Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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Overview of Invited Talks and Sessions

(Lecture rooms WIL B321 and GER 37; Poster P1C)

Invited Talks

DF 3.1	Mon	9:30–10:00	WIL B321	**Controlling core-shell formation in BNT-ST** — •Till Frömling, Azatuhi Ayrikyan, Matias Acosta, Leopoldo Molina-Luna, Michael Dürrschnabel, Hans-Joachim Kleebe, Herbert Hutter, Kyle Webber
DF 3.2	Mon	10:00–10:30	WIL B321	**Determining fundamental properties from diffraction: Electric field induced strain and piezoelectric coefficient** — •Manuel Hinterstein, Markus Hoelzel, Andrew Studer, Michael J. Hoffmann
DF 3.7	Mon	12:30–13:00	WIL B321	**Ferroic glasses: polar nanoregions in relaxor PMN vs. magnetic nanoparticles in a discontinuous multilayer** — •Wolfgang Kleemann
DF 7.1	Tue	9:30–10:00	GER 37	**Synthesis of large-area single-crystal diamond by heteroepitaxy for application as dielectric window material** — •Matthias Schreck, Stefan Gsell, Martin Fischer
DF 7.3	Tue	10:20–10:50	GER 37	**Design, materials composition and manufacturing of components for advanced modular gyrotron prototypes** — •Sebastian Ruess, Gaetano Aiello, Gerd Gantenbein, Tomasz Rzesnicki, Theo Scherer, Dirk Strauss, Manfred Thumm, Jörg Weggen, John Jelonnek
DF 7.4	Tue	11:10–11:40	GER 37	**Dielectric diamond window for the ITER EC H&CD Upper Launcher: design, analysis and qualification** — •Gaetano Aiello, Mario Gagliardi, Giovanni Grossetti, Francesco Mazzocchi, Andreas Meier, Gabriella Saibene, Sabine Schreck, Peter Spaeh, Dirk Strauss, Alessandro Vaccaro, Theo Scherer
DF 8.1	Tue	9:30–10:00	WIL B321	**Room temperature skyrmions and robust metastable skyrmion states in $Co_8Zn_8Mn_4$** — •Jonathan White, Kosuke Karube, Nicole Reynolds, Jorge Gavilano, Hiroshi Oike, Akiko Kikkawa, Fumitaka Kagawa, Yusuke Tokunaga, Henrik Ronnow, Yoshinori Tokura, Yasujiro Taguchi
DF 10.1	Wed	9:30–10:00	GER 37	**Mobile electronic excitations studied by ultrafast spectroscopy** — •Stefan Lochbrunner, Franziska Fennel, Steffen Wolter, Tim Völzer
DF 10.3	Wed	10:20–10:50	GER 37	**Time-resolved characterization of photoactive materials using terahertz spectroscopy** — •Rainer Eichberger
DF 10.4	Wed	11:10–11:40	GER 37	**Theoretical simulations of pump-probe spectroscopies in solids** — •Michael Sentef
DF 10.6	Wed	12:00–12:30	GER 37	**Accessing micro- and mesoscopic ultrafast electron dynamics in low-dimensional materials** — Michele Puppin, Christopher Nicholson, Melanie Müller, Roman Bertoni, Hannes Hübener, Angel Rubio, Claude Monney, Cephise Cacho, Martin Wolf, Alexander Paarmann, Laurenz Rettig, •Ralph Ernstorfer
DF 11.1	Wed	9:30–10:00	WIL B321	**Implications of domain evolution during the growth of ferroelectric superlattices** — Rui Liu, Benjamin Bein, Hsiang-Chun Hsing, Anna Gura, Mohammed Humed Yusuf, Giulia Bertino, Jin-Wen Lai, •Matthew Dawber

DF 11.9	Wed	12:15–12:45	WIL B321	**The electro-caloric effect in $BaTiO_3$ from first principles** — •Claude Ederer
DF 15.1	Wed	15:00–15:30	WIL B321	**Domain and fluctuation dynamics in magnetoelectric multiferroics** — •Joachim Hemberger
DF 17.1	Thu	9:30–10:00	WIL B321	**Magnetic and orbital excitations in the multiferroic skyrmion host GaV_4S_8** — Dieter Ehlers, Zhe Wang, Hans-Albrecht Krug von Nidda, Vladimir Tsurkan, Peter Lunkenheimer, Istvan Kézsmárki, Ioannis Stasinopoulos, Dirk Grundler, •Alois Loidl
DF 17.9	Thu	12:15–12:45	WIL B321	**Role of charged defects on conduction and dynamics of domain walls in $BiFeO_3$** — •Tadej Rojac, Andreja Bencan, Goran Drazic, Naonori Sakomoto, Hana Ursic, Bostian Jancar, Gasper Tavcar, Maja Makarovic, Julian Walker, Barbara Malic, Dragan Damjanovic

Tutorials

DF 1.1	Sun	16:00–16:50	HSZ 304	**Introduction to ferroic materials** — •Claude Ederer
DF 1.2	Sun	16:50–17:40	HSZ 304	**Skyrmions with ferroelectric polarization in multiferroic lacunar spinels** — •Alois Loidl
DF 1.3	Sun	17:40–18:30	HSZ 304	**Skyrmions in magnetic materials** — •Jonathan White

Invited talks of the joint symposium SYCE

See SYCE for the full program of the symposium.

SYCE 1.1	Mon	15:00–15:30	HSZ 02	**Ferroelectric domain walls: from conductors to insulators and back again** — •Petro Maksymovych
SYCE 1.2	Mon	15:30–16:00	HSZ 02	**Zoology of skyrmions and the role of magnetic anisotropy in the stability of skyrmions** — •Istvan Kezsmarki, Sandor Bordacs, Jonathan White, Vladimir Tsurkan, Alois Loidl, Peter Milde, Hiroyuki Nakamura, Andrey Leonov
SYCE 1.3	Mon	16:00–16:30	HSZ 02	**Magnetic imaging of topological phenomena in ferroic materials** — •Weida Wu
SYCE 1.4	Mon	17:00–17:30	HSZ 02	**Topological skyrmion textures in chiral magnets** — •Markus Garst
SYCE 1.5	Mon	17:30–18:00	HSZ 02	**Learning through ferroelectric domain dynamics in solidstate synapses** — Sören Boyn, Gwendal Lecerf, Stéphane Fusil, Sylvain Saïghi, Agnès Barthélémy, Julie Grollier, Vincent Garcia, •Manuel Bibes

Invited talks of the joint symposium SYNS

See SYNS for the full program of the symposium.

SYNS 1.1	Wed	15:00–15:30	HSZ 02	**The Limits to Lithography: How Electron-Beams Interact with Materials at the Smallest Length Scales** — •Karl K. Berggren
SYNS 1.2	Wed	15:30–16:00	HSZ 02	**High precision fabrication for light management at nanoscale** — •Saulius Juodkazis, Armandas Balcytis
SYNS 1.3	Wed	16:00–16:30	HSZ 02	**Directed self-assembly of performance materials** — •Paul Nealey
SYNS 1.4	Wed	16:45–17:15	HSZ 02	**Nanometer accurate topography patterning using thermal Scanning Probe Lithography** — •Armin W. Knoll
SYNS 1.5	Wed	17:15–17:45	HSZ 02	**High resolution 3D nanoimprint lithography** — •Hartmut Hillmer

Invited talks of the joint symposium SYBM

See SYBM for the full program of the symposium.

SYBM 1.1	Tue	9:30–10:00	HSZ 02	**New twists in biological photonics: circular polarisation and beyond.** — •Pete Vukusic, Luke McDonald, Ewan Finlayson
SYBM 1.2	Tue	10:00–10:30	HSZ 02	**Bio-inspired materials and structures for technology and architecture** — •Thomas Speck

SYBM 1.3	Tue	10:30–11:00	HSZ 02	**Cellulose bio-inspired hierarchical structures** — •Silvia Vignolini
SYBM 1.4	Tue	11:15–11:45	HSZ 02	**Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing** — •Vladimir Tsukuruk
SYBM 1.5	Tue	11:45–12:15	HSZ 02	**3D laser nano-printing of rationally designed materials** — •Martin Wegener

Sessions

DF 1.1–1.3	Sun	16:00–18:30	HSZ 304	**Tutorial: Ferroics and Skyrmions**
DF 2.1–2.8	Mon	9:30–12:30	GER 37	**Various Topics I**
DF 3.1–3.7	Mon	9:30–13:00	WIL B321	**Focus: Ferroics with Mesoscopic Order**
DF 4.1–4.1	Mon	14:00–14:45	HSZ 01	**PV V - Ramamoorthy Ramesh**
DF 5.1–5.5	Mon	15:00–18:00	HSZ 02	**SYCE - Novel Functionality and Topology-Driven Phenomena in Ferroics and Correlated Electron Systems (DF with MA, KR, MI, TT and DS)**
DF 6.1–6.5	Tue	9:30–12:15	HSZ 02	**SYBM - Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs (CPP with BP, MM, DF, DY und MI)**
DF 7.1–7.6	Tue	9:30–12:20	GER 37	**Focus: Microwave and THz Properties, Developments and Applications of Dielectric Materials**
DF 8.1–8.13	Tue	9:30–13:30	WIL B321	**Ferroics - Domains, Domain Walls and Skyrmions I**
DF 9.1–9.33	Tue	14:00–16:00	P1C	**Poster Session**
DF 10.1–10.6	Wed	9:30–12:30	GER 37	**Focus: Spatio-Temporal Multiscale Optical Spectroscopy Meets Functional Materials (DF with O, CPP)**
DF 11.1–11.10	Wed	9:30–13:00	WIL B321	**Ferroics - Domains, Domain Walls and Skyrmions II**
DF 12.1–12.1	Wed	13:15–13:45	HSZ 01	**PV XV - Dennis Meier**
DF 13.1–13.5	Wed	15:00–17:45	HSZ 02	**SYNS - Symposium Nanostructuring Beyond Conventional Lithography (MI with DS, DF, HL, MM and VA)**
DF 14.1–14.8	Wed	15:00–18:00	GER 37	**Various Topics II**
DF 15.1–15.8	Wed	15:00–17:30	WIL B321	**Ferroics - Domains, Domain Walls and Skyrmions III**
DF 16.1–16.6	Wed	18:00–20:00	P4	**Crystallography - Poster Session (KR with DF)**
DF 17.1–17.12	Thu	9:30–13:30	WIL B321	**Ferroics - Domains, Domain Walls and Skyrmions IV**
DF 18.1–18.8	Thu	15:00–17:15	WIL B321	**Multiferroics (DF and MA)**
DF 19.1–19.9	Fri	10:00–12:30	ZEU 118	**Glasses and Glass Transition (CPP with DF)**

Annual General Meeting of the Dielectric Solids Division

Mittwoch 18:00–19:00 GER 37

- Bericht
- Zukunft des Fachverbandes "Dielektrische Festkörper"
- Wahlen & Abstimmungen
- Verschiedenes

DF 1: Tutorial: Ferroics and Skyrmions

This tutorial combines the field of ferroics and domain engineering, their key concepts and materials with recent developments in strongly correlated systems, mainly focusing on skyrmions with polar textures. The basic concepts are introduced which intend to help non-specialists to get informed and involved in these interesting topics. This tutorial launches a 4-day focus (Plenary, Symposium, Focus Sessions and Posters) on ferroics, domain walls, multiferroics and skyrmion systems aiming at inspiring topical discussions to stimulate a vivid scientific exchange.

Organizers: Stephan Krohns, Dennis Meier, Elisabeth Soergel

Time: Sunday 16:00–18:30 Location: HSZ 304

Tutorial DF 1.1 Sun 16:00 HSZ 304

Introduction to ferroic materials — •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

In this tutorial talk I will give a general introduction to the physics of ferroic materials. I will discuss different cases such as ferro- and antiferromagnets, ferroelectrics, ferroelastics, and multiferroics. The basic phenomenology of ferroics will be introduced on the level of Landau theory, which allows to distinguish proper and improper ferroics and also to describe possible coupling between different ferroic order parameters. The important role of symmetry will be highlighted and microscopic mechanisms that drive the formation of ferroic orders will be mentioned.

Tutorial DF 1.2 Sun 16:50 HSZ 304

Skyrmions with ferroelectric polarization in multiferroic lacunar spinels — •Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

This tutorial will provide an introductory discussion of polar properties induced by topological spin order. Lacunar spinels will be taken as illuminating examples. They undergo orbital ordering and at low temperatures reveal complex magnetic phases. GaV_4S_8 and GaV_4Se_8 show ferromagnetic, cycloidal and Néel-type skyrmion lattice phases [1,2]. We provide a thorough study of the polar properties and show that the orbitally ordered phases are ferroelectric [3]. Moreover, spin-driven excess polarizations emerge in all magnetic phases. Hence, they host a zoo of multiferroic phases including the skyrmion lattice of spin vortices dressed with ferroelectric polarization [3]. The low-temperature magnetic phase diagrams document the importance of anisotropy: GaV_4S_8 is an easy axis magnet with a narrow skyrmion-lattice pocket only. In clear distinction, GaV_4Se_8 is governed by easy plane anisotropy, its skyrmion phase is drastically extended and reaches from the magnetic phase boundary down to the lowest temperatures.

[1] I. Kézsmárki *et al.*, Nature Materials **14**, 1116 (2015).
[2] S. Widmann *et al.*, Phil. Mag. (2016), in press.
[3] E. Ruff *et al.*, Science Advances **1**, E1500916 (2015).

Tutorial DF 1.3 Sun 17:40 HSZ 304

Skyrmions in magnetic materials — •Jonathan White — Paul Scherrer Institut, Switzerland

Research into magnetic Skyrmions currently attracts significant attention in topological condensed matter physics. Individual Skyrmions display a non-trivial twisted spin structure which, unlike simple ferromagnetic and antiferromagnetic spin structures, is described in terms of a finite topological index. We will introduce how this finite topology endows Skyrmions with remarkable properties, which moreover display a novel interplay with the general properties and dimensionality of the host magnet. We will also explain how the fascinating aspects of the physics of Skyrmions motivates the general expectation that topological spin structures will become pivotal components for future information technology and data storage.

DF 2: Various Topics I

Nano- and microstructured dielectrics / thin films
Optical and nonlinear optical properties, photonic
High- and low-k-dielectrics
Dielectric surfaces and interfaces

Chair: Martin Diestelhorst

Time: Monday 9:30–12:30 Location: GER 37

DF 2.1 Mon 9:30 GER 37

Octahedral tilt nanostructure in bismuth-based relaxors — •Wolfgang Donner[1], Florian Pforr[1], Marton Major[1], Uwe Stuhr[2], and Bertrand Roessli[2] — [1]Technische Universität Darmstadt, Germany — [2]Paul Scherrer Institut, Switzerland

Among the lead-free ferroelectrics, (1-x)$Na_{1/2}Bi_{1/2}TiO_3$-x $BaTiO_3$ is one of the most promising material systems. The dielectric properties around the morphotropic phase boundary at x = 0.06 are comparable to those of commonly used lead-containing ferroelectrics. However, the atomistic mechanisms leading to the relaxor properties are still unclear.

We performed a diffuse neutron scattering study in order to reveal the nanostructure of the octahedral tilt disorder of the oxygen anions. Our results show the coexistence of multiple tilt systems over a wide temperature range and a strong temperature dependence of the respective domain sizes. On this basis, we propose a model of the nanostructure featuring chemically pinned tetragonal platelets in a rhombohedral matrix. The different tilt domains are separated by a cubic intermediate phase. Furthermore, a strong temperature dependence of the planar defect density was found, which peaks at the depolarization temperature. These features react strongly to the application of an external electric field and their temperature dependence is clearly correlated with the dielectric permittivity.

DF 2.2 Mon 9:50 GER 37

Robust in-plane ferroelectricity over room temperature in atomic-thick SnTe — •Kai Chang[1,2], Junwei Liu[3,2], Haicheng Lin[2], Na Wang[2], Kun Zhao[2], Yong Zhong[2], Xiaopeng Hu[2], Wenhui Duan[2], Liang Fu[3], Qi-Kun Xue[2], Xi Chen[2], Shuai-Hua Ji[2], and Stuart Parkin[1] — [1]NISE, Max-Planck Institute of Microstructure Physics, Weinberg 2, Halle 06120, Germany — [2]State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Stable ferroelectricity with high transition temperature in nanostructures is needed for miniaturizing ferroelectric devices. Here, applying molecular beam epitaxy (MBE) and variant temperature scanning tunneling microscopy (VT-STM), we have studied the stable in-plane spontaneous polarization in atomic-thick SnTe, down to a 1-unit cell (UC) limit. The ferroelectric transition temperature T_c of 1-UC SnTe film is greatly enhanced from the bulk value of 98 K [1] and reaches as high as 270 K. Moreover, 2- to 4-UC SnTe films show robust ferroelectricity at room temperature [2]. Recent high temperature STM

experiments show that the ferroelectricity of 2- and 3-UC SnTe films persists even up to 380 K, comparable with the classical perovskite ferroelectric $BaTiO_3$. [1] M. Iizumi et al., J. Phys. Soc. Jpn. 38, 443 (1975). [2] K. Chang et al., Science, 353, 274 (2016).

DF 2.3 Mon 10:10 GER 37

Flexoelectric impact on the polarization switching dynamics in thin ferroelectric films — •Ivan Vorotiahin[1,2], Anna Morozovska[2], Eugene Eliseev[3], and Yuri Genenko[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Deutschland — [2]Institute of Physics, National Academy of Sciences of Ukraine, 46, pr. Nauky, 03028 Kyiv, Ukraine — [3]Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krjijanovskogo 3, 03142 Kyiv, Ukraine

Flexoelectric effect (or flexocoupling) is one of the properties of solid state materials that couples the gradient of electric polarization with the gradient of mechanical strain. It exists virtually in all solids, but has so small magnitude that it cannot be effectively observed in most of them. However, with the reduction of dielectric film thickness, it might obtain a significant influence on the properties of dielectrics.

A process of domainless polarization switching in the tetragonal ferroelectric $BaTiO_3$ has been modelled, using relations of Landau-Ginzburg mean-field theory. Static distributions of electric polarization and other relevant quantities, including electrostatic potential, donor and electron concentrations, as well as dynamics of polarization switching are obtained and analysed. A role of the flexocoupling is estimated for both statics and dynamics. It appeared, that whilst having a negligible influence on the static distributions, flexocoupling can remarkably affect polarization switching times and the values of critical fields under which the switching occurs.

DF 2.4 Mon 10:30 GER 37

Crystalline high-pressure phases in the Bi–Co system — •Leonore Wiehl[1], Shrikant Bhat[1], Iliya Radulov[1], Konstantin Skokov[1], Michael Dürrschnabel[1], Leopoldo Molina-Luna[1], Sabrina Sicolo[1], Leopold Diop[1], Dmitriy Karpenkov[1], Norimasa Nishiyama[2], Hans-Joachim Kleebe[1], Karsten Albe[1], Ralf Riedel[1], and Oliver Gutfleisch[1] — [1]Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, Darmstadt 64287, Germany — [2]DESY, Hamburg 22607, Germany

$RECo_5$ (RE = rare-earth) compounds are known as materials with high magnetocrystalline anisotropy [1]. They crystallize in the $CaCu_5$ structure type, space group $P\frac{6}{m}mm$. On searching for RE-free magnetic materials, which could replace the classical NdFeB magnets, MCo_5 type materials were considered as promising candidates. The existence of crystalline MCo_5 and MFe_5 (M = Bi, Ca, Zr) phases and their magnetic properties were explored. Here we report on the Bi-Co system. Samples with starting compositions 5:1 & 1:1 were subjected to high pressure (15.6 GPa) and temperature (900°C) in a multianvil press at DESY, Hamburg. The recovered products were characterized by X-ray diffraction with synchrotron radiation (ALS, Berkeley), SEM/EDX, and magnetic measurements. They proved to be a mixture of several crystalline phases, with the most prominent phase Bi_3Co [2]. The search for new phases was complemented by DFT calculations.

