Laboratory, Cornell University, Ithaca, NY 14853, USA — [4]Technische Universität Müunchen, Physik-Department, Physik weicher Materie, James-Franck-Straße 1, 85748 Garching, Germany.

The impact of 1-and 2-dimensional (2D) confinement on the structure and dynamics of poly(styrene-b-1,4–isoprene) P(S-b-I) diblock copolymer is investigated by a combination of Grazing–Incidence Small–Angle X–ray Scattering (GISAXS), Atomic Force Microscopy (AFM) and Broadband Dielectric Spectroscopy (BDS). 1D confinement is achieved by spin coating the P(S-b-I) to form nanometric thin films on silicon substrates, while in the 2D confinement, the copolymer is infiltrated into cylindrical anodized aluminum oxide (AAO) nanopores. GISAXS and AFM reveal hexagonally packed cylinders of PS in a PI matrix.The dynamic glass transition of the styrene and isoprene blocks is independent of the dimensionality and the finite sizes (down to 18 nm) of confinement but the normal mode is influenced by both factors with 2D geometrical constraints exerting greater impact.

DF 19.6 Fri 10:45 C 243

High frequency laser heated AC-chip calorimeter for dynamic glass transition investigation in room temperature ionic liquids — •Evgeni Shoifet[1,2,3,4], Heiko Huth[1], Sergey Verevkin[2,4], Christoph Schick[1,4], and Egon Hassel[3] — [1]Institute of Physics, University of Rostock, 18057 Rostock, Germany — [2]Institute of Physical Chemistry, University of Rostock, 18059 Ros-

tock, Germany — [3]Department of Technical Thermodynamics, Faculty of Mechanical Engineering and Marine Technology, Rostock, 18051 Rostock, Germany — [4]Faculty of Interdisciplinary Research, Department "Life, Light and Matter", University of Rostock, Germany

Many ionic liquids are good glass formers. Nevertheless, for the relaxation behavior only a few studies of the dynamic glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition (α-relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. In addition, dielectric spectroscopy is equally sensitive to the segmental relaxation (α-relaxation) and secondary relaxation but calorimetry is sensitive solely to segmental relaxation.

We try to use calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs. Particularly the influence of alkyl chain length on the α-relaxation in the frequency range from 1 mHz to 0.1 MHz [Shoifet. E. et. al. (2013)].

DF 19.7 Fri 11:00 C 243

Dynamic glass transition measurements on nm-thin films of Indomethacin using AC chip-nanocalorimetry — •Mathias Ahrenberg, Christoph Schick, and Gunnar Schulz — Institut für Physik, Universität Rostock

We are using AC chip nano-calorimetry for the in-situ investigation of the dynamic glass transition of vapor-deposited thin films of toluene and indomethacin of thicknesses between several hundred nm down to ten nm. With these experiments on low molecular mass substances we complement our data on similar thin polymer films. Firstly, the deposition-related thermodynamic state (stable glass) of each film is erased by transforming them into ordinary glasses. Secondly, upon reheating the thin ordinary glass films a direct comparison of the subsequently measured frequency-dependent dynamic glass transition temperatures becomes possible. The frequency of temperature modulation can be varied from 1 Hz up to about 1000 Hz. Film thicknesses for indomethacin are measured ex-situ with an atomic force microscope directly on the membrane of the chip-sensors. Similar to the thin polymer films no thickness dependence of the dynamic glass transition temperature (main relaxation) is seen. The results are in agreement with the explanation given by Cangialosi et al.