Crystallography Division
Fachgruppe Kristallographie (KR)

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Overview of Invited Talks and Sessions

(lecture rooms: H 0105, EB 107, EB 407; Posters: C)

Invited talks of the joint symposium SYDW (DF, DS, KR, MA, MI, TT)

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 of the joint sessions "Multiferroics II" and "Ceramics and Applications"

See DF for the full program.

DF 14.1	Wed	15:00–15:30	EB 107	**Low energy consumption spintronics using multiferroic heterostructures** — •Morgan Trassin
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

Sessions

KR 1.1–1.5	Mon	9:30–12:30	H 0105	**Symposium on Ferroic Domain walls (SYDW)**
KR 2.1–2.6	Mon	19:00–21:00	Poster C	**Poster Crystallography**
KR 3.1–3.30	Mon	19:00–21:00	Poster C	**Poster Session on Ferroic Domain Walls - Multiferroics (DF jointly with KR, MA, TT)**
KR 4.1–4.13	Wed	9:30–13:00	EB 107	**Multiferroics I (DF jointly with DS, KR, MA, TT)**
KR 5.1–5.13	Wed	15:00–18:50	EB 107	**Multiferroics II (DF jointly with DS, KR, MA,TT)**
KR 6.1–6.4	Wed	11:20–13:00	EB 407	**Ceramics and Applications (DF jointly with KR)**
KR 7.1–7.8	Wed	15:00–17:40	EB 407	**Optical and Nonlinear Optical Properties II (DF jointly with KR)**

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

Mittwoch 19:00–20:00 EB 107

- Bericht
- Verschiedenes

KR 1: Symposium on Ferroic Domain walls (SYDW)

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

Invited Talk KR 1.1 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 KR 1.2 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 KR 1.3 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 KR 1.4 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 KR 1.5 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)

KR 2: Poster Crystallography

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

KR 2.1 Mon 19:00 Poster C

Magnetic properties of high quality single crystals of the electron underdoped cuprate superconductor $Nd_{2-x}Ce_xCuO_4$ — •Alma Dorantes, Cai Qi, Mark Kartsovnik, and Andreas Erb — Walther-Meißner Institut, Walther-Meißnerstraße 8 D-85748 Garching

We present investigations of the magnetic properties of the electron-doped cuprate superconductor $Nd_{2-x}Ce_xCuO_4$ (NCCO) with particular attention to the underdoped regime of the phase diagram. Special attention is given to the region between the antiferromagnetic (AF) and superconducting (SC) state of the electron-doped cuprate superconductors. We tried to investigate whether the AF and SC regions are separated by an intrinsic phase separation or if a microscopic coexistence exists between these two states. Experiments on high quality single crystals were performed to probe the relation between the transition temperature (T_c) and dopant concentration x, and to estimate the superconducting volume fraction. The results indicated that a SC transition can be observed after an appropriate annealing process, even for highly underdoped samples and that bulk superconductivity is present. In addition we find indications of a deviation in the monotonic doping dependence of the transition temperature T_c between samples with 12% and 13% Ce doping, which could signify a first evidence of the so-called 1/8 anomaly in the electron-doped cuprate superconductors.

KR 2.2 Mon 19:00 Poster C

Towards neutron scattering experiments with microsecond time resolution — •Franz Alois Adlmann[1], Philipp Gutfreund[2], John Ankner[3], Jim Browning[3], Andre Parizzi[3], Bogdan Vacaliuc[3], Candice Halbert[3], Jason Rich[3], Andrew Dennison[2], and Max Wolff[1] — [1]Uppsala University, Box 516, 751 20, Uppsala, Sweden — [2]Institut Laue Langevin, BP 156, 38042, Grenoble, France — [3]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Due to the interaction with the nucleus, neutrons offer unique opportunities for the study of condensed matter. However, the neutron flux on nowadays source is relatively low. To overcome this limitation we have developed a new technique for periodic excitations. Our approach takes full advantage of data storage in list mode combined with the time dependent information on the excitation as meta-data in the event-stream of the neutron data. Re-binning of the neutron data with respect to the periodic excitation is done in the post processing. This has the advantage that the time slices and resolution can be defined after the experiment is completed. We applied our approach in a combined neutron reflectivity and rheology study to probe the solid-liquid interface of a micellar system. LAOS (Large Amplitude Oscillatory Shear) was applied to highlight the complex rheological behavior. We extract the intensity of a Bragg reflection with a time resolution of less than one millisecond and show that it follows the oscillatory shear.