Financial support by the excellence program LOEWE "RESPONSE" is gratefully acknowledged. [1] K. Strnat et al., J. Appl. Phys. 38 (1967) 1001 [2] S. Tencé et al., J.Phys.: Condens. Matter 26 (2014) 395701

20 min. break

DF 2.5 Mon 11:10 GER 37

Tunability of polymeric whispering gallery mode micro-lasers — •Tobias Siegle[1], S. Schierle[1], S. Krämmer[1], A. M. Flatae[1,2], M. Remmel[1], B. Richter[3], S. Nocentini[2], C. Parmeggiani[2], H. Zeng[2], M. Burresi[2], D. Wiersma[2], S. F. Wondimu[4], P. Schuch[4], C. Koos[4], and H. Kalt[1] — [1]Institute of Applied Physics, KIT, Karlsruhe, Germany — [2]European Laboratory for Non-Linear Spectroscopy, Sesto Fiorentino, FI, Italy — [3]Zoological Institute, KIT — [4]Institute of Microstructure Technology, KIT

Realizing tunable micro-optical devices, e.g., filters or lasers is a challenging task. A possibility is to use mechanically flexible structures. However, often lithographic fabrication and the rigidity of conventional materials induce an inflexibility. Here, we demonstrate that the flexibility of polymers can be utilized for widely tunable photonic circuits.

We review the fabrication of polymeric whispering gallery mode (WGM) micro-lasers and show their superiority in post-fabrication configuration tuning. The first example demonstrates resonance tuning by exploiting liquid crystal elastomers (LCE). When integrated into the cavity, a LCE cylinder can function as a micro-actuator modifying the resonator diameter and hence tuning the WGM resonances.

Polymers allow substrate-independent fabrication based on direct laser writing. As a second example we present the flexible coupling of WGM cavities structured on elastomer substrates. Reducing the inital inter-cavity gap through deformation of the substrate leads to the formation of photonic molecules. Tunable coupling is verified by exponential trends in the intensities of arising super-modes.

DF 2.6 Mon 11:30 GER 37

Interface engineering in all-oxide $Ba_xSr_{1-x}TiO_3$ thin-film varactors with highly conducting $SrMoO_3$ electrodes — •Patrick Salg[1], Aldin Radetinac[1], Dominik Walk[2], Holger Maune[2], Rolf Jacoby[2], Philipp Komissinskiy[1], and Lambert Alff[1] — [1]Institute of Materials Science, TU Darmstadt, Germany — [2]Institute for Microwave Engineering and Photonics, TU Darmstadt, Germany

We present epitaxial varactor heterostructures utilizing highly conducting oxide $SrMoO_3$ bottom electrodes with a room-temperature resistivity of 30 $\mu\Omega$cm [1] grown by pulsed laser deposition using $SrMoO_4$ targets. During thin film synthesis, highly reductive conditions are essential to achieve a Mo^{4+} state in the $SrMoO_3$ thin film. In contrast to the growth conditions of $SrMoO_3$, the growth of $Ba_xSr_{1-x}TiO_3$ films requires a high oxygen partial pressure of 1.5 mTorr. In order to prevent oxidation of the underlying $SrMoO_3$ layers during growth of $Ba_xSr_{1-x}TiO_3$, a $SrTiO_3$ layer was grown between $SrMoO_3$ and $Ba_xSr_{1-x}TiO_3$. The effectivity of this $SrTiO_3$ interlayer as an oxygen diffusion barrier was investigated by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The use of a $SrTiO_3$ interlayer allows a successful epitaxial growth of varactor heterostructures with high electric tunability of up to 80 % and low losses at microwave frequencies.

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

DF 2.7 Mon 11:50 GER 37

The pyroelectric coefficient of free standing GaN grown by HVPE — •Sven Jachalke[1], Patrick Hofmann[2], Gunnar Leibiger[3], Frank S. Habel[4], Erik Mehner[1], Tilmann Leisegang[1,4], Dirk C. Meyer[1], and Thomas Mikolajick[2,5] — [1]Institute for Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany — [2]NaMLab gGmbH, Nöthnitzer Str. 64, 01187 Dresden, Germany — [3]Freiberger Compound Materials GmbH, Am-Junger-Löwe-Schacht 5, 09599 Freiberg, Germany — [4]Samara National Research University, Moskovskoye Shosse 34, Samara 443086, Russia — [5]Institute for Semiconductors and Microsystems, TU Dresden, Nöthnitzer Str. 64, 01187 Dresden, Germany

Here, we present the first temperature dependent measurements of the pyroelectric coefficient of free standing, and strain free GaN grown by hydride vapour phase epitaxy (HVPE). The Sharp-Garn method is applied to extract the pyroelectric coefficient from the electrical current response of the crystals subjected to a sinusoidal temperature excitation in a range of 0°C to 160°C. To avoid compensation of the pyroelectric response by an internal conductivity, insulating GaN crystals were used by applying carbon, manganese and iron doping during HVPE growth. Different pyroelectric coefficients observed at room temperature due to the doping correlate well with the change of the lattice parameter c. The obtained data is compared to previously published theoretical and experimental values of thin film GaN and discussed in terms of a strained lattice.

DF 2.8 Mon 12:10 GER 37

Confocal Raman analysis of diffusion profiles in ion exchanged waveguides in PPKTP — •Julian Brockmeier, Michael Rüsing, Christof Eigner, Laura Padberg, Gerhard Berth, Christine Silberhorn, and Artur Zrenner — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

KTP presents a promising material system for integrated quantum optical applications. Integrated quantum optical devices require the fabrication of waveguides, which can be achieved in this material via the ion exchange of Potassium by Rubidium. An optimized fabrication of these structures requires a detailed understanding of the induced changes in the material structure, such as the diffusion profile. Here

the confocal Raman imaging technique presents one of the foremost methods for a three dimensional spatial analysis of the material properties. Within this work periodically poled KTP (PPKTP) waveguides have been visualized by Raman imaging. For a more detailed analysis of the induced material changes the data processing has been improved and now allows to map the changes of the FWHM shift and intensity of peaks in the Raman spectra. Based on this optimized method, spectral features have been identified, which are sensitive to the concentration of the ion exchanged Rubidium.

DF 3: Focus: Ferroics with Mesoscopic Order

This focus session aims at bringing together scientists from both magnetism and dielectric communities to stimulate discussions about similarities and differences between mesoscopic phenomena in both fields.

Organizer: Leonard Henrichs KIT Karlsruhe

Time: Monday 9:30–13:00 Location: WIL B321

Topical Talk DF 3.1 Mon 9:30 WIL B321

Controlling core-shell formation in BNT-ST — •Till Frömling[1], Azatuhi Ayrikyan[2], Matias Acosta[1], Leopoldo Molina-Luna[1], Michael Dürrschnabel[1], Hans-Joachim Kleebe[1], Herbert Hutter[3], and Kyle Webber[2] — [1]Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, Darmstadt, Germany, 64287 — [2]Institute of Materials Science and Engineering, Friedrich-Alexander-Universität, Martensstraße 5, Erlangen, Germany, 91054 — [3]Institute of Chemical Technologies and Analytics, Technische Universität Wien, Getreidemarkt 9, Vienna, Austria, 1060

Apart from synthesizing solid solutions and doping of ferroelectric materials tailoring core-shell microstructures is an excellent opportunity for modifying ferroelectric and dielectric properties. Recently, the core-shell development in $Bi_{1/2}Na_{1/2}TiO_3$-$SrTiO_3$ (BNT-ST) and its extraordinary impact on achievable strain has been evaluated. About 3% strain at 4 kV/mm was reached which exceeds values obtained for commercially available soft $Pb(Zr,Ti)O_3$ (PZT). It is of major importance to gain more knowledge about possible ways to control the core-shell microstructure to actually be able to tailor the physical properties. Hence, the mechanism of core-shell formation in BNT-ST will be discussed in this work. With the help of secondary ion mass spectrometry (SIMS) and energy dispersive X-ray spectroscopy (EDX) interdiffusion experiments of BNT and ST diffusion couples are investigated. As a result, the species dominating the mass transport during sintering are qualitatively and quantitatively evaluated.

Topical Talk DF 3.2 Mon 10:00 WIL B321

Determining fundamental properties from diffraction: Electric field induced strain and piezoelectric coefficient — •Manuel Hinterstein[1,2], Markus Hoelzel[3], Andrew Studer[4], and Michael J. Hoffmann[1] — [1]Institut für Angewandte Materialien, Karlsruher Institut für Technologie, Haid-und-Neu Straße 7, 76131 Karlsruhe, Germany — [2]School of Materials Science and Engineering, UNSW Australia, Sydney, New South Wales 2052, Australia — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [4]Bragg Institute, Australian Nuclear Science and Technology Organization, Locked Bag 2001, Kirrawee DC NSW 2232, Australia

Piezoelectric ceramics exhibit the remarkable property to couple elastic strain and polarization. Especially actuators rely on high electric fields to generate high strains and forces. The two most important characteristics of this class of materials are macroscopic strain and piezoelectric coefficient. Despite extensive studies and elaborated measurement techniques, the correlation between macroscopic strain and structural response is still not fully understood. Most of the relevant systems found up to now are compositions close to phase boundaries linking highly correlated phases. Apart from the well-known field induced structural responses such as domain switching and the converse piezoelectric effect we recently identified field induced phase transitions in different systems as an additional poling mechanism. The results not only separately reveal the contributions of each poling mechanism to the macroscopic strain, but also different behaviours of the phases.

DF 3.3 Mon 10:30 WIL B321

Mechanisms of thermal depolarization and electromechanical response of lead-free relaxor/semiconductor composites — Lukas Riemer, Lalitha Kodumudi Venkataraman, Jürgen Rödel, and •Jurij Koruza — Technische Universität Darmstadt, Darmstadt, Germany

Thermal depolarization, i.e., vanishing of the macroscopic piezoelectric properties, is one of the major issues limiting the wide application of many lead-free piezoelectrics based on non-ergodic relaxors [1]. An increase of the depolarization temperature, T_d, was recently achieved by the formation of (3-0) composites of the $(Na_{0.5}Bi_{0.5})TiO_3$-based relaxor phase and the ZnO semiconductor phase [2]. The aim of our work was to investigate the mechanisms responsible for this behaviour.

Composites consisting of the non-ergodic relaxor $0.94(Na_{0.5}Bi_{0.5})TiO_3 - 0.06BaTiO_3$ as the matrix phase and ZnO inclusions were prepared and a ferroelectric long-range order was found to be induced in virgin samples by residual thermal stresses. Moreover, an increase in the T_d of up to $\approx 40°C$ was observed. The ZnO inclusions had two counteracting influences on the thermal depolarization: stabilization of the induced ferroelectric state due to additional charges provided by the semiconductor and depolarization induced by residual thermal stresses. The results indicate possibilities for enhancing the thermal stability and operational range of lead-free relaxor piezoelectrics.

[1] J. Rödel et al., J. Eur. Ceram. Soc., 35, 1659 (2015)
[2] J. Zhang et al., Nat. Commun., 6, 6615 (2015)

DF 3.4 Mon 10:50 WIL B321

On the Jahn-Teller ferroelectric transition of GaV_4S_8 — •Jiri Hlinka — Institute of Physics, Czech Acad. Sci., Prague

Recently, the crystal of GaV_4S_8, a multiferroic system hosting a skyrmion lattice phase, has been investigated by polarized Raman and IR spectroscopy above and below the ferroelectric phase transition[1]. Phonon spectra were interpreted with the aid of ab initio calculations of the phonon spectra in the ferroelectric phase.

In this contribution, we shall mostly discuss the relevance of Jahn-Teller distortion for the mesoscopic phases and the character of phonon vibrations directly related to the Jahn-Teller distortion.

[1] J. Hlinka, F. Borodavka, I. Rafalovskyi, Z. Docekalova, J. Pokorny, I. Gregora, V. Tsurkan, H. Nakamura, F. Mayr, C. A. Kuntscher, A. Loidl, S. Bordacs, D. Szaller, H.-J. Lee, J. H. Lee, and I. Kezsmarki, Lattice modes and the Jahn-Teller ferroelectric transition of GaV4S8, Phys. Rev. B 94 060104(R) (2016).

20 min. break

DF 3.5 Mon 11:30 WIL B321

Multiferroic effects in nanoparticulate systems — •Soma Salamon[1], Joachim Landers[1], Marianela Escobar[2], Muhammad Naveed-Ul-Haq[2], Vladimir Shvartsman[2], Morad Etier[2], Doru C. Lupascu[2], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Institute for Materials Science and CENIDE, University of Duisburg-Essen

Both intrinsic and composite multiferroic nanoparticles have been investigated using a variety of measurement methods. Representing an intrinsic multiferroic, bismuth ferrite ($BiFeO_3$) nanoparticles were examined by Mössbauer spectroscopy to analyze the size and temperature dependence of the cycloidal spin structure and its anharmonicity. This was done to investigate whether the cycloid can be inhibited by sufficiently small particle diameters, potentially inducing a net magnetic moment in the otherwise antiferromagnetic material. Results indicate that the spin cycloid exists even in particles small compared to the period length of the cycloid (ca. 62 nm). Representing a composite multiferroic, cobalt ferrite-barium titanate ($CoFe_2O_4$-$BaTiO_3$) core-shell nanoparticles were synthesized, resulting in a ferroelectric

$BaTiO_3$ shell and a ferrimagnetic $CoFe_2O_4$ core. This was followed by the preparation of ceramics through sintering techniques, producing magnetostrictive regions in a piezoelectric matrix. The strain coupling between the two constituents was verified by successful measurements of the direct and converse magnetoelectric effect on these samples. This work was supported by the DFG (FOR 1509) and Stiftung Mercator (MERCUR).

DF 3.6 Mon 12:00 WIL B321

Superparamagnetism induced by polar nano region in relaxor magnet — •Minoru Soda — ISSP, Univ. of Tokyo, Japan

Strong coupling between magnetism and dielectricity has attracted much attention in the fundamental and applied physics. In order to search novel system exhibiting enhanced coupling between the dielectric and magnetic properties, we focused on relaxor ferroelectrics having magnetic ions, relaxor magnet. In the relaxor ferroelectrics, there is the concept of Polar Nano Regions (PNRs), where ordered polarizations in nanoscale domains are randomly oriented. In the present study, the interaction between PNRs and the magnetic correlation was studied both by macroscopic properties and microscopic neutron-scattering measurements for two different compounds; perovskite $2/3\ BiFeO_3 - 1/3\ BaTiO_3$ and triangular lattice system $LuFeCoO_4$. As a result, the obvious coupling between nuclear and magnetic correlations was identified, and a novel type of superparamagnetism induced by PNR was discovered. The growth of the antiferromagnetic correlation with ferromagnetic component is restricted inside the PNRs and the magnetic moments in nano-magnetic domain behave as superparamagnetic moments. For relaxor magnet, the dielectric and magnetic properties were dominated by the Multiferroic Nano Region.

Topical Talk DF 3.7 Mon 12:30 WIL B321

Ferroic glasses: polar nanoregions in relaxor PMN vs. magnetic nanoparticles in a discontinuous multilayer — •Wolfgang Kleemann — Fakultät Physik, Universität Duisburg-Essen, 47048 Duisburg

The term "ferroic glass" was coined [1] for martensitic, magnetic, and relaxor ferroelectric nanodomain states, which undergo glassy dynamic criticality at $T > T_g$ and non-ergodicity at $T < T_g$. While these features are also found in "superspin glass" systems of matrix isolated magnetic nanoparticles as in $[Co_{80}Fe_{20}(0.9nm)/Al_2O_3(3nm)]$ 10 multilayers [2], the mesoscopic "ferroic glasses" are generally more complex due to the much closer relationship of the nanodomains to the embedding matrix. This is shown for the archetypical relaxor PbMg(1/3)Nb(2/3)O(3) [3], where quenched electric random fields (RF) give rise to creation and growth of polar nanoregions (PNR) on cooling toward Tg with a spectrum of relaxation frequencies skewing from Lacroix-Béné to Cole-Davidson-type. It becomes replaced by relaxation and creep-like domain wall dynamics below Tg, where the PNR percolate and form a ferroelectric microdomain state under the control of the ferroelectric soft lattice mode.

[1] X. B. Ren, Phys. Stat. Sol. B 251, 1982 (2014).

[2] S. Bedanta, O. Petracic and W. Kleemann, Handbook Magn. Mater. 23, 1 (2015).

[3] W. Kleemann and J. Dec, Phys. Rev. B 94, 174203 (2016).

DF 4: PV V - Ramamoorthy Ramesh

Time: Monday 14:00–14:45 Location: HSZ 01

Plenary Talk DF 4.1 Mon 14:00 HSZ 01

Electric Field Control of Magnetism — •Ramamoorthy Ramesh — University of California, Berkeley

Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. The basic materials physics of such materials provide the ideal playground for interdisciplinary scientific exploration. Over the past decade we have been exploring the science of such materials (for example, colossal magnetoresistance, ferroelectricity, etc) in thin film form by creating epitaxial heterostructures and nanostructures. Among the large number of materials systems, there exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics. Using our work in the field of ferroelectric(FE) and ferromagnetic oxides as the background, we are now exploring such materials, as epitaxial thin films as well as nanostructures. We have been able to demonstrate electric field control of both antiferromagnetism and ferromagnetism at room temperature. Current work is focused on ultralow energy (1 attoJoule/operation) electric field manipulation of magnetism. We are also exploring artificially designed multiferroics. In this talk, I will describe our progress to date on this exciting possibility.

DF 5: SYCE - Novel Functionality and Topology-Driven Phenomena in Ferroics and Correlated Electron Systems (DF with MA, KR, MI, TT and DS)

Time: Monday 15:00–18:00 Location: HSZ 02

Invited Talk DF 5.1 Mon 15:00 HSZ 02

Ferroelectric domain walls: from conductors to insulators and back again — •Petro Maksymovych — Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA

The root cause of uncertainty around conducting ferroelectric domain walls (DWs) is the contact problem, which may be intrinsic to the polarization topology and may not be resolved by doping ferroelectric films. We revealed how contact effects are responsible for apparent DW conductance in ultrathin BiFeO3, wherein the DW electrostatically gates the interface, but is not itself a conductor. At the same time, we explored AC conductance of DWs to eliminate contact effects. DWs in both BiFeO3 and Pb(Zr0.2Ti0.8)O3 revealed robust conductivity at 3 GHz with remarkably large values of 2-6 S/m. Using the Ginzburg-Landau-Devonshire model for ferroelectric semiconductor, the effect is traced to local charge of nominally straight DWs due to defect-induced roughening and/or an intrinsic flexoelectric effect. Microwave regime opens new opportunities for device integration and carrier-density and dielectric effects at DWs.

Support provided by U.S. Department of Energy, BES, Materials Science and Technology Division. Microscopy experiments performed at the Center for Nanophase Materials Sciences, a DOE Office of Science User Facility.

[1] R. K. Vasudevan, et al., and P. Maksymovych, submitted (2016) [2] A. Tselev, P. Yu, Y. Cao, L. R. Dedon, L. W. Martin, S. V. Kalinin, and P. Maksymovych, Nat. Comms., 7 (2016) 11630.

Invited Talk DF 5.2 Mon 15:30 HSZ 02

Zoology of skyrmions and the role of magnetic anisotropy in the stability of skyrmions — •Istvan Kezsmarki[1], Sandor Bordacs[1], Jonathan White[2], Vladimir Tsurkan[3], Alois Loidl[3], Peter Milde[4], Hiroyuki Nakamura[5], and Andrey Leonov[6] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Paul Scherrer Institute, Villingen, Switzerland — [3]University of Augsburg, Augsburg, Germany — [4]Technical University of Dresden, Dresden, Germany — [5]University of Kyoto, Kyoto, Japan — [6]University of Hiroshima, Hiroshima, Japan

Skyrmions are nanometric magnetic objects with high stability owing to their topological structures. The internal spin pattern of skyrmions depends on the crystal symmetry of the host materials. While we know many chiral crystals hosting Bloch-type skyrmions, Néel-type skyrmions have only recently observed in polar compounds. On experimental basis, I am going to compare the main characteristics of the

two types of skyrmions and discuss the effect of magnetic anisotropy on the thermal stability range of the corresponding Bloch- and Néel-type skyrmion lattices.

Invited Talk DF 5.3 Mon 16:00 HSZ 02

Magnetic imaging of topological phenomena in ferroic materials — •Weida Wu — Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA

Topology is a pervasive concept in condensed matter physics. Topological phenomena such as vortices, Skyrmions and chiral edge states are mesoscopic textures that are crucial for the physical properties and functionalities. Thus, it is imperative to directly visualize these mesoscopic phenomena. In this talk, I will present our recent discovery of alternating uncompensated magnetic moments at Z6 vortex domain walls in hexagonal manganites, which demonstrates the coupling between ferroelectric and antiferromagnetic orders. Furthermore, magnetoelectric response of the vortex domains were directly visualized by Magnetoelectric Force Microscopy (MeFM), a combination of MFM with in-situ modulating high electric fields. Our MeFM results reveal a giant enhancement of magnetoelectric response of a lattice mediated magnetoelectric effect near a spin-reorientation critical point.

This work is supported by US DOE under grant DE-SC0008147.

30 min. break

Invited Talk DF 5.4 Mon 17:00 HSZ 02

Topological skyrmion textures in chiral magnets — •Markus Garst — Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

A magnetization that spatially varies within a plane can be characterized by a topological skyrmion number specifying how often the magnetization vector covers the unit sphere. Magnetic skyrmion textures with such a non-trivial winding number are endowed with additional functionality as they efficiently couple to magnon- and itinerant spin currents allowing for novel spintronic applications. Such textures arise, in particular, in chiral magnets where the Dzyaloshinskii-Moriya interaction favours a spatially modulated magnetization. This stabilizes magnetic solitons that carry an integer skyrmion charge as well as regular arrangements thereof, i.e., skyrmion crystals. We demonstrate that defects of helimagnetic order can carry half-integer skyrmion numbers. In analogy to cholesteric liquid crystals, such defects can be interpreted as disclinations and dislocations that are instrumental for the magnetic relaxation process in these systems. We also show that an array of such defects might arise in topological domain walls of helimagnetic order permitting an efficient manipulation by spin currents.

Invited Talk DF 5.5 Mon 17:30 HSZ 02

Learning through ferroelectric domain dynamics in solidstate synapses — Sören Boyn[1], Gwendal Lecerf[2], Stéphane Fusil[1], Sylvain Saïghi[2], Agnès Barthélémy[1], Julie Grollier[1], Vincent Garcia[1], and •Manuel Bibes[1] — [1]Unité Mixte de Physique CNRS/Thales, Palaiseau FRANCE — [2]IMS Laboratory, U. Bordeaux FRANCE

In the brain, learning is achieved through the ability of synapses to reconfigure the strength by which they connect two neurons. Artificial hardware with performances emulating those of biological systems require electronic nanosynapses endowed with such plasticity. Promising solid-state synapses are memristors, simple two-terminal nanodevices that can be finely tuned by voltage pulses. Their conductance evolves according to a learning rule called spike-timing-dependent plasticity, conjectured to underlie unsupervised learning in our brains. We will report on purely electronic ferroelectric synapses and show that spike timing-dependent plasticity can be harnessed and tuned from intrinsically inhomogeneous ferroelectric polarisation switching. Through combined scanning probe imaging and electrical transport experiments, we demonstrate that conductance variations in such BiFeO3-based ferroelectric memristors can be accurately controlled and modelled by the nucleation-dominated electric-feld switching of domains with different polarisations. Our results show that ferroelectric nanosynapses are able to learn in a reliable and predictable way, opening the way towards unsupervised learning in spiking neural networks.

DF 6: SYBM - Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs (CPP with BP, MM, DF, DY und MI)

Time: Tuesday 9:30–12:15 Location: HSZ 02

Invited Talk DF 6.1 Tue 9:30 HSZ 02

New twists in biological photonics: circular polarisation and beyond. — •Pete Vukusic, Luke McDonald, and Ewan Finlayson — University of Exeter, Exeter, UK.

The evolution of structural colour mechanisms in many biological systems has given rise to many specialised and often highly functional optical effects both in animals and in plants. Recent scientific works yielded several examples that are being developed for use across technology. Among many thousands of biological systems, a distinctive example involving circular polarisation (CP) was described by Michelson himself: the scarab beetle Chrysina resplendens. Its exoskeleton has a bright, golden appearance that reflects both right-handed and left-handed CP light. The chiral nanostructure responsible for this is a helicoid comprising twisted birefringent dielectric planes. This presentation revisits the C. resplendens beetle, correlating details of its CP reflectance spectra directly with detailed analysis of its morphology that includes a chiral multilayer configuration comprising two chirped, left-handed, helicoids separated by a birefringent retarder. The system's optical behaviour is modelled using a scattering matrix simulation, where the optical roles of each component of the morphological substructure are elucidated. The C. resplendens' model is presented here, alongside summaries of other inspirational biological structural colour generation strategies, as a key example of highly adapted optical design.

Invited Talk DF 6.2 Tue 10:00 HSZ 02

Bio-inspired materials and structures for technology and architecture — •Thomas Speck — Plant Biomechanics Group & Botanic Garden, University of Freiburg

Biological structures and materials are typically multi-layered, hierarchically structured, finely tuned and highly differentiated based on the combination of a few basic molecular components. This leads to materials and structures that are characterized by multiple networked functions and (often) possess excellent mechanical properties, a pronounced adaptability to changing environmental conditions and manyfold self-x-properties.

During the last decades biomimetics, i.e. using living organisms as inspiration for technical developments products, has attracted increasing attention as well from basic and applied research as from various fields of industry. Biomimetics has a high innovation potential and offers the possibility for the development of sustainable technical products and production chains. On the one hand, novel sophisticated methods for quantitatively analyzing and simulating the form-structure-function-relationship on various hierarchical levels allow new fascination insights in multi-scale mechanics and other functions of biological structures, materials and surfaces. On the other hand, recent developments in computational design and simulation together with new production methods enable for the first time the transfer of many outstanding properties of the biological role models into innovative biomimetic products for reasonable costs which makes them interesting for applications in many fields of technology and building construction.

Invited Talk DF 6.3 Tue 10:30 HSZ 02

Cellulose bio-inspired hierarchical structures — •Silvia Vignolini — Lensfield Road Cambridge CB2 1EW UK

Nature's most vivid colours rely on the ability to produce complex and hierarchical photonic structures with lattice constants on the order of the wavelength of visible radiation. A recurring strategy design that is found both in the animal and plant kingdoms for producing such effects is the helicoidal multilayers. In such structures, a series

of individual nano-fibers (made of natural polymers as cellulose and chitin) are arranged parallel to each other in stacked planes. When distance between such planes is comparable to the wavelength of light, a strong polarised, colour selective response can be obtained. These helicoidal multilayers are generally structured on the micro-scale and macroscopic scale giving rise to complex hierarchical structures.

Biomimetic with cellulose-based architectures enables us to fabricate novel photonic structures using low cost materials in ambient conditions. Importantly, it also allows us to understand the biological processes at work during the growth of these structures in plants. In this talk the route for the fabrication of complex bio-mimetic cellulose-based photonic structures will be presented and the optical properties of artificial structures will be analyzed and compared with the natural ones.

15 min break

Invited Talk DF 6.4 Tue 11:15 HSZ 02

Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing — •Vladimir Tsukuruk — School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, USA

I discuss recent results from our research group on designing flexible and strong responsive polymer and biopolymer nanocomposite materials and structures for advanced flexible sensing and electronic applications. Ultrathin silk fibroin proteins and chemically modified cellulose nanocrystals were assembled in order to control intimate assembly with graphene oxide sheets with controlled surface chemical composition on planar and curved substrates. We demonstrated flexible laminated bionanocomposites with developed biointerphases that facilitate extremely high elastic modulus, bending flexibility, and toughness. Both experimental and computational methods were undertaken to address silk fibroin adsorption at heterogeneous surfaces of graphene oxide with different degrees of oxidation. Graphene oxide and reduced graphene oxide sheets at various levels of oxidation were compared with silicon dioxide (SiO2) as a benchmark substrate. We concluded that silk fibroin readily forms single molecule proto-nanofibrils with β-sheet structures on oxidized graphene oxide surfaces but aggregated globular structures on the hydrophobic surfaces. Finally, electrochemical-assisted photolithography has been utilized for high spatial resolution conductive patterning of these nanocomposites with high local electrical conductivity, sharp boundaries, and optical transparency. Some peculiar features of these flexible bionanocomposites can be explored for tactile recognition, remote sensing, and low-noise SERS substrates.

Invited Talk DF 6.5 Tue 11:45 HSZ 02

3D laser nano-printing of rationally designed materials — •Martin Wegener — Karlsruhe Institute of Technology, Karlsruhe, Germany

Broadly speaking, 3D structures and materials can be designed by using the human brain, computer-based (topology) optimization, or inspiration from nature. Regardless of how a 3D blueprint has been obtained, it eventually needs to be manufactured. 3D laser printing on the micro- and nanometer scale has become a versatile and reliable workhorse for accomplishing this task. Here, we review recent examples from our group. This includes micropolar metamaterials with behavior beyond ordinary continuum mechanics, metamaterials with effectively negative thermal expansion from positive constituents, and electrical metamaterials with unusual direction and sign of the Hall voltage.

DF 7: Focus: Microwave and THz Properties, Developments and Applications of Dielectric Materials

This dedicated focus session represents applications of dielectric materials from electronics up to Mega-Watt Fusion Heating systems. Part of the session are the different applications of dielectrics and the production and properties of these materials as well. Goal of the session is to join different fields to generate new ideas for dielectric applications and developments.

Organizer: Theo Scherer KIT Karlsruhe

Time: Tuesday 9:30–12:20 Location: GER 37

Topical Talk DF 7.1 Tue 9:30 GER 37

Synthesis of large-area single-crystal diamond by heteroepitaxy for application as dielectric window material — •Matthias Schreck, Stefan Gsell, and Martin Fischer — Institut für Physik, Universität Augsburg, 86135 Augsburg, GERMANY

Due to ist low dielectric loss tangent in combination with excellent mechanical properties and the unrivalled thermal conductivity, diamond is the optimum window material for the transmission of high power millimeter waves. Polycrystalline discs with diameters of about 100 mm synthesized by microwave plasma chemical vapor deposition (MWPCVD) are already in use as gyrotron exit windows or as injection windows for future thermonuclear fusion reactors. Since imperfections like graphitic bonds and C-H groups at grain boundaries still give rise to power absorption, the use of single crystals promises even lower loss tangents thus facilitating higher power levels. The present contribution reviews the efforts towards the synthesis of wafer-scale single-crystal diamond by heteroepitaxial growth using MWPCVD. The search for the optimum substrate material, the development of appropriate nucleation methods and the concepts for the scaling to wafer size are described. Particular attention is paid to dislocations which represent the crucial defect type. The role of dislocations in the development of intrinsic stress, the reduction of their density by growth of thick layers and by advanced deposition concepts is broadly discussed. Finally, the present state-of-the-art in terms of crystal quality and sample size is described.

DF 7.2 Tue 10:00 GER 37

Electron Cyclotron systems in future Fusion Power Plants, using dielectric microwave transmission windows — •Giovanni Grossetti, Gaetano Aiello, Francesco Mazzocchi, Andreas Meier, Theo Scherer, Sabine Schreck, Peter Spaeh, Dirk Strauss, and Alessandro Vaccaro — KIT, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein Leopoldshafen

Nuclear fusion has the potential to be a nearly unlimited, safe and CO2-free friendly energy source which would allow coping with the increasing demand in energy consumption, currently heavily based on the fast depleting fossil fuels (over 80%). Fusion devices are ring-shaped metal vessels provided with numerous openings for diagnostic systems and additional heating systems. One of the most important one is the Electron Cyclotron Heating and Current Drive system (ECH&CD), that aims to provide high power (several MW) in the rage of hundreds of GHz into the plasma, a hot gas composed by Deuterium and Tritium nuclei. In this paper we present the possible configurations of ECH&CD systems required by future fusion power plants. The focus will be on launching antenna systems without movable parts close to the plasma (i.e. remote steering concepts and truncated waveguides) and chemical vapor deposition (CVD) diamond windows. The latter are crucial to ensure flexibility in operation of Radio Frequency source (Gyrotrons), when the latter are capable to tune the beam frequency to the desired resonance.

Topical Talk DF 7.3 Tue 10:20 GER 37

Design, materials composition and manufacturing of components for advanced modular gyrotron prototypes — •Sebastian Ruess[1], Gaetano Aiello[2], Gerd Gantenbein[1], Tomasz Rzesnicki[1], Theo Scherer[2], Dirk Strauss[2], Manfred Thumm[1], Jörg Weggen[1], and John Jelonnek[1] — [1]IHM, — [2]IAM-WAP, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

In frame of EUROfusion, Karlsruhe Institute of Technology (KIT) is

performing major research on future gyrotrons for microwave heating of fusion plasma. Major factor for the success is to gain a fundamental understanding about the basic physics, the right materials composition in the assembly and, finally, the manufacturing technologies for future 2-MW gyrotrons operating in the frequency range from 170 GHz up to 240 GHz. The components of a first pre-prototype 2-MW, 170 GHz long-pulse gyrotron were already successfully in-house manufactured with an excellent quality. Furthermore, welding and solder joints have been achieved with an excellent leakage rate below $<$ 10-12 mbar l/s. In particular, excellent solder joints between CVD diamond and copper as well as stainless steel and dispersion strengthened copper (Glidcop) were achieved. In addition, KIT is strongly involved in the development of ultra-low loss diamond discs for high power gyrotrons and fusion power plants. The ongoing KIT developments are focusing on the manufacturing, joining technologies and cooling concepts for advanced broadband CVD diamond double-disk and Brewster-angle windows.

20 min. break

Topical Talk DF 7.4 Tue 11:10 GER 37

Dielectric diamond window for the ITER EC H&CD Upper Launcher: design, analysis and qualification — •Gaetano Aiello[1], Mario Gagliardi[2], Giovanni Grossetti[1], Francesco Mazzocchi[1], Andreas Meier[1], Gabriella Saibene[2], Sabine Schreck[1], Peter Spaeh[1], Dirk Strauss[1], Alessandro Vaccaro[1], and Theo Scherer[1] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, D-76021 Karlsruhe, Germany — [2]Fusion for Energy, E-08019 Barcelona, Spain

The diamond window is a sub-component of the EC H&CD Upper Launcher and it is part of the ITER first vacuum and tritium confinement system while allowing the transmission of high power microwave beams from the gyrotrons into the plasma. The window consists of an ultra-low loss CVD diamond disc brazed to two copper cuffs and this structure is then integrated into a metallic housing by welding. Being a Protection Important Component, the most stringent requirements in the ITER safety, quality, seismic, vacuum and tritium classifications apply. In this work, we present the development of the window design and the qualification process aiming to meet the requirements via the applicable ASME code and a dedicated program. The window is in fact a unique component that cannot be entirely covered by Codes and Standards. At KIT, FABRY-PEROT resonators measure the loss tangent of the diamond disc which is then used as input to the FEM analyses aiming to validate the design. In the context of the OPE467 contract with F4E, technical specifications are approaching the final phase for the manufacturing and testing of two window prototypes.

DF 7.5 Tue 11:40 GER 37

THz Diagnostics for fusion - A new challenge for dielectric windows — •Francesco Mazzocchi, Giovanni Grossetti, Dirk Strauss, and Theo Scherer — Karlsruhe Institüt für Technologie, Hermann Von Helmholtz Platz 1, 76344, Eggenstein Leopoldshafen

Polarimetry is a reliable methodology to estimate fundamental plasma parameters such as electronic density and poloidal field from the measure of the Faraday rotation angle. In this work we present a conceptual study of an innovative polarimetric system. The device foresees multiple lines of sight, so that the estimation of the aforementioned parameters can be performed at different cords. Dielectric windows play a fundamental role in this case, given the number beamlines that require access to the vacuum vessel. In order to have an appreciable Faraday rotation, sources in the range of the low THz are needed. Quantum Cascade Lasers represent a very promising solution but to work at low frequency (around 1.6 THz) they require cryogenic temperatures. The power output of such devices is still several order of magnitudes below the level guaranteed by the more common laser sources employed so far, such as DCN gas lasers. Therefore a strong focus on the production and characterization of ultra low loss dielectric materials (e.g. diamond, sapphire) for the cryostat and torus windows in the THz range is mandatory, to ensure the polarimeter probe beam absorption to be negligible and the device to work correctly.

DF 7.6 Tue 12:00 GER 37

Dielectric investigation methods in the THz frequency range — •Theo Scherer, Francesco Mazzocchi, and Giovanni Grossetti — Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

CVD diamond disks for high power heating applications are being investigated by different low- and high power measurement setups in the frequency range of $>$ 100 GHz. To understand the loss mechanisms in diamond material the determination of the frequency dependence of dielectric constant and loss tangent at higher frequencies up to several THz is essential. It is well known from the experience with other window materials for high power fusion applications (ECRH) like silicon or sapphire, electrons and phonons are responsible for microwave losses. In diamond the sp2-carbon content and surface roughness determines surface losses. Additionally, the electronic surface states of such dielectrics for different chemical finishing of the diamond disks can be studied in the THz region. Different resonator setups to determine dielectric properties in the THz-range will be discussed.

DF 8: Ferroics - Domains, Domain Walls and Skyrmions I

Subsequently to the symposium "Novel functionality and topology-driven phenomena in ferroics and correlated electron systems" four Focus Sessions "Ferroics - Domains, Domain Walls and Skyrmions I - IV" cover recent developments in analyzing (multi-)ferroic materials, investigations of domain and domain-wall phenomena, the introduction of novel key concepts as well as methods for advanced characterization.

Chairs: Markus Garst and Manuel Bibes

Time: Tuesday 9:30–13:30 Location: WIL B321

Topical Talk DF 8.1 Tue 9:30 WIL B321

Room temperature skyrmions and robust metastable skyrmion states in $Co_8Zn_8Mn_4$ — •Jonathan White[1], Kosuke Karube[2], Nicole Reynolds[1,3], Jorge Gavilano[1], Hiroshi Oike[2], Akiko Kikkawa[2], Fumitaka Kagawa[2], Yusuke Tokunaga[4], Henrik Ronnow[3], Yoshinori Tokura[2,5], and Yasujiro Taguchi[2] — [1]Paul Scherrer Institut, Switzerland — [2]RIKEN CEMS, Wako, Japan — [3]EPFL, Switzerland — [4]Department of Advanced Materials Science, University of Tokyo, Japan — [5]Department of Applied Physics, University of Tokyo, Japan

Magnetic skyrmions are being intensely studied in various noncentrosymmetric magnets. Among them, the chiral cubic magnets are well-known to host a hexagonal skyrmion lattice as a thermodynamic equilibrium state. However, this state exists only over a narrow temperature and magnetic field region just below the magnetic transition temperature. Using both ac susceptibility and neutron scattering, we study metastable Skyrmion states in the room-temperature skyrmion host material $Co_8Zn_8Mn_4$. These states, created by a conventional field-cooling through the equilibrium skyrmion state, survive over the major part of the phase diagram, including down to zero temperature and up to the critical magnetic-field of the ferromagnetic transition. Furthermore, the metastable skyrmion lattice is observed to transform between conventional hexagonal and a novel square-like coordinations upon varying the temperature and magnetic field. These findings exemplify the topological robustness of the once-created skyrmions, and establish metastable states as a promising technological platform.