KR 2.3 Mon 19:00 Poster C

Application of polychromatic X-ray Laue diffraction for the analysis of dislocation structures using a PNCCD — •Ali Abboud[1], Sebastian Send[1], Ullrich Pietsch[1], Christoph Kirchlechner[2], Lothar Strüder[4], Jean Sebastian Micha[5], and Jozef Keckes[3] — [1]Department of Physics, University of Siegen, Siegen, 57072, Germany — [2]Max Planck Institut für Eisenforschung GmbH, Max-Planck-Str.1, 40237 Düsseldorf, Germany — [3]Montanuniversität Leoben, Leoben, 8700, Austria — [4]PNSensor GmbH, Munich, 80803, Germany — [5]CEA-Grenoble/DRFMC/SprAM, 17 rue des Martyrs, Grenoble Cedex 9, F-38054, France

uLaue diffraction with a polychromatic X-ray beam can be used to measure strain fields and crystal orientations of micro crystals. In the vicinity of a Bragg reflection the intensity distribution of the reciprocal space is sensitive to the distribution and type of dislocations. By using a pnCCD, the energy and the 2D intensity distribution of the Bragg reflections can be measure simultaneously. This allows to obtain the hydrostatic strain and the deviatoric strain tensors. We present an application of white beam uLaue X-ray diffraction on a bent Copper crystal to measure local strain along the bending beam by using a PNCCD detector.

KR 2.4 Mon 19:00 Poster C

Structural Information Beyond the Ensemble Average From Colloidal Crystals Using X-Ray Cross-Correlation Analysis — •Matthias Kampmann[1,2], Michael Sprung[1], Bill Pedrini[3], Tushar Sant[2], Falko Ziegert[4], and Christian Gutt[2] — [1]DESY, Hamburg, Germany — [2]Universität Siegen, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]Universität Rostock, Germany

Fluctuations in X-ray scattering intensity from particle ensembles carry structural information beyond the pure ensemble average, which can be mined using X-ray cross correlation analysis (XCCA). Kam was the first to propose applying higher order intensity correlation functions to solution scattering data of macromolecules for obtaining structural information [Kam1]. His ideas were far beyond the power of X-ray sources and detectors in the 1970s. But they gained new interest with the ultrafast snapshot capabilities of X-ray free-electron laser sources, not only for solving particle structures but also in a more statistical context for densely packed systems [Wochner].

Here we present an XCCA analysis of diluted suspensions of small micrometer sized colloidal crystals. In a coherent X-ray scattering experiment we have measured several thousand diffraction patterns of colloidal sample systems and calculated the corresponding higher order correlation functions. The data reveal strong angular modulations of the XCCA signal, which are a fingerprint of the single particle diffraction properties.

Kam1: Z. Kam, Macromolecules 10, 927-934 (1977)
Wochner: P. Wochner et al., PNAS 106, 11511-11514 (2009)

KR 2.5 Mon 19:00 Poster C

Kinetics of the hydrogen defect in lithium niobate and lithium tantalate — •Thomas Köhler, Erik Mehner, Juliane Hanzig, Günter Gärtner, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, 09596 Freiberg, Germany

$LiNbO_3$ and $LiTaO_3$ crystals are used in many optical devices, therefore, understanding the structural defects is helpful to control optical and electrical properties. The incorporation of hydrogen in the two materials is investigated by FT-IR and UV/VIS spectroscopy using different crystallographic orientations and excitation polarisations. The aim of the study is the development of a structural model for the kinetic and the diffusion of the OH defect. The examined congruent crystals are cube shaped, cut and polished along the $[2\bar{1}\bar{1}0]$, $[01\bar{1}0]$ and [0001] directions. The used stoichiometric crystals are plates, polished and cut in [0001]. Depending on the stoichiometry the hydrogen defect causes an OH band with several sub-bands, at different spectral positions. In congruent material two sub-bands are detectable, whereas near stoichiometric material exhibits four. The composition of the OH band with respect to formation or decline of sub-bands under oxidizing and reducing conditions shows the transport mechanisms within the crystals. The protonation in hot water shows a formation of new sub-bands at higher energies. We have found three and six sub-bands in congruent and near stoichiometric crystals, respectively. The results show that the hydrogen is disordered and can migrate to different binding sites within the crystal.