DF 8.2 Tue 10:00 WIL B321

Universal relations between electromagnetic response functions: towards a first-principles description of magnetoelectric materials — •Giulio Schober[1] and Ronald Starke[2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]Institut für Theoretische

Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg

Based on modern microscopic approaches to electrodynamics of materials, we systematically investigate the mutual functional dependencies of induced, external and total electromagnetic field quantities. This allows for a unified, relativistic description of the electromagnetic response without assuming the material to be composed of electric or magnetic dipoles. Using this approach, we derive universal (material-independent) relations between electromagnetic response functions such as the dielectric tensor, the magnetic susceptibility and the microscopic conductivity tensor. Our formulae can be reduced to well-known identities in special cases, but more generally include the effects of inhomogeneity, anisotropy, magneto-electric cross-coupling and relativistic retardation. If combined with the Kubo formalism, they would therefore lend themselves to the ab initio calculation of all linear electromagnetic response functions, thus paving the way for a first-principles description of magneto-electric materials for spintronics applications.

DF 8.3 Tue 10:15 WIL B321

Giant Rashba effect in ferroelectrics from first principles — •Louis Ponet[1,2], Urko Petralanda[1], Silvia Picozzi[3], and Sergey Artyukhin[1] — [1]Quantum Materials Theory, Istituto Italiano di Tecnologia, Via Morego, 30, Genova, Italy. — [2]Scuola Normale Superiore, Piazza dei Cavalieri, 7, Pisa — [3]CNR-SPIN, UOS L'Aquila, Via Vetoio, 10, Coppito, L'Aquila (IT)

Spintronics has been an exciting area in the last decades, due to a promise for devices that exploit the existence of spin-polarized states [1]. Important applications include storage media, where the use of spins to store data has been widespread since the earliest days of computing. However, these storage devices use magnetic fields to orient magnetic domains, an approach that is making further miniaturization increasingly difficult. A possible solution could be using spin torques provided by spin-polarized currents for more fine-grained and efficient control of magnetic domains. However, to access these states in electronics, there is also a pressing need for electric control of the states, which was recently demonstrated in materials that showcase an anomalously large Rashba-effect [2]. This effect allows for electric control of very highly spin-polarized states, but the origin of the behaviour is not thoroughly understood yet. We used model Hamiltonians and ab-initio calculations to examine the effect.

[1] S. D. Bader and S. S. P. Parkin, Spintronics, Ann. Rev. Cond. Matt. Phys. 1, 71 (2010).

[2] D. Di Sante, P. Barone, R. Bertacco, S. Picozzi, Advanced Materials, 25, 509 (2013).

15 min. break

DF 8.4 Tue 10:45 WIL B321

Constant-current calligraphic domain-inversion in lithium-niobate crystals — •Christoph S. Werner[1], Simon J. Herr[1], Karsten Buse[1,2], and Ingo Breunig[1] — [1]Department of Microsystems Engineering, University of Freiburg — [2]Fraunhofer Institute for Physical Measurement Techniques, Freiburg, Germany

Lithium-niobate is commonly applied as a nonlinear crystal in nonlinear, optical frequency converters. In order to phase-match the interacting waves, a periodic domain inversion of the crystal is often necessary. The standard method to create the necessary domain pattern uses a structured electrode which defines the position of the domains. While this method is good in batch-processing large quantities of crystals, it is unflexible for prototyping domain patterns since every pattern requires an individual photolithographic mask. We present a technique to rapidly create high-quality domain-structures in congruent-melting, MgO-doped lithium-niobate crystals by defining the position of the domain with a metallic needle. Therefore, the needle is moved along the desired position of the domain. A current-control-loop maintains a constant current and adjusts the necessary poling-voltage accordingly while the needle moves across the crystal. This ensures a high-quality domain-formation independent of the crystal orientation. This method is especially useful for creation of radially-poled domains which are suited for whispering-gallery resonators.

DF 8.5 Tue 11:00 WIL B321

Giant charged-domain-wall conductivity in lithium-nioabte — •Simon J. Herr[1], Christioph S. Werner[1], Cina Razzaghi[2], Elisabeth Soergel[2], Boris Sturman[3], Karsten Buse[4], and Ingo Breunig[1] — [1]Department of Microsystems Engineering, University of Freiburg — [2]University of Bonn, Bonn, Germany — [3]Institute for Automation and Electrometry of Russian Academy of Science, Novosibirsk, Russia — [4]Fraunhofer Institute for Physical Measurement Techniques, Freiburg, Germany

Charged-domain-walls in ferroelectric materials are known to show increased conductivity compared to the bulk-material. These domain-walls could play the key-role in a new type of electronic or electro-optic devices making use of the functional features of the host crystals. So far, the limiting factors are the high resistivity of the domain walls and the lack of a mechanism to create an ohmic interface to the domain-wall. Based on our method of calligraphic domain-inversion, we were able to create conducting domain-walls in lithium-niobate which show a highly increased conductivity, comparable to that of semiconductor materials. Further, we demonstrate that we can achieve diode-like behaviour as well as ohmic conduction.

DF 8.6 Tue 11:15 WIL B321

Functional electronic inversion layers at ferroelectric domain walls — •Jakob Schaab[1], Julia A. Mundy[2], Yu Kumagai[1], Andres Cano[3], Massimiliano Stengel[4], Darrel G. Schlom[2], David A. Muller[2], Ramamoorthy Ramesh[5], Manfred Fiebig[1], Nicola A. Spaldin[1], and Dennis Meier[6] — [1]ETH Zürich — [2]Cornell University — [3]CNRS, Université de Bordeaux — [4]ICMAB-CSIC Barcelona — [5]UC Berkeley — [6]NTNU Trondheim

Ferroelectric domain walls hold great promise as functional 2D-materials because of their unusual electronic properties. Particularly intriguing are the so-called charged walls where a polarity mismatch causes local, diverging electrostatic potentials requiring charge compensation and hence a change in the electronic structure. These walls can exhibit significantly enhanced conductivity and serve as a circuit path. The development of all-domain-wall devices, however, also requires walls with controllable output to emulate electronic nanocomponents such as diodes and transistors.

Here, we will present electric-field control of the electronic transport at ferroelectric domain walls. We reversibly switch from resistive to conductive behavior at charged walls in semiconducting $ErMnO_3$. We relate the transition to the formation - and eventual activation - of an inversion layer that acts as the channel for the charge transport. Our conductive atomic force microscopy (cAFM) and electron energy loss spectroscopy (EELS) data provide new insight to the domain-wall physics in ferroelectrics and foreshadow the possibility to design elementary digital components for all-domain-wall circuitry.

DF 8.7 Tue 11:30 WIL B321

In-situ 3D observation of the domain wall dynamics of triglycine sulfate upon ferroelectric phase transition — •Lukas Wehmeier, Thomas Kämpfe, Alexander Haussmann, and Lukas M. Eng — Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

Second harmonic generation microscopy (SHGM), also known as Cherenkov-SHG, allows for the 3-dimensional (3D) observation of ferroelectric domain walls (DWs) across millimeter-thick bulk materials [1,2]. We apply here SHGM in order to quantify the DW dynamics in triglycine sulfate (TGS) single crystals upon the ferroelectric-to-paraelectric phase transition around Tc = 49°C. Although having been in the focus of many works, this second-order phase transition is still of fundamental interest, especially in the view of our novel 3D techniques at hand or with respect to explore charged domain walls [3-5] in bulk single crystals. SHGM allows, for the first time, to watch the time-resolved dynamics in real time and in 3D, here when crossing the Curie temperature Tc. Furthermore, we also monitor the spike domain growth in TGS using SHGM. Spike domains are an excellent example of transient charged domain walls that topologically differ completely from the equilibrium bulk domain structure.

[1] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014)
[2] T. Kämpfe et al., Appl. Phys. Lett. 107, 152905 (2015)
[3] M. Schröder et al., Mater. Res. Express 1, 035012 (2014)
[4] M. Schröder et al., Adv. Funct. Mater. 22, 3963 (2012)
[5] T. Sluka et al., Nat. Commun. 3, 748 (2012)

DF 8.8 Tue 11:45 WIL B321

Anisotropic domain wall conductivity (DWC) of neighboring 180° DWs in $LiNbO_3$ single crystals — •Shuyu Xiao[1,2], Thomas Kaempfe[2], Yaming Jin[1], Alexander Haussman[2], Xiaomei Lu[1], and Lukas Eng[2] — [1]Physics School, Nanjing University, 210093 Nanjing, P. R. China — [2]Institute of Applied Physics, Technical University of Dresden, George-Baehr-Strasse 1, Dresden, Germany

Investigating the origin and nature of the domain wall conductivity (DWC) in different ferroelectric materials such as $BiFeO_3$ [1], $ErMnO_3$ [2] and $LiNbO_3$ (LNO) [3] is of a major scientific interest today. Here, we report on anisotropic DWC, as found between neighboring head-to-head (h2h) and tail-to-tail (t2t) 180° DWs in z-cut LNO single crystals. We applied conductive atomic force microscopy (cAFM) to quantify the local DW currents, probed the local polarization by piezo-response force microscopy (PFM), and mapped the 3D domain topology via Cherenkov Second Harmonic Generation (CSHG) microscopy [4]. The origin of the different DWC between h2h and t2t is studied by both phenomenological theories and dipole modelling assuming a quantum-mechanical tunneling process for electron transport. The domain wall inclination is found to account for the different conductivities in neighboring 180° DWs, while the material symmetry determines whether h2h or t2t DW becomes more conductive. In addition, domain wall roughness plays an important role in DWC as well.

[1] J. Seidel et al., Nat. Mater., 8 (2009), 229 [2] D. Meier et al., Nat, Mater., 11 (2012), 284 [3] M. Schroeder et al., Mater. Res. Express., 1 (2014), 035012 [4] T. Kaempfe et al., Phys. Rev. B, 89 (2014), 035314

15 min. break

DF 8.9 Tue 12:15 WIL B321

Electric conduction and dynamics of ferroelectric domain walls in $SrTiO_3$ — •Haijiao Harsan Ma, Daniel Kohlberger, Matthias Lange, Sebastian Scharinger, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany

Domain walls in $SrTiO_3$ could play a significant role in future oxide electronics, given their small size at the nanoscale as well as the fact that their occurrence can be controlled by an external electric field. Here, we report on the low-temperature electric conductance properties of domain walls in $SrTiO_3$ and their response to an external electric field. These properties are probed by using a combination of low-temperature scanning electron microscopy, polarized light microscopy and electric transport measurements. Our measurements show that above the threshold electric field $\sim 1\,kV/cm$ for field-induced electric order [1], the domain walls show strongly increased conductance as compared to the bulk $SrTiO_3$. We will also address observations of complex dynamic behavior of the domain wall conductance properties.

[1] H. J. Harsan Ma *et al.*, Phys. Rev. Lett. **116**, 257601 (2016).

DF 8.10 Tue 12:30 WIL B321

Conductive domain walls in $SrMnO_3$ thin films under epitaxial tensile strain — •Lokamani Lokamani[1], Carina Faber[3], Peter Zahn[1], Nicola Spaldin[3], and Sibylle Gemming[1,2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01314 Dresden, Germany — [2]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — [3]Materials Theory, ETH, 8093 Zürich, Switzerland

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

Here, we present a first-principle investigation of the domain wall formation in epitaxially strained $SrMnO_3$ and a discussion of the electronic properties.

[1] J. H. Lee et al., PRL 104, 207204 (2010)
[2] C. Becher et al., Nature Nanotechnology 10, 661 (2015)
Funding by VI Memriox(VH-VI-422) & Nanonet(VH-KO-606)

DF 8.11 Tue 12:45 WIL B321

Local probe studies of switching and current dynamics in $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films — •Philippe Tückmantel[1], Iaroslav Gaponenko[1], Stefano Gariglio[1], Benedikt Ziegler[1], Joshua Agar[2], Lane W. Martin[2], and Patrycja Paruch[1] — [1]DQMP, University of Geneva, Geneva, Switzerland — [2]DMSE, University of California, Berkeley, USA

Defects and electrostatic boundary conditions have been shown to greatly impact the intrinsic configuration, geometry and growth dynamics of polarization domains in ferroelectric thin films. Indeed, defects can induce different switching dynamics, where the polarization reversal can be dominated by the nucleation of new domains or by the lateral growth of existing domains. Defects such as oxygen vacancies can also play an important role in controlling the electrical conduction at ferroelectric domain walls and, in conjunction with electrostatic boundary conditions can even allow fully reversible control of this phenomenon.

Here, we present our results on $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films showing both different switching dynamics and different domain wall current behaviours in samples grown by pulsed laser deposition and off-axis RF magnetron sputtering. Using piezoresponse force microscopy (PFM) and conductive atomic force microscopy (c-AFM) in ultra-high vacuum, we study the nanoscale nucleation and motion of domains as a function of applied tip voltage and their relation to the corresponding currents and defect densities.

DF 8.12 Tue 13:00 WIL B321

Enhancement of local photovoltaic current at ferroelectric domain walls in $BiFeO_3$ — •Ming-Min Yang and Marin Alexe — Department of Physics, University of Warwick, Coventry, UK

Domain walls, which are intrinsically two-dimensional nano-objects exhibiting nontrivial electronic and magnetic behaviors, have been proven to play a crucial role in photovoltaic properties of ferroelectrics. Despite this recognition, the electronic properties of domain walls under illumination until now have been accessible only to macroscopic studies and their effects upon the conduction of photovoltaic current still remain elusive. The lack of understanding hinders the developing of nanoscale devices based on ferroelectric domain walls. Here, we directly characterize the local photovoltaic and photoconductive properties of 71 degree domain walls on $BiFeO_3$ thin films with a nanoscale resolution. Local photovoltaic current, proven to be driven by the bulk photovoltaic effect, has been probed over the whole illuminated surface by using a specially designed photoelectric atomic force microscopy and found to be significantly enhanced at domain walls. Additionally, spatially resolved photoconductive current distribution reveals a higher density of excited carriers at domain walls in comparison with domains. Our measurements demonstrate that domain wall enhanced photovoltaic current originates from its high conduction rather than the internal electric field. This photoconduction facilitated local photovoltaic current is likely to be a universal property of topological defects in ferroelectric semiconductors.

DF 8.13 Tue 13:15 WIL B321

Reconfigurable domain wall conductance by inclination tuning — •Thomas Kämpfe[1], Bo Wang[2], Scott Johnston[3], Eric Y. Ma[3], Alexander Haussmann[1], Hui Hu[4], Zhi-Xun Shen[3], Long-Qing Chen[2], and Lukas M. Eng[1] — [1]Institute of Applied Physics and Center for Advancing Electronics (CFAED), TU Dresden, Germany — [2]Department of Materials Science and Engineering, Pennsylvania State University, University Park, USA — [3]Department of Applied Physics and Geballe Laboratory for Advanced Materials (GLAM), Stanford University, USA — [4]School of Physics, Shandong University, Jinan, China

We report on ferroelectric domain wall (DW) conductance in lithium niobate thin films that allows reproducibly writing/erasing DWs by proper voltage adjustment. The DWs are conductive and show persistent DWC at least for two months. Mandatory to DW conductance is a minimal DW inclination that promotes electron transport without illumination [1]. We proof this dependence indirectly: we compare cAFM measurements for domains written at various writing voltages and compare it with the simulated inclination angles obtained from phase-field modeling, which shows a decrease in inclination the larger the writing voltage. The conductance was further investigated by scanning-microwave impedance microscopy (sMIM) revealing a conductivity of about 100 to $1000\,S/m$ at 1 GHz, hence an increase of about 10^{11} to the bulk conductivity of about 10^{-8} S/m.

[1] M.Schröder et.al., Adv. Funct. Mater. 22, (18), 3936 (2012)

DF 9: Poster Session

Many thanks to NT-MDT for providing sustenance.

1-6:	Optical and nonlinear optical properties, photonic
7-12:	Nano- and microstructured dielectrics / thin films
13-14:	Dielectric surfaces and interfaces
15:	High- and low-k-dielectrics
16:	Developments and applications of Dielectric Materials
17-24:	Ferroic domains and domain walls
25-33:	Multiferroics

Time: Tuesday 14:00–16:00 Location: P1C

DF 9.1 Tue 14:00 P1C

Wave vector dependent dielectric function and ab initio materials physics — •René Wirnata[1], Ronald Starke[1], Giulio Schober[2], and Jens Kortus[1] — [1]Institut für Theoretische Physik, TU Freiberg — [2]Institut für Theoretische Physik, Uni Heidelberg

We study the wave vector dependence of the dielectric function for a set of crystallographically simple materials (such as C, Si, AlP, GaAs, LiF in fcc structure). For this purpose, the FP-LAPW method in Density Functional Theory (DFT) has been combined with the Kubo formula in order to connect quantum mechanical ab initio calculations with quantities from classical electrodynamics. Conceptually, our work is motivated by the rising importance of modern microscopic approaches to electrodynamics in materials, which lead to universal though wave vector dependent response relations between different electromagnetic material properties.

DF 9.2 Tue 14:00 P1C

Second-Harmonic analysis of ion-implanted $LiNbO_3$: Effect of ion-implantation on the nonlinear susceptibility — •Kai J. Spychala[1], Lei Wang[2], Gerhard Berth[1], and Artur Zrenner[1] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]School of physics, Shandong University, 250100 Shandong, PR China

On the way to integrated $LiNbO_3$ optics a key technology is the fabrication of high quality optical waveguides. The formation of waveguides is accompanied by a severe modification of the crystal structure, which may substantially change the optical properties of the used material. Within this work, the effective nonlinear coefficients in ion-implanted $LiNbO_3$ waveguides have been studied via surface-near Second-Harmonic (SH) analysis for single domains as well as for periodically poled structures. The studies have been performed on a set of samples with different implantation dose and energy. The analysis was carried out in backscattering geometry on wedged samples to acquire depth-resolved information. The experimental data shows that a characteristic SH-signal drop is produced for all samples in the implanted region. A comparison with simulation data calculated with the software package "SRIM" by Ziegler et al. suggests that the characteristic drop can be traced back to the implantation-induced defects. In particular, it is possible to correlate the used ion-dose and energy to specific features of the modified optical properties. In a second step a thermally annealed sample series was examined with the same method, revealing that the induced damage can be healed partially.

DF 9.3 Tue 14:00 P1C

Hopping transport of small strong-coupling polarons in magnesium doped lithium niobate — •Tobias Noerenberg[1,2], Lukas M. Eng[1], Simon Messerschmidt[2], Andreas Krampf[2], and Mirco Imlau[2] — [1]Institut für Angewandte Physik, Technische Universität Dresden, Germany — [2]School of Physics, Osnabrück University, Germany

Lithium niobate is an important, widely used ferroelectric in optics and photonics. Its nonlinear optical properties and electrical conductivity are largely influenced by small strong-coupling polarons [M. Imlau *et al.* Appl. Phys. Rev. **2**, 040606 (2015)]. Their microscopic movement is usually investigated in the high-temperature regime and therefore described by a thermally activated hopping transport.

For the first time we were able to measure the polaron transport for magnesium doped lithium niobate (above and below the optical damage resistance threshold) via light-induced absorption in a temperature regime where the thermal energy does not suffice to provide the hopping's activation energy, i.e. as low as 40 K.

The results will be qualitatively compared to Emin's hopping theory [Emin. *Polarons.* Cambridge (2013)] who predicted three different temperature dependent hopping processes: the well-known Arrhenius behaviour at high temperatures, the multiphonon freezeout and at low temperatures the atomic tunneling regime.

Financial support by the DFG (project numbers: IM 37/5-2, INST 190/137-1 FUGG, INST 190/165-1) is gratefully acknowledged.

DF 9.4 Tue 14:00 P1C

A field-theoretical approach to light propagation and lasing in disordered photonic media — •Zhong Yuan Lai, Oleg Zaitsev, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Random lasing is a phenomena which has continuously received attention since its experimental discovery in 2000. We study the propagation of light in an optically active, nonlinear and dielectrically disordered medium using a functional integral formalism, which enables the derivation of an effective low-energy action, known as the Keldysh nonlinear sigma model [1]. In addition, we were able to calculate explicit transport quantities in the form of counting statistics [2] which we could show, in the case of nonactive media, to be quantitatively the same as previous diagrammatical calculations. Finally we study random lasing by including the full matter-light interacting picture and integrating out the matter fields, thus exposing the nonlinear nature of effective photonic interactions in our theory. By obtaining the full interacting saddlepoint of the nonlinear sigma model and systematically taking into account fluctuations around the saddlepoint we obtain the diffusive modes. In this manner we are able to obtain the photonic density correlation function with a correlation length which we intepret as the average lasing spot size, and the single-particle Green's function which yields information about the average laser linewidth.

[1] Lai, Z. Y. and Zaitsev, O., Phys. Rev. A **85**, 043838 (2012).

[2] Lai, Z. Y. and Zaitsev, O., Phys. Rev. A **88**, 023861 (2013)

DF 9.5 Tue 14:00 P1C

Rogue wave generation due to inelastic quasi-soliton collisions in optical fibers — •rudolf a. roemer[1], antonino savojardo[1], marc eberhard[2], and akihiro maruta[3] — [1]Department of Physics, The University of Warwick, United Kingdom — [2]School of Engineering and Applied Science, Aston University, United Kingdom — [3]Graduate School of Engineering, Osaka University, Japan

Optical rogue waves (RW) are rare and extremely high power pulses. Experimental results in optical fibers and numerical data suggest that these giant waves are due to at least two mechanisms of amplification, modulation instability, which leads to the creation of quasi-solitons, and multiple inelastic quasi-soliton collisions. Based on statistics from more than 17×10^6 quasi-soliton collisions, we establish unambiguously the fat-tail character of the probability distribution function (PDF). We also investigate single pair-wise inelastic quasi-soliton collisions and describe the energy transfer as a resonant-like scattering processes. This allows us to implement a novel cascade model that simulates the RW generation process directly giving quantitative agreement with a full numerical integration of the non-linear Schroedinger equation (gNLSE). This highlights the importance of quasi-soliton energy exchange in giving rise to RWs. Time series analysis for the gNLSE and the cascade model show calm before the storm behavior a few picoseconds before they pass. Surprisingly the cascade model predicts such signature with the only assumption of energy transfer between

quasi-solitons, not further ingredients are needed.

DF 9.6 Tue 14:00 P1C

Global modelling of strong-coupling carriers in lithium niobate — Simon Messerschmidt[1], Andreas Krampf[1], •Tobias Nörenberg[1], Felix Freytag[1], Mirco Imlau[1], Laura Vittadello[2], and Marco Bazzan[2] — [1]School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany — [2]Dipartimento di Fisica e Astronomia, Università di Padova, Via Marzolo 8, 35131 Padova, Italy

Strong-coupling carriers, such as small polarons and/or self-trapped excitons (STE), are of increasing importance for a variety of dielectric applications. Although, the properties of these quasiparticles have been studied individually over decades in a variety of oxide dielectrics, a comprehensive model for the excitation, transport and transformation between different types of strong-coupling carriers and the mutual interplay is missing. We have addressed this question by considering small, strong-coupling polarons together with self-trapped excitons in the model system lithium niobate, $LiNbO_3$ (LN) [Imlau, M. *et al.* Appl. Phys. Rev. 2 (2015)]. Our studies comprise different measurement techniques and experimental conditions, i.e., transient absorption and luminescence analysis in a temperature range from (15-300) K, involving nominally undoped, Fe-, and Mg-doped LN samples. We succeeded in global modelling of all data using a single set of parameters by considering the various types of strong-coupling carriers and show the importance of a blue-green absorption of STEs, so far not been considered in literature. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

DF 9.7 Tue 14:00 P1C

Enhancing the sensitivity of polymeric whispering gallery mode micro-disks by structuring notches in the outer cavity rim — •Michael Remmel, Tobias Siegle, Sarah Krämmer, Carolin Klusmann, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

We present the usage of active, dye-doped, polymeric whispering gallery mode resonators as sensors. Pyrromethene 597 is embedded into PMMA (poly (methyl methacrylate)) micro-disks. If pumped optically the micro-disks exhibit sharp lasing peaks allowing easy tracking of the resonance modes via free-space excitation (fluorescence coupling) and read-out. In this way the sensors can be characterized regarding their bulk refractive index sensitivity (BRIS).

The disks are structured by electron-beam lithography on a silicon substrate. Designing notches in the outer section of the micro-disk cavities leads to enhanced interaction of the electric field with the environment due to partial free-space propagation of the cavity mode. The BRIS is determined for resonators with a varying number of notches. A sensitivity enhancement with increasing number of notches is found and compared to conventional disk cavities.

DF 9.8 Tue 14:00 P1C

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

Whispering gallery mode (WGM) resonators build a promising platform for sensing applications due to their high quality factors in combination with small modal volumes. Coupling plasmonic nanoparticles to WGM resonators has recently been suggested to further improve their sensitivity by utilizing local field enhancements around metallic nanoparticles immobilized within the evanescent field of the WGM. However, the underlying physical mechanism is not fully understood yet. Using generalized Mie theory we theoretically analyze the interplay between spherical WGM resonators and plasmonic nanoparticles to provide a deeper understanding of the physical properties of such hybrid systems. We show that the wavelength-detuning between plasmonic resonance and WGM plays a crucial role in the coupling process and deduce engineering guidelines to enhance the sensitivity of such systems.

DF 9.9 Tue 14:00 P1C

Properties of metal-coated polymeric whispering gallery mode resonators — •Patrick Forster[1], Carolin Klusmann[1], Jens Oppermann[2], Carsten Rockstuhl[2,3], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

Whispering-gallery mode resonators are characterized by high Q-factors and a small mode volume V. This renders them promising candidates for devices in biological sensing applications or in nonlinear optics. A unique quantity, the figure-of-merit defined as Q/V, is usually used to judge the suitability of a given structure for these applications. Here, we study whether the figure-of-merit can be notably improved by coating the resonator with a noble metal such as silver or gold. At the interface between the dielectric medium of the cavity and the metal coating, surface plasmon polaritons (SPP) can be sustained. They possess a high field confinement and show large field enhancements at the interface. In addition, hybrid modes occur due to the coupling of plasmonic and dielectric modes. Hybrid modes fuse the advantage of both modes and show, therefore, strong field localization while preserving fairly high Q-factors. In this study that combines theory and experiment, we investigate the influence of different cavity geometries and characteristic parameters of the resonator to obtain a fundamental understanding of the hybrid system operated at near-infrared frequencies.

DF 9.10 Tue 14:00 P1C

Fabrication of silicon nano-structures for dielectric laser accelerators — •Peyman Yousefi[1], Joshua McNeur[1], Martin Kozák[1], Florentina Gannott[2], and Peter Hommelhoff[1,2] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen — [2]Max-Planck-Institut für die Physik des Lichts, Erlangen

Dielectric laser accelerators (DLA) - a novel class of accelerator in which electrons interact with laser-induced accelerating near-fields in the vicinity of dielectric nanostructures - have recently demonstrated accelerating gradients in the GeV/m regime. As such, DLAs may enable accelerator applications not available to classical RF accelerators [1,2]. However there are still major challenges in order to maintain the interaction between electrons and near-fields over longer distances (necessary for larger energy gains) and to achieve even higher accelerating gradients. Developing new nano-structures is essential to solve these issues. In this work we discuss the fabrication of different geometries of silicon such as single side gratings, dual circular pillars and sinusoidal pillars gratings that aim to achieve high gradients and energy gains. E-beam lithography and reactive ion etching (RIE) are used to fabricate the nano-structures. Future designs to address focusing and tapered structures are also discussed.

[1]England R. Joel, et al. Dielectric laser accelerators. Reviews of Modern Physics 2014, 86(4): 1337-1389.

[2]John Breuer, Peter Hommelhoff. Laser-Based Acceleration of Nonrelativistic Electrons at a Dielectric Structure. PRL 2013, 111: 134803.

DF 9.11 Tue 14:00 P1C

Sub-micrometer structuring of sapphire surface applying nanosecond IR laser irradiation — •Igor Zagoranskiy, Pierre Lorenz, Lukas Bayer, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, 04318 Leipzig, Germany

Laser treatment of surfaces finds nowadays a lot of applications. It is also possible to fabricate various, periodic and stochastic micrometer and nanometer structures into substrate surfaces. By modifying of dielectric surfaces the IPSM-LIFE methodic (laser-induced front side etching using in situ pre-structured metal structures) was developed and optimized in applying the fiber laser with wavelength of 1064 nm and adjustable pulse duration from 1 to 600 ns. The IPSM-LIFE includes 2 steps. First step is laser induced pre-structuring of metal layer, which covered dielectric surface. In the second step the produced metal structures are transferred into dielectric substrate. As example 10 nm molybdenum covered sapphire (Al_2O_3 (1-102)) wafer was tested. Modified dielectric surfaces were analyzed by atomic force (AFM) and scanning electron microscopy (SEM) as well as contact angle measurements. Down to nanometer scale the resultant surface topography can be adjusted due to variation of follow laser parameter: number of pulses, pulse duration and fluence.

DF 9.12 Tue 14:00 P1C

Modelling electrode shape deformations of a dielectric elas-

tomer actuator with finite elements — •Philipp J. Mehner, Markus Franke, Andreas Voigt, Uwe Marschner, and Andreas Richter — Chair of Polymeric Microsystems, Technische Universität Dresden, Germany

The concept of dielectric elastomer actuators is used for tuning an optical micro-mirror for low-cost laser development. The basic elements are a flexible top electrode, a transparent dielectric elastomer based on PDMS and a fixed bottom electrode. The employed PDMS has an extremely low elastic modulus, to keep the driving voltage under $U_{\max} = 100\,\mathrm{V}$. Experimental investigations have shown that the shape of the micro-cavity under stress highly depends on the width of the top electrode and the bonding process increases the stiffness of the layer underneath. Due to the micro scale of the setup and the nanoscale thickness of the electrodes, 3d shape measurements are difficult to perform. Computer aided models, based on finite elements, will help to understand and visualize the shape deformations.

We propose a finite element method implemented in ANSYS which utilizes coupled elements for accurate and time efficient simulation runs. A concept of how to implement a depth dependent elastic stiffness will be presented. The simulated results are in accordance with the conducted experiments. This approach helps to formulate novel design parameters to optimize the developed of dielectric elastomer actuators.

DF 9.13 Tue 14:00 P1C

Water-lithium niobate interface studied from first-principles calculations — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — Universität Paderborn

Its piezoelectric, pyroelectric, and photorefractive properties make lithium niobate ($LiNbO_3$, LN) the material of choice for various optical and acoustic applications. The strong and switchable ferroelectric polarization of LN is expected to strongly influence its surface reactivity. This may open the possibility for domain-specific chemistry and the realization of molecular detectors [1].

The water-lithium niobate interface beyond the (sub)monolayer adsorption [2] is largely unexplored. Recent findings suggest, however, that the water freezing temperature is dependent on the surface polarization [3]. Here density-functional theory calculations on the adsorption of water films on both the positive and the negative Z-cut as well as the X-Cut surface of LN are presented. The temperature-dependent interface atomic structure is explored using ab-initio molecular dynamics and the influence of the surface polarity on the water layer is investigated in detail.

[1] D. Li, et al., Nature Materials 7 (2008) 473.
[2] S. Sanna, R. Hölscher, W.G. Schmidt, PRB 86 (2012) 205407.
[3] D. Ehre et al., Science 327 (2010) 672.

DF 9.14 Tue 14:00 P1C

Oxygen exchange behaviour of implanted singles crystals $SrTiO_3$ for energy storage applications — Max Stöber[1], •Charaf Cherkouk[1], Tilmann Leiseganga[1], Matthias Schelter[2], Jens Zosel[2], Slawomir Prucnal[3], and Dirk C. Meyer[1] — [1]Institute for Experimental Physics, TU Bergakademie Freiberg, Germany — [2]Kurt-Schwabe Institute for Measuring and Sensor Technology Meinsberg, Germany — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden Rossendorf,Dresden, Germany

In this work a solid-state-air battery based on thin-film technology containing an oxygen cathode is addressed. Since the efficiency of metal-air batteries is significantly limited by the activation of oxygen reduction reaction (ORR) as well as the ion and electron conductivities, an adequate porosity and a controlled metal doping is required. The ion implantation of promising transition metal oxides is a key technology to achieve this goal. The single crystal $SrTiO_3$ were implanted with Ni, Ag, O_2 and N_2 ions. The time resolved measurements of oxygen exchange behaviour by means of coloumetric titration on the ion implanted single crystal $SrTiO_3$ surface were investigated. In order to understand the defect chemistry and structure of those samples after the ion beam implantation their morphology was studied for example by TEM and sputter XPS. It was shown that the quantitative measurement of oxygen reduction rate on Ni implanted samples revealed an increase on oxygen exchange rate compared to non-treated $SrTiO_3$ single crystals. Keywords: Energy, solid-state battery, $SrTiO_3$, ORR

DF 9.15 Tue 14:00 P1C

Structural analysis of Ba_2SiO_4 thin films grown on Si(100) — •Julian Koch and Herbert Pfnür — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

Crystalline Ba_2SiO_4 is a very promising candidate as a high-k dielectric. Films grown in a previous study [1] have shown a dielectric constant of 22.8 ± 0.2, band offsets to p-Si(100) of over 2 eV, a high temperature stability up to desorption at around 750 °C and an acceptable leakage current of 3 $\mathrm{mA/cm^2}$ at -1 V. Unfortunately, these films still feature a high density of interface traps. The primary cause of this is most likely the growth mode of the silicate films, which were produced by heating the Si(100) substrate during the growth of a BaO film, so that a diffusion of Si from the substrate to the film occured turning the BaO into Ba_2SiO_4. This process resulted in an atomically rough interface in a geometric and possibly also in a chemichal sense. Moreover, only the first 5 nm close to the interface turned out to be crystalline.

This study aims to improve the structural quality of the Ba_2SiO_4 films by employing a co-deposition growth method, in which Ba and Si are evaporated simultaneously in an oxygen atmosphere. This eliminates the need for the Si diffusion. The chemical composition and the crystallinity of the films are investigated using XPS and SPA-LEED, respectively. To further investigate the crystalline growth, crystal orientation and thickness HRTEM is used.

[1] S. Islam, K. R. Hofmann, A. Feldhoff, H. Pfnür, Phys. Rev. Applied **5**, 054006 (2016)

DF 9.16 Tue 14:00 P1C

Strong field scattering from lattice defects — •Lukas Medišauskas, Ulf Saalmann, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems Nöthnitzer Straße 38 D-01187 Dresden

Electron scattering from point defects in dielectrics driven by strong and low frequency laser fields close to the dielectric breakdown of the solid is investigated. The results reveal a strongly non-perturbative nature of the scattering process. Namely, multiphoton absorption to several bands and multiple scattering plateaus reminiscent of strong-field scattering in atoms can be observed in the energy resolved spectra. Intensity scaling of the spectra reveals band structure modification due top the strong laser field.

Kramers-Henneberger frame and Floquet approaches are employed. An efficient numerical method is developed to describe the scattering process in a regime where hundreds of Floquet states become important. This approach allows to compare scattering in different physical systems that may have very different final state.

DF 9.17 Tue 14:00 P1C

Implementing conductive domain walls in $LiNbO_3$ for optoelectronic applications in OLEDs — •Tillmann Stralka, Christian Godau, Alexander Haussmann, Thomas Kämpfe, and Lukas Eng — Institute of Applied Physics, Technische Universität Dresden, Germany

The research on ferroelectric domain walls (DWs) has focused for the last years on their unique property of electronic charge transport when being properly tuned. In fact, domain wall conductivity (DWC) was reported for both thin-film [1] and bulk-single-crystalline [2] ferroelectrics. In lithium niobate ($LiNbO_3$: LNO), DWC can be reversibly tuned through high-voltage treatment [3,4] or super-band-gap illumination [5], rendering this material ideal for the integration into optoelectronic devices. The present work reports on the development of such an optoelectronic device that combines conductive DWs with organic light emission diode (OLEDs). OLEDs are built in vertical stacks, with the charge-carrier mobility being optimized perpendicular to the stacks while becoming very restricted parallel to these layers [6] hence affecting the local light emission dramatically. Here, we implement conductive DWs as so-called local vias contacting the electron- and hole-transport layers in such an OLED.

[1] J. Seidel et al., Nature Mater. **8** (2009), 229. [2] T Sluka et al., Nature Comm. **4** (2013), 1808. [3] C. Godau et al., (2016), submitted. [4] T. Kämpfe et al., Phys. Rev. B **89** (2014), 035314. [5] M. Schröder et al., Adv. Func. Mater. **22** (2012), 3926. [6] Shu-Hao Wen et al., J. Phys. Chem. B **113** (2009), 8813.

DF 9.18 Tue 14:00 P1C

Raman spectroscopic investigations of domains in multiferroic $BiFeO_3$ crystals — •Jan Rix[1], Cameliu Himcinschi[1], Jens Kortus[1], Christian Röder[1], and Marin Alexe[2] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]Department of Physics, University of Warwick,

Coventry CV4 7AL, United Kingdom

Multiferroic $BiFeO_3$ crystals were investigated at room temperature by means of Raman spectroscopy using the 442 nm line of a HeCd laser. Considering the direction of polarisation of the incoming and the scattered beam, characteristic spectra were revealed. These spectra can be attributed to two different types of domains, which differ in the orientation of the pseudo-cubic $<111>_{pc}$ direction. The strong intensity variation of the polar Raman mode at 175 cm^{-1} (A_1(LO) -> E(LO)) was used for domain identification by line scans and mappings. In addition, simulations by means of the Raman tensor formalism proof the experimental findings. This method is a viable alternative to polarisation microscopy and offers opportunities for further studies of ferroelastic domains in $BiFeO_3$.

DF 9.19 Tue 14:00 P1C

Real-time observations of ferroelectric switching by ultrafast x-ray diffraction — •Christelle Kwamen[2], Matthias Reinhardt[2], Wolfram Leitenberger[1], Matthias Roessle[1], Flavio Zamponi[1], Marin Alexe[3], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Uni Potsdam — [2]Helmholtz-Zentrum Berlin — [3]Department of Physics, University of Warwick

We present time-resolved x-ray diffraction experiments on the ferroelectric switching of Lead-Titanate films with a thickness of 150 nm.

The Bragg peak position directly measures the piezoelectric strain during the switching process, while the peak width derived from reciprocal space maps yields a detailed picture of the domain wall propagation dynamics. The scattering intensity yields the structure factor of the unit cells, which is a direct measure of the poling process.

We discuss how the switching speed can be increased from nanosecond to several picoseconds.

DF 9.20 Tue 14:00 P1C

Influence of ferroelectric domain walls on the dielectric permittivity of $BiFeO_3$ — Marek Pasciak, Pavel Marton, •Sabine Körbel, and Jiři Hlinka — Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

$BiFeO_3$ with its coexistence of structural distortions (polar displacements, tilting of oxygen octahedra) and magnetic ordering has been a favourite playground for investigating structure-property relationships in multiferroics. Domain engineering adds another level of complexity, with many recent experimental and theoretical works showing rather spectacular changes in material properties. In this work we use a shell model to study how dynamics related to ferroelectric domain walls change the dielectric permittivity.

DF 9.21 Tue 14:00 P1C

Giant resisitive switching by charged domain walls — •Thomas Kämpfe[1], Bo Wang[2], Scott Johnston[3], Eric Y. Ma[3], Alexander Haussmann[1], Hui Hu[4], Zhi-Xun Shen[3], Long-Qing Chen[2], and Lukas M. Eng[1] — [1]Institute of Applied Physics and Center for Advancing Electronics (CFAED), TU Dresden, Germany — [2]Department of Materials Science and Engineering, Pennsylvania State University, University Park, USA — [3]Department of Applied Physics and Geballe Laboratory for Advanced Materials (GLAM), Stanford University, USA — [4]School of Physics, Shandong University, Jinan, China

We investigate the application of conductive domain walls (CDWs) in exfoliated thin-film lithium niobate (LNO) for resistive switching in a standard metal-ferroelectric-metal stack. An abrupt increase over at least 5 orders of magnitude in the unidirectional conductivity is observed when the voltage sweep approaches the coercive voltage. Local-scale measurements involving AFM techniques confirm that the conductivity indeed correlates with the formation of CDWs. The high- and low-resistance-states show a retention of $> 10^4$ s and an endurance over 10^5 cycles with a resistance window of 10^4 and a high device homogeneity. The non-volatile current is tunable both by varying the writing voltage and exposure time, and indeed decreases for larger writing voltage. The transport mechanism was found to be space-charge limited, with temperature-dependent transport measurements confirming a small-electron polaron hopping. All these experiments are in good agreement with the developed phase-field modeling.