KR 2.6 Mon 19:00 Poster C

Impact of temperature and barometric pressure fluctuations on X-ray beam intensities — •Tina Weigel[1], Matthias Zschornak[1], Marco Herrmann[2], Manuel Rothenberger[1], Tilmann Leisegang[2], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany — [2]Saxray GmbH, Maria-Reiche-Str. 1, 01109 Dresden, Germany

Essential to X-ray analysis in crystallography, such as diffractometry and spectrometry, is a stable and reproducible X-ray beam intensity. Particularly, changes in environmental conditions, such as temperature, humidity and barometric pressure, and cooling water fluctuations can affect the beam intensity significantly. In this comprehensive qualitative as well as quantitative study, the impact of the environmental conditions and cooling water fluctuations on the primary beam intensity of a sealed tube with Cu anode are determined. This should be of wide interest for all who are dealing with X-ray analyzes, in particular in the field of crystallography, where accurate experimental data are

a prerequisite for deriving high-quality structure parameters. With a common set-up, the X-ray intensities are detected by a scintillation counter. Laboratory as well as external conditions are monitored simultaneously. Their individual influence on the X-ray intensity and their correlations are evaluated by statistical analysis including time lag. The study shows significant correlations in respect to ambient conditions and in particular with daily and weekly cycles, which affect the intensity nearly instantaneous.

KR 3: Poster Session on Ferroic Domain Walls - Multiferroics (DF jointly 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

KR 3.1 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.

KR 3.2 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.

KR 3.3 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.

KR 3.4 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.

KR 3.5 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.

KR 3.6 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)

KR 3.7 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).

KR 3.8 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.

KR 3.9 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.

KR 3.10 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.

KR 3.11 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.

KR 3.12 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 measure-

ment 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.

KR 3.13 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.

KR 3.14 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.

KR 3.15 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.

KR 3.16 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.

KR 3.17 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).

KR 3.18 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 interference 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.

KR 3.19 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).

KR 3.20 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.

KR 3.21 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.

KR 3.22 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.

KR 3.23 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.

KR 3.24 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).

KR 3.25 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.

KR 3.26 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.

KR 3.27 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.

KR 3.28 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.

KR 3.29 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.

KR 3.30 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).

KR 4: Multiferroics I (DF jointly with DS, KR, MA, TT)

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

KR 4.1 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.

KR 4.2 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.

KR 4.3 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.

KR 4.4 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

KR 4.5 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.

KR 4.6 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)

KR 4.7 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

KR 4.8 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.

KR 4.9 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.

KR 4.10 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.

KR 4.11 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.

KR 4.12 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)

KR 4.13 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.

KR 5: Multiferroics II (DF jointly with DS, KR, MA,TT)

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

Invited Talk KR 5.1 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.

KR 5.2 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)

KR 5.3 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

KR 5.4 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)

KR 5.5 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).

KR 5.6 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).

KR 5.7 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

KR 5.8 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.

KR 5.9 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 magnetically 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.

KR 5.10 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.

KR 5.11 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.

KR 5.12 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.

KR 5.13 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).

KR 6: Ceramics and Applications (DF jointly with KR)

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

Invited Talk KR 6.1 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|$SrTiO_3$-δ|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.

KR 6.2 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 University, 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.

KR 6.3 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 $Pb(Mg_{1/3}Nb_{2/3})O_3$- x$PbTiO_3$ 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 KR 6.4 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 σ(t) as well as the resulting surface potential V0(t) due to internal currents j(x,t), charges ρ(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)

KR 7: Optical and Nonlinear Optical Properties II (DF jointly with KR)

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

KR 7.1 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.

KR 7.2 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)

KR 7.3 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.

KR 7.4 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)

KR 7.5 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)

KR 7.6 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.

KR 7.7 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

KR 7.8 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 photorefraction. 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.