DF 9.22 Tue 14:00 P1C

Electrical current measurements at head-to-head domain walls in $LiNbO_3$ — •Manuel Becker and Elisabeth Soergel — University of Bonn, Bonn, Germany

Besides its pyroelectric, photorefractive, electrooptic and nonlinear optical properties, $LiNbO_3$ is observed to exhibit an enhanced electrical conductivity at certain domain wall configurations, although the crystal itself is an insulator. Especially head-to-head DWs show a significant conductivity which is related to a larger charge density compared to the bulk. The electrical currents at these DWs turn out to be in the order of several pA only, being difficult to detect by usual DC measurement techmiques. Therefore, low-noise AC current measurements using a lock-in amplifier are more suitable. By this means, DW currents are shown to be ohmic and an estimate for the resistance of a head-to-head DW is proposed.

DF 9.23 Tue 14:00 P1C

Creation of ferroelectric domain walls — •Cina Razzaghi[1] and Elisabeth Soergel[2] — [1]Physikalisches Institut, University of Bonn — [2]Physikalisches Institut, University of Bonn

The properties of ferroeletric domains are of great interest in modern research. In the case of $LiNbO_3$ mainly domain walls (DWs) with inclination angles of 180°, as well as head-to-head DWs, are investigated. For a deeper understanding of the properties of DWs it is necessary to study DWs that exhibit other inclination angles α. The electrical conductivity of a DW is expected to be dependent on α. Therefore, one must find techniques for a controlled creation of DWs with various inclination angles.

DF 9.24 Tue 14:00 P1C

Frequency analysis in scanning probe microscopy — •Sarmed Hussain and Elisabeth Soergel — Physics Institute of Bonn University, Bonn, Germany

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

DF 9.25 Tue 14:00 P1C

Time-resolved analysis of multiferroic switching in $Ni_3V_2O_8$, $MnWO_4$, $DyMnO_3$, and $TbMnO_3$ — Jonas Stein[1], •Sebastian Biesenkamp[1], Tobias Fröhlich[1], Tobias Cronert[1], Jeannis Leist[2], A Agung Nugroho[6], Ladislav Bohatý[5], Petra Becker[5], Navid Qureshi[4], Karin Schmalzl[3], Götz Eckold[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Universität Göttingen — [3]JCNS at ILL, France — [4]ILL Grenoble, France — [5]Kristallographie, Universität zu Köln — [6]Institut Teknologi Bandung, Indonesia

We control multiferroic domains with electric fields in the order of several kV/mm to investigate the rise time in dependency of temperature and field strength and analyze the spatial extend and the dynamics of the chiral domains in the multiferroic phase and in vicinity of the multiferroic transition. Polarized neutrons are the ideal tool to investigate the multiferroic domains and complete the dielectric data. With our time-resolved setup it is possible to follow the reversion of chiral domains in the timescale of a few hundred microseconds to hours and record full Bragg scans for peak profile analysis in the time domain. In $TbMnO_3$ we find a clear logarithmic relation between the rise time and temperature that is fulfilled over 5 orders of magnitude. In $DyMnO_3$ the multiferroic switching is slowed down by Mn-Dy coupling.
[1] Niermann et al. **PRB 89**, 134412 (2014) [2] Baum et al. **PRB 89**, 144406 (2014) [3] Holbein et al. **PRB 91**, 014432 (2015) [4] Stein et al. **JPC 27**, 446001 (2015)

DF 9.26 Tue 14:00 P1C

Magnetic correlations in $Eu_{1-x}Ho_xMnO_3$ ($0 \leq x \leq 0.5$) probed by Raman spectroscopy — •Sebastian Elsässer[1], Anatoly M. Balbashov[2], Alexander A. Mukhin[3], and Jean Geurts[1] — [1]Exp. Phys. III, University of Würzburg, Germany — [2]Prokhorov GPI, Russian Academy of Sciences, Moscow, Russia — [3]General Physics Institute of the Russian Academy of Sciences, Moscow, Russia

The perovskite-like rare-earth manganites $RMnO_3$ are among the most widely studied compounds in multiferroics, where the magnetically in-

duced ferroelectricity of, for example, $TbMnO_3$, $DyMnO_3$ is induced via the inverse Dzyaloshinskii - Moriya (DM) interaction. The mixed stoichiometry compounds like $Eu_{1-x}Ho_xMnO_3$ allow fine-tuning of the competing ferro- and antiferromagnetic interactions to achieve the cycloidal spin order patterns needed for this mechanism. The presence of magnetic Ho^{3+} introduces an additional coupling that leads to a complete flip of the spin cycloid plane for Ho-contents of $x > 0.35$ from the *c*- to the *b*-axis (Pnma). Specific Raman-active phonon modes are prime candidates to probe the temperature- and composition dependent developement of magnetic correlations on a quasi-local level via spin-phonon coupling (SPC). Upon cooling, this is observed as a SPC-induced phonon frequency renormalization which reveals magnetic coupling effects even up to $\approx 100\,K$, despite the much lower Néel Temperature $T_N \approx 45\,K$. This is interpreted as the formation of locally correlated spin cycloids, oriented with random helicity, which explains the absence of global magnetic order.

DF 9.27 Tue 14:00 P1C

Interplay of oxygen vacancies and conductance in $SrMnO_3$ thin films under epitaxial tensile strain — •Lokamani Lokamani[1], Carina Faber[3], Peter Zahn[2], Nicola Spaldin[3], and Sibylle Gemming[1,2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01314 Dresden, Germany — [2]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — [3]Materials Theory, ETH, 8093 Zürich, Switzerland

Strontium manganate ($SrMnO_3$), a perovskite polymorph, exhibits cubic structure at low temperatures, which transforms under tensile strain into a G-type-antiferromagnetic (G-AFM) antiferrodistortive polar phase in the plane parallel to the substrate[1]. Recently, ferroelectric domains have been observed experimentally in 20nm thin films of $SrMnO_3$ under 1.7% tensile strain on (001)-oriented LSAT grown in an oxygen-deficient atmosphere[2]. Strikingly, the individual domains show different conductance features, whereas the domain walls were found to be electrically insulating, rendering the domains to form stable nano-capacitors with high charge rention times.

Here, we present a detailed first-principle investigation of the domain wall formation in strained $SrMnO_3$, their electronic properties and the influence of oxygen vacancies on the 2D-electron gas at the polar domain walls. Preliminary results on the migration energetics of the oxygen vacancies are expected.

[1] J. H. Lee et al., PRL 104, 207204 (2010)
[2] C. Becher et al., Nature Nanotechnology 10, 661 (2015)
Funding by VI Memriox(VH-VI-422) & Nanonet(VH-KO-606)

DF 9.28 Tue 14:00 P1C

Dielectric properties of the spin driven multiferroics linarite and $LiCuVO_4$ — •Alexander Ruff, Theresa Mack, Stephan Krohns, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

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

Here we present the dielectric properties as well as the ferroelectric polarization from pyro- and magnetocurrent measurements, both in external magnetic fields up to 12 T. Finally, we provide (H,T)-diagrams for the multiferroic phase of linarite and the new high-temperature phase of $LiCuVO_4$.

DF 9.29 Tue 14:00 P1C

Strong magnetoelectric coupling within ceramic core-shell structures — •Leonard Henrichs[1], Torsten Scherer[1], James Benett[2], Andrew Bell[2], Oscar Cespedes[2], and Christian Kübel[1] — [1]Karlsruhe Insitute of Technology, Karlsruhe, Germany — [2]University of Leeds, Leeds, United Kingdom

In perovskite ceramics of the composition $BiFe_{0.9}Co_{0.1}O_3)_{0.4} - Bi_{1/2}K_{1/2}TiO_3)_{0.6}$, novel nano-sized regions called multiferroic clusters (MFC) were recently discovered. These MFC belong to so-called core-shell structures as known from other relaxor ferroelectrics, where $BiFe_{1-x}Co_xO_3$-rich cores are surrounded by a $Bi_{1/2}K_{1/2}TiO_3$-rich shell within one grain. The MFC exhibit exceptionally large direct and converse local ME coupling. The observed electric-field induced switching of magnetization is especially interesting in terms of applications, since it enables in principle electrically driven magnetic memory, one of the 'holy grails' in information technology research. It is assumed that the strong magnetism stems from ferrimagnetic order of Fe and Co in MFC, which requires a superstructure of Fe and Co on the B lattice site. The main unsolved question in this system is, why the exceptional multiferroic properties occur in the $BiFe_{1-x}Co_xO_3$-rich Cores, but have never been observed in pure $BiFe_{1-x}Co_xO_3$ compounds. An explanation might be epitaxial strain originating from the core-shell structure. It is anticipated, that deeper understanding of the MFC might give valuable insights for the design e.g. of a thin-film material with similar multiferroic properties like the MFC.

DF 9.30 Tue 14:00 P1C

Exchange coupling in multiferroic $Bi_{1-x}Ba_xFeO_3$/ferromagnet heterostructures — •Sven Becker, Mehran Vafaee, Mathias Kläui, and Gerhard Jakob — Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

The $BiFeO_3$/ferromagnet interface has been target of numerous researches. The effect of exchange coupling was often weak at room temperature [1] or dies after some time because of oxidation of the interface[2]. Multiferroic $Bi_{1-x}Ba_xFeO_3$/ferromagnet heterostructures have been fabricated using pulsed laser deposition (PLD). The focus laid on $Bi_{0.75}Ba_{0.15}FeO_3$(BB15FO), which promises to have a larger magnetic moment than undoped $BiFeO_3$ (BFO).[3] As ferromagnetic layers $La_{0.7}Sr_{0.3}MnO_3$ and ferrimagnetic Sr_2FeMoO_6 have been deposited. Single crystal growth has been confirmed using XRD. Ferroelectric properties of BB15FO have been proven by piezoresponse force microscopy (PFM). Heterostructures have been investigated with regard to the exchange coupling using a SQUID magnetometer. [1] M. Vafaee Appl. Phys. Lett. **108**, 072401 (2016) [2] J. T. Heron, Nature **516**, 370 (2014) [3] R. Das, J. Magn. Magn. Mater. **324**, 1913 (2012)

DF 9.31 Tue 14:00 P1C

Tuning spin and charge orders in geometrically frustrated rare earth ferrites — •Sabreen Hammouda, Thomas Müller, Jörg Persson, and Manuel Angst — JCNS-2, Forschungszentrum ,Jülich, Germany

Rare earth ferrites RFe_2O_4 have attracted a lot of attention as prototypical examples of multiferroics, which have a potential use in information technology in particular due to their proposed new mechanism of ferroelectricity arising from charge ordering (CO) of Fe^{2+} and Fe^{3+} in the Fe/O bilayers [1]. The $YbFe_2O_4$ exhibits a behavior very similar to $LuFe_2O_4$ [2], consistent with the primary importance of the rare earth ion size, which is comparable for both Yb^{3+} and Lu^{3+}. Alternatively, the Y^{3+} ionic radius is much larger, and a completely different charge order was found [3].

Given the completely different CO in $LuFe_2O_4$, and YFe_2O_4, it is of high interest to study "how charge and spin orders change while tuning the relevant interactions by gradually increasing the rare earth ion radius, made by substitution", i.e. the substitution $Lu_xY_{1-x}Fe_2O_4$. However, a critical aspect have to be considered in such a study is that, for each substitution level x, the oxygen-stoichiometry needs to be fine-tuned, as otherwise O-stoichiometry changes are impossible to cleanly disentangle from the rare earth substitution.

I will present results from substituting Y (larger ion size) by the smaller Lu i.e. $Lu_xY_{1-x}Fe_2O_4$, particularly for $x = 0.5$.

[1] Ikeda et al., Nature 436, 1136 (2005). [2] Williamson et al., unpublished. [3] T. Mueller et al., J. Crystal Growth 428, 40 (2015).

DF 9.32 Tue 14:00 P1C

Synthesis and characterization of Bi - based double perovskites — •D. E. Saavedra Mesa[1,2], J. Roa-Rojas[1], A. U.B. Wolter[2], S. Aswartham[2], S. Wurmehl[2,3], and B. Büchner[2,3] — [1]Universidad Nacional de Colombia, Bogotá, Colombia — [2]Leibniz Institute for Solid State and Material Research, Dresden, Germany — [3]Institute of Solid State Physics TU Dresden, Dresden, Germany

The complex perovskite-type oxides with formula A2BB°O6 have been extensively investigated due to their wide range of physical properties. However, only four of them with Bi in the A position have been reported. Bi-based double perovskites are highly interesting because of their magneto-electric effects, where e.g. Bi2NiMnO6 has been found

to be ferroelectric below 480 K. Here, we present a systematic investigation of synthesis and characterization of new Bi-based double perovskites such as Bi2BB°O6 (B=Ho, Dy & B° = Mn, Co). Polycrystalline samples of Bi2HoMnO6 were synthesized by the conventional solid state reaction method. The structural analysis was carried out with powder X-ray diffraction (XRD) experiments. The surface morphology was studied by scanning electron microscopy (SEM), and the composition was analyzed using energy dispersive spectrometry (EDX).

DF 9.33 Tue 14:00 P1C

Directional dichroism via optical para-magnetoelectric effect in high magnetic fields — •David Szaller[1], Daniel G. Farkas[1], Vilmos Kocsis[1,4], Sandor Bordacs[1], Urmas Nagel[2], Toomas Room[2], Bence Bernath[3], Hiroshi Murakawa[4], and Istvan Kezsmarki[1] — [1]Dept. of Phys., Budapest Uni. of Tech. and MTA-BME Lendület Magn.-opt. Spect. Gr., Hungary — [2]Nat. Inst. of Chem. Phys. and Biophys., Estonia — [3]High Field Magnet Lab., Inst. for Molecules and Materials, The Netherlands — [4]RIKEN Center for Emergent Matter Science, Japan

Magnetoelectric multiferroics, i.e. materials simultaneously hosting ferroelectric and magnetic order, attract enormous interest due to their potential in IT applications. The magnetoelectric coupling present in these materials appears in the optical regime as the difference of absorption coefficients of counter-propagating light beams, which effect is termed as directional dichroism. This exotic phenomenon has been reported for spin excitations in multiferroic melilite single crystals and proposed as a new principle of directional light switches operating in the GHz-THz region. Applications seem to be limited to low temperatures where electric and magnetic order coexist. However, recent studies on melilites revealed that an external magnetic field can recover the electric polarization via the para-magnetoelectric effect far above the material's ordering temperature. Based on these static results we found strong directional dichroism in the paramagnetic phase of $Sr_2CoSi_2O_7$. The strength of the effect grows with the magnetic field, in accordance with the magnetoelectric sum rule.

DF 10: Focus: Spatio-Temporal Multiscale Optical Spectroscopy Meets Functional Materials (DF with O, CPP)

In this Focus Session, we want to bring together scientists from transient spectroscopy as well as materials scientists, concentrating on the physics of (light-induced) excitation, transport, and relaxation in functional materials. Besides presentation of experimental techniques for spatio-temporal multiscale spectroscopy, the emphasis is laid on models and analysis tools needed to understand experimental findings beyond time constants. The Focus Session is meant to join insights and interests, potentially establishing new collaborations between "different" communities.

Organizer: Christoph Merschjann TU Berlin

Time: Wednesday 9:30–12:30 Location: GER 37

Topical Talk DF 10.1 Wed 9:30 GER 37

Mobile electronic excitations studied by ultrafast spectroscopy — •Stefan Lochbrunner, Franziska Fennel, Steffen Wolter, and Tim Völzer — Institute of Physics, University of Rostock, Albert-Einstein-Str. 23, 18059 Rostock, Germany

The design of materials with specific photonic properties attracts currently intense scientific attention since they are the basis for many future applications in the fields of solar cells, detectors or light emitting devices. Understanding the behavior of light induced excitations in the materials is crucial for developing promising strategies. We apply time resolved spectroscopy on time scales ranging from femto- to milliseconds to characterize the sequence of processes and appearing species which result from the absorption of light. Two examples are presented in the talk. The migration of excitons due to Förster energy transfer is studied using a guest-host system based on dye molecules incorporated with a high concentration in PMMA. We characterized the influence of energetic disorder on the exciton mobility and developed a modified Förster theory which takes this effect correctly into account [1]. The dynamics of charge recombination in transition metal dichalcogenides is investigated by means of MoS_2. Evidence for defect assisted, bimolecular recombination is found by modelling the excitation dependent signal decay with corresponding rate equations.

[1] F. Fennel and S. Lochbrunner, Phys. Rev. B **92** (2015), 140301.

DF 10.2 Wed 10:00 GER 37

Diffuse transient absorption: a tool for investigation of powdery functional materials — •Christoph Merschjann — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, D-14195 Berlin, Germany — Universität Rostock, Institut für Physik, Albert-Einstein-Straße 23-24, D-18059 Rostock, Germany

Transient absorption (TA) spectroscopy is a wide-spread and versatile tool for investigating dynamic processes induced in functional materials. Typical quantities of interest include generation, spatial transport, separation (e.g. at interfaces), and ultimate recombination of (photo)excited charge-carriers, polarons, excitons, etc.
However, most novel functional solids are initially synthesized in powder form, and many applications (e.g. catalysis) demand for rather sponge-like or otherwise rough morphologies. Standard TA spectroscopy, which typically utilizes either direct transmission or specular reflection geometries, does not perform too well for such highly scattering materials.

Here, we present a femtosecond TA spectroscopy setup using diffuse reflection/transmission geometry, showing good results for a variety of functional materials, like polymeric carbon nitrides and TaON. A major challenge is the analysis of the retrieved data. Contrary to standard TA, a simple application of Lambert-Beer's law is not possible due to a wide distribution of optical pathlengths in the sample. Models and tools for photon propagation and mutual as well as light-matter interaction, to be used alongside those models needed for the kinetics of the excited states themselves, will be discussed.

Topical Talk DF 10.3 Wed 10:20 GER 37

Time-resolved characterization of photoactive materials using terahertz spectroscopy — •Rainer Eichberger — Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Charge carrier mobility and lifetime are key properties of photoactive semiconductor materials. To develop and better understand novel functional materials that enable direct conversion of sunlight into electricity or chemical fuels it is essential to characterize charge generation and separation as well as carrier transport and recombination processes with high time resolution and sensitivity. In conjunction, time-resolved terahertz spectroscopy (TRTS) and microwave conductivity (TRMC) can probe a broad photoconductivity time window from a few hundred femtoseconds to milliseconds. An additional advantage of TRTS is the possibility to measure frequency-dependent conductivity or mobility spectra by transferring the signal into the Fourier space, which gives a deeper insight into the nature of carrier transport and localization. We discuss the dynamics of photo-induced processes such as polaron formation in metal oxides and charge transport issues in polycrystalline chalcopyrite and kesterite thin films arising from carrier localization caused by bandgap fluctuations.

20 min. break

Topical Talk DF 10.4 Wed 11:10 GER 37

Theoretical simulations of pump-probe spectroscopies in solids — •Michael Sentef — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

In this talk I will discuss recent progress of theoretical simulations of the nonequilibrium dynamics following laser excitations on femtosecond time scales. I will show two examples: (i) the nonequilibrium dynamics following laser stimulation in a cuprate high-Tc superconductor, where an electron-boson dissipation pathway could be identified in a theoretical-experimental collaboration [1,2,3]; and (ii) the proposed generation of Floquet states in solids with the prospect of engineering effective Hamiltonians [4,5]. I will use this to discuss different theoretical approaches to the nonequilibrium many-body problem - from models to materials - and the future opportunities they offer for the field of pump-probe spectroscopies.

[1] M. A. Sentef et al., Phys. Rev. X 3, 041033 (2013)
[2] A. F. Kemper et al., Phys. Rev. B 90, 075126 (2014)
[3] J. D. Rameau et al., arXiv:1505.07055 → Nature Communcations
[4] M. A. Sentef et al., Nature Communications 6, 7047 (2015)
[5] H. Hübener et al., arXiv:1604.03399 → Nature Communications

DF 10.5 Wed 11:40 GER 37

Time-dependent quantum transport in nanosystems: A nonequilibrium Green's function approach — •Riku Tuovinen — Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — Department of Physics, Nanoscience Center, FIN 40014, University of Jyväskylä, Finland

Quantum transport is often discussed in the steady-state regime where the characteristics of the system are described in terms of the energy-dependent transmission or conductance. It is not guaranteed, however, that this description would capture the essential physics in, say, atomic-scale junction operating at high frequencies. Therefore, we consider the full time-dependence which also provides us with "transient spectroscopy" giving detailed information about the nanosystems out of equilibrium. A time-dependent extension to the Landauer–Büttiker approach is presented. The nonequilibrium Green's function approach is employed for describing the charge and heat transport dynamics. The importance of the method is that it provides a closed formula for the time-dependent density matrix in both electronic and phononic systems. In the electronic case the nonequilibrium conditions are due to a switch-on of a bias voltage in the leads or a perturbation in the junction whereas in the phononic case the junction is coupled to reservoirs of different temperatures. In both cases time-dependent transport properties, such as local charge and heat currents, may be evaluated without any propagation. Some applications with, e.g., graphene-based circuitries are presented and discussed.

Topical Talk DF 10.6 Wed 12:00 GER 37

Accessing micro- and mesoscopic ultrafast electron dynamics in low-dimensional materials — Michele Puppin[1], Christopher Nicholson[1], Melanie Müller[1], Roman Bertoni[1], Hannes Hübener[2], Angel Rubio[2], Claude Monney[3], Cephise Cacho[4], Martin Wolf[1], Alexander Paarmann[1], Laurenz Rettig[1], and •Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [3]Universität Zürich, CH — [4]STFC Rutherford Appleton Laboratory, UK

The coupling of electronic, phononic and spin degrees of freedom is at the heart of most phenomena in condensed matter and governs the flow and relaxation of charge carriers in out-of-equilibrium conditions. Microscopic coupling and correlation effects can be accessed quantitatively by time-, energy- and momentum-resolved information on ultrafast electron dynamics as obtained by time- and angle-resolved photoelectron spectroscopy (trARPES). I will discuss the generation of spin-, valley- and layer-polarized excited states in the semiconductor WSe_2 [1], their ultrafast evolution from 2D to 3D states, and the signatures of transient excited-state many-body interactions. In addition, the visualization of the spatio-temporal evolution of photocurrents in a nanowire by means of femtosecond point-projection microscopy will be discussed [2,3].

[1] Bertoni *et al.*, Phys. Rev. Lett., in print, arXiv:1606.03218.
[2] Müller *et al.*, Nature Comm. 5, 5292 (2014).
[3] Müller *et al.*, ACS Photonics 3, 611 (2016).

DF 11: Ferroics - Domains, Domain Walls and Skyrmions II

Chairs: Tadej Rojac and Istvan Keszmarki

Time: Wednesday 9:30–13:00 Location: WIL B321

Topical Talk DF 11.1 Wed 9:30 WIL B321

Implications of domain evolution during the growth of ferroelectric superlattices — Rui Liu, Benjamin Bein, Hsiang-Chun Hsing, Anna Gura, Mohammed Humed Yusuf, Giulia Bertino, Jin-Wen Lai, and •Matthew Dawber — Dept of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA

In ferroelectric superlattices the constituent materials are often under considerable epitaxial strain, raising their ferroelectric transition temperatures to the point where they are comparable to or exceed the growth temperature. This has a number of important consequences for the growth of the superlattice and it's eventual properties. For example, the polarization domain structure is markedly different depending on whether the overall structure's transition temperature lies constantly below, constantly above, or oscillates around the growth temperature. Perhaps more surprisingly, we have found that the ferroelectric polarization of a growing structure has a strong effect on the rate at which it grows, which is critical information if high quality samples with well defined layer thicknesses are to be achieved. A useful approach to investigating these questions is x-ray diffraction performed in-situ during the growth process. The precise control of both layer thicknesses and the arrangement of polarization domains are particularly important for applications of ferroelectric materials that rely on their polar surface structure, such as photocatalysis or the nanoscale control of the charge state of 2D materials.

DF 11.2 Wed 10:00 WIL B321

Probing in situ the polar states in growing multiferroic heterostructures — •Morgan Trassin, Gabriele De Luca, Sebastian Manz, and Manfred Fiebig — ETH Zurich, Switzerland

In ferroelectric thin films, the polarization state, i. e. orientation and domain architecture, defines the macroscopic ferroelectric properties such as the switching dynamics. Ferroelectric domain engineering is in permanent evolution from the epitaxial strain tuning to the chemical control on interface atomic termination. Technology promising complex polar flux closure or vortices architecture have been recently demonstrated in ferroelectric heterostructures. However the determination of the role of depolarizing field and local strain in the formation of these complex polar states remains challenging. The optical second harmonic generation process is an efficient and non-invasive tool for thin films ferroic properties probing. Here, we investigate the emergence of the ferroelectric polarization in ultra-thin ferroelectric and multiferroic films and monitor in situ the optical non-linear response of the film during the growth. We find that, the ferroelectric critical thickness and domain state can be measured in situ during the film deposition. Using a combination of epitaxial strain engineering and surface termination control in $(BiFeO_3/SrRuO_3)_n$ multilayers, we determine the $BiFeO_3$ net polarization orientation in each layer and in real-time, exempt from substrate contribution. Our work provides direct observation of ferroelectric states during the growth as well as new insights towards further control of ferroelectric based heterostructure.

DF 11.3 Wed 10:15 WIL B321

Early stage of ferroelectricity in $BaTiO_3$ multilayers — •Nives Bonacic[1], Gabriele De Luca[1], Marco Campanini[2], Marta D Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zürich, Department of Materials — [2]EMPA, Switzerland

Progress in the growth quality of transition-metal oxide heterostructures by pulsed-laser deposition greatly faciliated research of ultra-thin ferroelectrics with respect to their technological potential. In the thickness regime of a few unit cells, maintaining a large, stable and switchable ferroelectric polarization relies on the control of the strain state, thickness and interface termination in multilayers. Due to the complex interplay of these parameters, open questions remain about the intrinsic ferroelectric properties in the ultra-thin thickness regime. In order to understand the emergence of the ferroelectric polarization and determine the critical thicknesses involved, we use optical second harmonic

generation (SHG) during the film deposition to probe the formation of the ferroelectric order directly. Taking $(BaTiO_3\text{-}SrRuO_3)_n$-based multilayers as an example, we access the polarization of each ferroelectric layer separately and of the ferroelectric interlayer coupling using SHG. Within each $BaTiO_3$ layer, an abrupt transition from single domain to multi-domain state is evidenced. By tracking the SHG signal during growth continuously, we show that reduced dimension and electrostatic environment induce intermediate polar states not visible in the final structure. Following the dynamics of ferroelectricity emergence and evolution in-situ paves the way to definite answers on size-reduction effects and the dynamics of complex domain formation.

15 min. break

DF 11.4 Wed 10:45 WIL B321

Domain wall architecture in tetragonal ferroelectric thin films — •Gabriele De Luca[1], Marta D. Rossell[2], Jakob Schaab[1], Nathalie Viart[3], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, EMPA, Switzerland — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, France

Ferroic domain walls separate regions with a different orientation of the order parameter. The resulting lowering of the local symmetry enables properties that are otherwise not allowed in the bulk rendering them attractive for potential applications. Lead Zirconate Titanate (PZT) is the most important ferroelectric material to date, and its performance largely depends on the behaviour of its domains and domain walls. For example, in PZT thin films, out-of-plane-polarized c-domains are typically interspersed by in-plane-polarized a-domains that obstructs the controlled migration of 180° domain walls due to pinning at surface dislocations. Combining scanning transmission electron microscopy and nonlinear optics we determine the relation between strain, film thickness, local electric fields and the resulting domain and domain-wall structure across the entire thickness of various PZT films [1]. We find that the voltage-induced c-domain walls are inclined and exhibit a mixed Ising-Néel-type rotation of polarization across the wall with a specific nonlinear optical response. The domain wall tilt leads to a macroscopic tail-to-tail polarization component where accumulation of screening charges can be expected.

[1] G. De Luca et al., Adv. Mater. 28 (2016)

DF 11.5 Wed 11:00 WIL B321

Monoclinic superdomains in ferroelectric $K_{0.7}Na_{0.3}NbO_3$ thin films on $TbScO_3$ — •Leonard von Helden[1], Martin Schmidbauer[1], Dorothee Braun[1], Christoph Feldt[1], Michael Hanke[2], and Jutta Schwarzkopf[1] — [1]Leibniz Institut für Kristallzüchtung, Max-Born-Str. 2, 12389 Berlin — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteipl. 5-7, 10117 Berlin

$K_xNa_{1-x}NbO_3$ is a promising material for lead free ferro- and piezoelectric applications. Enhanced piezoelectric properties can be achieved by incorporating anisotropic lattice strain in epitaxial thin films. Monoclinic domains, which are favorable as they enable a continuous rotation of the polarization vector within the monoclinic mirror plane, were shown to be stabilized in $K_{0.7}Na_{0.3}NbO_3$ thin films grown by MOCVD on $TbScO_3$ substrates.[1]

In this study we present the coexistence of four variants of superdomains in $(001)_{pc}$ oriented $K_{0.7}Na_{0.3}NbO_3$ films on $TbScO_3$ with a film thickness of 30 nm. Below this thickness, only two types of superdomains occur. Each superdomain consists of periodically ordered stripe domains which are characterized by their vertical and lateral response in piezoresponse force micrographs (PFM) indicating different local piezoelectric coefficients. The domain structure can tentatively be described by monoclinically distorted unit cells, whose in-plane orientation is rotated by 90° between the stripe domains. A domain model is presented based on X-Ray diffraction experiments using a nano-focused beam.

[1] J. Schwarzkopf et al., J. Appl. Crys., 49, 375-384, (2016)

DF 11.6 Wed 11:15 WIL B321

Controlling the intrinsic polarization state in RF sputtering grown ferroelectric ultrathin films — •Christian Weymann, Céline Lichtensteiger, Stéphanie Fernandez, Jean-Marc Triscone, and Patrycja Paruch — DQMP, University of Geneva, Geneva, Switzerland

Ferroelectric ultrathin films are technologically promising. Crucial to all applications is their intrinsic polarization state. To maintain a uniform polarization state, the depolarizing field must be compensated either by external free charges or by internal mobile charges from within the ferroelectric itself. The built-in field also affects the polarization state, as it favors one polarization direction over the other. It results from an asymmetry in the screening or from internal sources, such as trapped charges or strain gradients leading to flexoelectricity.

We show that we can manipulate both these fields, acting on the electrostatic boundary conditions via the use of dielectric spacer layers to increase the depolarizing field, or modulating the built-in field through changes in the growth temperature of PbTiO3 thin films.

Quality and production costs are also major issues for applications. Off-axis radio frequency (RF) magnetron sputtering is a reliable technique to grow these structures. However, the relatively low cost of such a system compared to other thin film deposition techniques traditionally brings the disadvantage of lower control over the sample quality. Here we present a slow kinetics intermittent sputtering (SKIS) approach which greatly enhances the sample quality, opening a pathway towards an affordable method to grow high quality epitaxial thin films.

DF 11.7 Wed 11:30 WIL B321

Analysing the orientation distribution function of ferroelectric domains using vector piezoresponse force microscopy — •Markus Kratzer[1], Michael Lasnik[1,2], Felice Bombieri[1,2], Sören Röhrig[2], Marco Deluca[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Aiustria — [2]Materials Center Leoben Forschung GmbH, Austria

An important figure of merit for analyzing and improving the behavior of commercial piezoelectric actuators is the orientation distribution function (ODF) of the domains in ferroelectric ceramics. A common method to visualize piezoelectric domain orientations is Piezoresponse Force Microscopy (PFM). In principle, a three-dimensional reconstruction of the domain polarization can be obtained by measuring the out-of-plane and in-plane components of the domains (Vector PFM). On the basis of the material's piezoelectric tensor and multiple measurements on one sample, the vertical (1D) and lateral (2D) orientations of the domains are obtained, and the ODF can be reconstructed. Utilizing Vector PFM we investigated differently polarized lead zirconate titanate ceramics and commercial piezoceramic actuators. A newly developed data treatment algorithm allowed fast and reliable reconstruction of the domain ODF from three-dimensional Vector PFM data.

DF 11.8 Wed 11:45 WIL B321

Smart correction of SPM time series: can data analytics help us extract correlations? — •Iaroslav Gaponenko[1], Philippe Tückmantel[1], Benedikt Ziegler[2], Guillaume Rapin[1], Manisha Chhikara[1], and Patrycja Paruch[1] — [1]Department of Quantum Matter Physics, University of Geneva, 1211 Geneva, Switzerland — [2]Combine AB, 413 04 Gothenburg, Sweden

Since its inception, scanning probe microscopy (SPM) has established itself as the tool of choice for probing surfaces and functionalities at the nanoscale. Although recent developments in the instrumentation have greatly improved the metrological aspects of SPM, it is still plagued by the drifts and nonlinearities of the piezoelectric actuators underlying the precise nanoscale motion.

In this work, we present a novel computer-vision-based distortion correction algorithm for offline processing of functional SPM images, allowing two images to be directly overlaid with minimal error - correlating the position with time evolution and local functionality.

The algorithm is applied to two very different systems. First, the characteristics of surface folds and wrinkles in CVD graphene deposited on a polyethylene substrate are probed as a function of applied strain. Secondly, we demonstrate the tracking of polarization switching in an epitaxial $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin film during high-speed continuous scanning under applied tip bias. Thanks to the precise time-location-polarization correlation we can extract the regions of domain nucleation and track the motion of domain walls until the merging of the latter in avalanche-like events.

15 min. break

Topical Talk DF 11.9 Wed 12:15 WIL B321

The electro-caloric effect in $BaTiO_3$ from first principles — •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The electro-caloric effect (ECE), a temperature change observed in certain materials under application or removal of an electric field, provides an attractive perspective for future solid state cooling. Here, we

use molecular dynamics simulations for a first-principles-based effective Hamiltonian to study the ECE in the prototypical ferroelectric (FE) material $BaTiO_3$. Our simulations allow to gain a better understanding of the underlying mechanisms and to identify routes for optimizing the electro-caloric response towards future device applications. In particular, we discuss the anisotropy of the ECE for different directions of the applied electric field, and analyze the origin of an inverse effect (i.e. decreasing temperature under application of an electric field) that occurs at FE-FE phase transitions for certain orientations of the applied field. Finally, we explore ways to optimize the caloric response through epitaxial strain in thin films of $BaTiO_3$. We show that strain can be used to shift the largest caloric response to both higher and lower temperatures, depending both on the type of strain (compressive or tensile) and on the orientation of the applied field.

DF 11.10 Wed 12:45 WIL B321

Influence of domain walls on the electrocaloric effect — •Anna Grünebohm[1], Madhura Marathe[2], and Claude Marathe[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Materials Theory, ETH Zürich, Switzerland

The electrocaloric effect (ECE) is the adiabatic temperature change of a material in a varying external electrical field which is promising for novel cooling devices [1]. However, a large ECE is restricted to a small temperature range, which is above room temperature for standard ferroelectrics such as $BaTiO_3$. One way to shift the operation temperature is epitaxial strain [2,3]. Most important, tensile strain stabilizes a multi-domain ferroelectric phase which can enhance the caloric response in a broad temperature interval. We discuss the coupling between ferroelectric domains and the external electric field and its impact on the ECE by means of *ab initio* based simulations.

[1] X. Moya, *et al.*, Nature Mater. **13**, 439 (2014).
[2] M. Marathe, *et al.*, Appl.Phys.Lett, **104**, 212902 (2014).
[3] A. Grünebohm *et al.* Euro. Phys. Lett. **115**, 47002 (2016).

DF 12: PV XV - Dennis Meier

Time: Wednesday 13:15–13:45 Location: HSZ 01

Prize Talk DF 12.1 Wed 13:15 HSZ 01

Functional domain walls in multiferroic oxides — •Dennis Meier — Department of Materials Science and Engineering, NTNU, Trondheim, Norway — Laureate of the Gustav-Hertz-Prize

Oxide materials exhibit a broad range of tunable phenomena, including magnetism, multiferroicity, and superconductivity. Oxide interfaces are particularly intriguing. The low local symmetry combined with the sensitivity to electrostatics and strain leads to unusual physical properties beyond the bulk properties. Recently, ferroelectric domain walls have attracted attention as a novel type of oxide interface. These walls are spatially mobile and can be created, moved, and erased on demand. The additional degree of flexibility enables domain walls to take an active role in future devices and hold a great potential as multifunctional 2D systems for nanoelectronics.

In my talk I will discuss unique features that occur at ferroelectric domain walls in multiferroic oxides. In the first part, I will address geometrically driven charged domain walls in hexagonal manganites and show how their local electronic properties can be optimized and controlled. In the second part, I will consider domain walls in spin-spiral multiferroics with strong magnetoelectric couplings and additional functionality that arises from the interplay of charge and spin degrees of freedom. The goal is to provide insight into the exotic and fascinating physics at domain walls in multiferroics and their great application potential for next-generation devices.

DF 13: SYNS - Symposium Nanostructuring Beyond Conventional Lithography (MI with DS, DF, HL, MM and VA)

Time: Wednesday 15:00–17:45 Location: HSZ 02

Invited Talk DF 13.1 Wed 15:00 HSZ 02

The Limits to Lithography: How Electron-Beams Interact with Materials at the Smallest Length Scales — •Karl K. Berggren — Massachusetts Institute of Technology (MIT), 77 Massachusetts Ave., Cambridge, MA, USA

Electron-beam lithography is a ubiquitous tool required by the modern industry and research enterprise. The semiconductor industry relies on it for mask making, while researchers use it for prototyping advanced device concepts and structuring materials to achieve desired form and function. However, surprisingly the impact of the underlying physics of the interaction of electrons with radiolytic materials such as photoresist has been somewhat neglected in describing the limits of lithography. It has been known for some time that, lithographic systems suffer from spatial blurring due to the creation of secondary electrons and the propagation of these secondary electrons in space. What was not as well understood was the role of electro-galvanic effects–plasmons–in the limiting the performance of sub-10-nanometer lithography.

In this talk, I will describe efforts to improve the resolution and performance of sub-10-nm lithographic systems based on enhancement of resist processing. I will then point out the role plasmons (primarily in the bulk) play in limiting the resolution of lithography at the sub-10-nm scale. Finally, I will present some key applications of lithographic patterning at this length scale, and discuss the future implications of the work to related fields such as optical lithography, microscopy, and electromagnetic radiation generation.

Invited Talk DF 13.2 Wed 15:30 HSZ 02

High precision fabrication for light management at nanoscale — •Saulius Juodkazis[1,2] and Armandas Balcytis[1] — [1]Swinburne University of Technology, Melbourne, Australia — [2]Melbourne Center for Nanofabrication, Melbourne, Australia

For control of light-matter interactions occurring on molecular level we need to develop tools with nanoscale precision via nano-fabrication. Recent advances in high precision nanofabrication using 3D approaches and combining standard cleanroom tools with laser direct writing capabilities will be presented. Combination of electron beam lithography (EBL) with post-processing of nanoparticles with Ga-ion milling opens a possibility of sub-20 nm direct write of nano-inscriptions on nanoparticles. Arrays of identical chiral nanoparticles were fabricated with high fidelity and with uniform nano-features. Controlled resizing of ion-milled nanopores over the range of sizes from 100 nm to several nanometers in nano-membranes is achieved using electron beam scanning. Surface charging which is a common problem in applications of ion milling and electron imaging is resolved with co-illumination of deep UV light whose photons have energy larger than the electron work function for a given material. EBL and IBL can be both optimized for a high throughput for simple sample geometries. 3D laser fabrication of micro-optical elements and nano-textured surfaces adds new applications in lab-on-chip and sensing.

Invited Talk DF 13.3 Wed 16:00 HSZ 02

Directed self-assembly of performance materials — •Paul Nealey — University of Chicago and Argonne National Laboratory, Chicago, IL USA

Directed self-assembly (DSA) is arguably the most promising strategy for high-volume cost-effective manufacturing at the nanoscale. Over the past decades, manufacturing techniques have been developed with such remarkable efficiency that it is now possible to engineer complex systems of heterogeneous materials at the scale of a few tens of nanometers. Further evolution of these techniques, however, is faced with difficult challenges in terms of feasibility of implementation at the scale of 10 nm and below, and prohibitively high capital equipment costs. Materials that self-assemble, on the other hand, spontaneously form nanostructures down to length scales at the molecular

scale, but the micrometer areas or volumes over which the materials self-assemble with adequate perfection in structure is incommensurate with the macroscopic dimensions of devices and systems of devices of industrial relevance. Directed self-assembly (DSA) refers to the integration of self-assembling materials with traditional manufacturing processes to enhance and augment capabilities. Here I will discuss the use of lithographically-defined chemically patterned surfaces to direct the assembly of block copolymer films for semiconductor manufacturing and ion-conducting membranes, liquid crystal based systems for optoelectronics, and nanoparticles for applications in nanophotonics.

15 min. break

Invited Talk DF 13.4 Wed 16:45 HSZ 02

Nanometer accurate topography patterning using thermal Scanning Probe Lithography — •Armin W. Knoll — IBM Research - Zurich, Switzerland

In thermal Scanning Probe Lithography (t-SPL) [1-5] a heated tip with an apex radius of less than 5 nanometers is used to locally evaporate organic resists and thereby create well defined patterns. Key features of t-SPL are linear patterning speeds of up to 20 mm/s [3] and a resolution of $<$ 10 nm half pitch in resist and $<$ 15 nm after pattern transfer to the substrate [4]. High precision device fabrication is possible due to overlay accuracies of $<$ 5 nm [5]. In addition, 3D topography patterning with ˜1 nm (1 sigma) depth accuracy was demonstrated [2].

Examples of unique devices fabricated by t-SPL will be discussed, such as Gaussian shaped mesas in optical micro-cavities for light confinement and Brownian motors for transport and separation of nanoparticles in fluids.

References:
[1] D. Pires et al. Science, 328, 732-735 (2010).
[2] R. Garcia et al. Nature Nanotechnology 9, 577-587 (2014).
[3] P. Paul et al. Nanotechnology, 22, 275306 (2011).
[4] H. Wolf et al. J. Vac. Sci. Technol. B, 33, 02B102 (2015).
[5] C. Rawlings et al. ACS Nano, 9, 6188-6195 (2015).

Invited Talk DF 13.5 Wed 17:15 HSZ 02

High resolution 3D nanoimprint lithography — •Hartmut Hillmer — Institute of Nanostructure Technologies and Analytics (INA), University of Kassel, Germany

2D nanoimprint technologies have been widely investigated and are well established today, although huge research and development tasks have to be tackled in future since many scientific problems are not yet fully solved. In contrary, studies dealing with 3D nanoimprint technologies are still rare. This talk presents imprints of 3D structures:

1) 3D structures on substrates with very high spatial resolution in the vertical direction on substrates. Mesa arrays of laterally arbitrary shape with nominally perpendicular side walls towards the vertical direction have been fabricated by Substrate Conformal Imprint Lithography (SCIL). The height differences between the mesas are in the range of 2-3 nm and is some cases in the sub-nm range. These structures are embedded between Distributed Bragg Reflectors (DBRs) and define the cavities. These arrays of Fabry-Pérot Filters are applied as spectrometers. Since the entire different cavity heights are implemented by a single nanoimprint step, we label the device a nanospectrometer. The 3D templates have been fabricated using digital lithography. Applications of the imprinted nanospectrometer are demonstrated in food monitoring.

2) Released full 3D micro and 3D nano particles with arbitrary shape have been fabricated using our Self-Aligned NanoShaping (SANS) technology. The technological process involves a dual mold "waffle iron" principle. The novel SANS nanoimprint technology allows arbitrarily shaped 3D nanoparticles with precise size and shape control. Applications are intended in the field of pulmonal drug application in future.

References:
S. Schudy, M. Smolarczyk, H. Hillmer, N. Worpattrakul, F. Pilger, Patent application DE 10 2011 054 789.4
A. Albrecht, X. Wang, H.H. Mai, T. Schotzko, I. Memon, M. Bartels, M. Hornung and H. Hillmer, Nonlinear Optics and Quantum Optics 43, 339-353 (2012).

DF 14: Various Topics II

Nano- and microstructured dielectrics / thin films
Optical and nonlinear optical properties, photonic
High- and low-k-dielectrics
Dielectric surfaces and interfaces

Chair: Leonore Wiehl

Time: Wednesday 15:00–18:00 Location: GER 37

DF 14.1 Wed 15:00 GER 37

Applying of UV and IR nanosecond laser radiation for the nanostructuring of dielectric surfaces — •Pierre Lorenz, Igor Zagoranskiy, Lukas Bayer, Joachim Zajadacz, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, 04318 Leipzig, Germany

Dielectric nanostructures have a widespread field of applications. However, a fast and cost-effective production is still a challenge. Laser structuring methods using self-organized processes can solve the technological difficulties. The so-called ISPM-LIFE (laser-induced front side etching using in-situ pre-structured metal layer) method allows the nanostructuring of dielectric surfaces assisted by a laser-induced nanostructured metal film. The IPSM-LIFE can be separated into two steps: First, a low laser fluence treatment results in a nanopattern formation of the metal film, caused by instabilities of a thin molten metal. Second, a high-fluence treatment of the pre-structured metal film results in nanostructuring of the dielectric surface. Different metal layer (Cr, Mo, Ti) / dielectric substrate (fused silica, sapphire, BK7) systems were tested with UV laser (KrF excimer laser $\lambda = 248\,\mathrm{nm}$, $\Delta t_p = 25\,\mathrm{ns}$, $f = 1 - 200\,\mathrm{Hz}$) and IR laser (fiber laser $\lambda = 1064\,\mathrm{nm}$, $\Delta t_p = 1 - 600\,\mathrm{ns}$ with a time resolution of $1\,\mathrm{ns}$, $f = 2 - 100\,\mathrm{kHz}$). The resultant structures were investigated by atomic force (AFM) and scanning electron microscopy (SEM). The structuring process was simulated using a heat equation to describe the laser-heating of the solid and a kind of Navier-Stokes equation to describe the mass transport in the liquid.

DF 14.2 Wed 15:20 GER 37

Local charge injection and extraction on surface-modified Al_2O_3 nanoparticles in LDPE — •Riccardo Borgani[1], Love K. H. Pallon[2], Mikael S. Hedenqvist[2], Ulf W. Gedde[2], and David B. Haviland[1] — [1]Nanostructure Physics, KTH Royal Institute of Technology, Stockholm, Sweden — [2]Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

Nanocomposite polymer insulators are promising materials for high voltage direct current power transmission, due to their very low leakage current. We image the injection of charges around surface-modified aluminum oxide nanoparticles in a low-density polyethylene (LDPE) matrix[1] using a recently developed atomic force microscopy technique. Intermodulation Electrostatic Force Microscopy[2] allows us to image the surface potential around the individual nanoparticles under different bias conditions. The experimental results are consistent with the presence of shallow trap states (localized electronic states) in the LDPE near the nanoparticles, providing experimental evidence for a previously proposed explanation of the enhanced insulating properties of nanocomposite LDPE.

[1] R. Borgani, L.K.H. Pallon, M.S. Hedenqvist, U.W. Gedde, and D.B. Haviland, Nano Lett. 16, 5934 (2016).
[2] R. Borgani, D. Forchheimer, J. Bergqvist, P.-A. Thorén, O. Inganäs, and D. B. Haviland, Appl. Phys. Lett. 105, 143113 (2014).

DF 14.3 Wed 15:40 GER 37

In situ hard x-ray photoemission spectroscopy of barrier-height control at metal/PMN-PT interfaces — Erik Kröger[1], Adrian Petraru[2], Arndt Quer[2], Rohit Soni[2], Matthias Kalläne[1,3], Nikolay Pertsev[4], •Hermann Kohlstedt[2], and

Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, D-24143 Kiel, Germany — [3]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [4]Ioffe Institute, St. Petersburg, Russia

Metal-ferroelectric interfaces form the basis of novel electronic devices. A key effect determining the device functionality is the bias-dependent change of the electronic energy-level alignment at the interface. Here, hard x-ray photoelectron spectroscopy (HAXPES) is used to determine the energy-level alignment at two metalferroelectric interfaces Au versus SrRuO3 on the relaxor ferroelectric Pb(Mg1/3Nb2/3)0.72Ti0.28O3 (PMN-PT) directly in situ as a function of electrical bias. The bias-dependent average shifts of the PMN-PT core levels are found to have two dominant contributions on the 0.1 to 1 eV energy scale: one depending on the metal electrode and the remanent electric polarization and the other correlated with electric-field-induced strain. The results suggest electric-field-induced modifications of the polarization distribution as a novel way to control the barrier height at such interfaces.

E. Kröger et al., Phys. Rev. B 93, 235415 (2016).

DF 14.4 Wed 16:00 GER 37

The work function for Li^+-Ion Emission from Spodumene - a complete characterization of thermionic emission — •Martin Schäfer, Stephan Schuld, Mira Diekmann, and Karl-Michael Weitzel — Philipps-Universität Marburg

Experiments with ion beams have manifold applications, e.g. in surface structuring, in focused ion beam microscopy and micromachining, in micro-propulsion for space vehicles and for depth profiling in secondary ion mass spectrometry. Most of these applications rely on a strong and stable ion source. A classical means for generating strong ion beams is thermionic emission. In the current work [1], thermionic emission of Li+ from synthetic spodumene ($LiAlSi_2O_6$) has been investigated as a function of temperature and electric field. The data presented cover the entire range from space charge limited Child-Langmuir regime, to the Richardson-Dushman regime and finally the field assisted Schottky regime. From a self-consistent analysis of all data measured the work function for Li+ emission from synthetic spodumene is determined as (2.47 ± 0.015),eV. The thermionic currents exhibit a voltage offset of (1.7 ± 0.1) eV, which can be traced to a combination of the ionic work function of the emitter, the recombination energy Li^{++} electron, the electronic work function of the detector and the contact potential between detector and filament. Fundamental differences between ion emission and electron emission and their relevance for properties of Li-electrolytes in battery materials are discussed. [1] S. Schuld, M. Diekmann, M. Schäfer, and K. M. Weitzel, J. Appl. Phys. 120, (2016) 185102

20 min. break

DF 14.5 Wed 16:40 GER 37

Luminescent glasses for LED lighting — •Juliane Schuppich[1], Peter W. Nolte[2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Luebecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Luebecker Ring 2, 59494 Soest

Light emitting diodes (LEDs) are currently revolutionizing the lighting market. White LEDs are commonly realized by a blue emitting LED chip combined with a yellow emitting phosphor powder embedded in an organic polymer on top of the chip. However, the polymers are prone to aging due to high temperatures and high light intensities. This work describes an approach to replace the powder/polymer composite by a luminescent glass which offers a significantly higher thermal and chemical stability. Luminescent glasses have attracted much attention in the last decades, in particular for applications such as lasers, optical fibres, and optical amplifiers. Glass is very versatile and a good host for luminescent lanthanide ions; it provides high optical transparency, good lanthanide ion solubility, and it can be cast in almost any shape or size. Here, investigations performed on a blue LED covered with luminescent borate glass are presented. The glasses are analyzed for their optical parameters such as transmittance, reflectance, and quantum efficiency to provide a basis for subsequent optical simulations. The simulations are compared to photometric far-field measurements of the luminous intensity distributions and discussed in detail.

DF 14.6 Wed 17:00 GER 37

Tailoring metal-organic frameworks for enhanced two-photon absorption — •Lydia Nemec, Raghavender Medishetty, Roland A. Fischer, and Karsten Reuter — Technische Universität München

Two-photon absorption (2PA) is exploited in a wide range of applications such as photonics, three-dimensional data storage or fluorescence microscopy. The performance of typical molecular 2PA materials is often hindered by low molecular stability and concentration. A promising new material class to overcome these limitations are metal-organic frameworks (MOFs). In a joined experimental and theoretical venture, we demonstrate how MOFs can be tuned for enhanced 2PA properties, outperforming any currently known solid-state material with 2PA values of up to 3600 GM. We investigate the origin of the enhanced 2PA cross section through time-dependent density-functional theory calculations on the level of van der Waals corrected hybrid exchange-correlation functionals. Systematically exploring the influence of charge transfer, molecular strain and constraints, as well as structural arrangement, we identify five design criteria to enhance 2PA in MOFs.

DF 14.7 Wed 17:20 GER 37

Mid-infrared optical and plasmonic devices enabled by area-selective ion beam doping of silicon — •Martin Hafermann[1], Jad Salman[2], Raymond Wambold[2], Chenghao Wan[2], Jura Rensberg[1], Mikhail A. Kats[2], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Department of Electrical and Computer Engineering, University of Wisconsin - Madison, 1415 Engineering Drive, Madison, WI 53706, USA

The free charge carrier concentration of semiconductors is tunable over several orders of magnitude by impurity doping. Comparable to noble metals in the ultraviolet-visible spectral region, highly doped semiconductors possess "metal-like" optical properties but in the mid-infrared regime. Thus, the plasma frequency of these materials can be adjusted over a wide range by controlling the doping concentration. In this work, we fabricated optical and plasmonic devices in the mid-infrared using area-selective ion implantation of phosphorous through lithographically defined masks into silicon and subsequent annealing. Reaching doping concentrations on the order of 10^{21} cm^{-3} resulted in cross-over frequencies (where $\varepsilon_{\mathrm{real}} = 0$) in the range of 4 μm. Thus, we demonstrate diffractive optical elements such as Fresnel zone plates and diffraction gratings, as well as plasmonic devices like frequency selective surfaces. Our process results in optical devices that are CMOS compatible, completely planar and monolithic, thus stackable, as well as robust against high temperatures and physical erosion.

DF 14.8 Wed 17:40 GER 37

Self-consistent theory of Anderson localization for vector waves in disordered photonic media — •Zhong Yuan Lai, Michael Golor, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Anderson localization of light in a random dielectric system is still a controversial issue due to the vector nature of light. We investigate the effects of the vector nature of light on propagation properties in photonic crystals with binary disorder. Due to the transverse nature of light ($\nabla \cdot \vec{D} = 0$), the three vector components reduce to the well-known, two-fold polarization degrees of freedom, that is, in two orthogonal polarization modes on each lattice site in a three-dimensional lattice. It can be described as a pseudospin-$\frac{1}{2}$ degree of freedom. Hopping in the random lattice induces flipping of the pseudospin (mixing of the polarization modes) in analogy to random spin-orbit scattering in electronic systems. We generalize the photonic Coherent Potential Approximation (CPA) to this pseudospin system in order to calculate single-photon properties like the self-energy and density of states (DOS). To calculate transport properties, we generalize the Vollhardt-Wölfle theory of Anderson localization to the case of vector waves, using the pseudospin representation. We find localizing and antilocalizing contributions to the diffusion coefficient $D(\Omega)$ in the pseudospin singlet and triplet channels, analogous to random spin orbit scattering. We calculate the corresponding phase diagram of Anderson localization. Our results may provide a systematic way of analyzing the difficulties in achieving light localization in experiments.

DF 15: Ferroics - Domains, Domain Walls and Skyrmions III

Chair: Weida Wu

Time: Wednesday 15:00–17:30 Location: WIL B321

Topical Talk DF 15.1 Wed 15:00 WIL B321

Domain and fluctuation dynamics in magnetoelectric multiferroics — •Joachim Hemberger — Institute of Physics II, University of Cologne, Germany

Multiferroic systems comprise hybrid order parameters which couple e.g. non-collinear spin structures to ferroelectric polarization. This talk raises the question concerning the the dynamics of the corresponding fluctuations and discusses results for exemplary magnetoelectric systems on the basis of broadband linear and non-linear dielectric spectroscopy.

E.g. in $MnWO_4$ one observes a critical slowing down of a magnetoelectric soft-mode above the multiferroic transition [1], while the dielectric response within the ordered phase is dominated by the dynamics of domains [2]. Thus both electric field driven phenomena resemble the behavior of canonical ferroelectrics, but an analysis of the corresponding dynamical exponents reveals differences reflecting the magnetic nature of the underlying order parameter.

Similar findings can be reported for other spin-spiral multiferroics like $TbMnO_3$, $Ni_3V_2O_8$, or even the spin chain $LiCuVO_4$ effected by quantum fluctuations. In addition, the merely magnetic field induced domain and fluctuation dynamics in the non-multiferroic but linear magnetoelectric $TbPO_4$ shall be discussed.

[1] D. Niermann, C.P. Grams, P. Becker, L. Bohatý, H. Schenck, and J. Hemberger, Phys. Rev. Lett. **114**, 037204 (2015)

[2] D. Niermann, C.P. Grams, M. Schalenbach, P. Becker, L. Bohatý, J. Stein, M. Braden, and J.H., Phys. Rev. B **89**, 134412 (2014)

DF 15.2 Wed 15:30 WIL B321

Probing polar order in improper ferroelectric thin films using SHG — •Johanna Nordlander[1], Gabriele De Luca[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Departments of Materials, ETH Zürich, Switzerland — [2]Electron Microscopy Center, EMPA, Switzerland

Improper ferroelectrics are materials whose ferroelectricity is driven by a non-polar order parameter. This type of ferroelectricity can lead to exotic properties which do not exist in standard ferroelectrics. For example, improper ferroelectricity in hexagonal $YMnO_3$ (YMO), which is geometrically driven through a lattice trimerization, leads to a topological domain vortex pattern. There has been a revival in the growth of improper ferroelectric thin films, and these bulk-like ferroelectric domain vortices were also reported in YMO thin epitaxial layers. In order to understand the behavior of ultrathin YMO, and in particular in order to investigate the influence of epitaxial strain on the ferroelectric trimerization, we use optical second harmonic generation (SHG) to non-invasively probe the ferroic state of these thin films for different epitaxial growth conditions. Here, we demonstrate the growth of highly oriented, epitaxial hexagonal YMO thin films by pulsed laser deposition on various substrates. We report reversible scanning-probe-tip-induced ferroelectric switching and the subsequent spatially resolved SHG analysis. The temperature-dependent emergence of the coexisting magnetic and electric orders is investigated by SHG. Ultimately, we provide a deeper insight into the mechanism of ferroelectric domain vortex formation and antiferromagnetism in thin film YMO.

DF 15.3 Wed 15:45 WIL B321

Inner structure of topological defects in hexagonal manganites — Kostantin Shapovalov[1], Megan Holtz[2], Julia Mundy[2], David Muller[2], Zewu Yan[3], Edith Bourret-Courchesne[3], Dennis Meier[4], and •Andrés Cano[1] — [1]CNRS, Univ. Bordeaux, ICMCB, Bordeaux, France — [2]Cornell University, Ithaca, NY, USA — [3]Lawrence Berkeley National Laboratory, Berkeley, CA — [4]Norwegian University of Science and Technology, Trondheim, Norway

Structural domain walls and vortices are two different incarnations of topological defects in the hexagonal manganites RMnO3. These entities display intriguing functional features related to their local transport properties and can be regarded as analog systems for the study of the formation of cosmic strings in the early universe. We develop a field-theory description of their inner structure supporting the experimental characterization of these defects by means of HAADF scanning transmission electron microscopy. Our theory reveals novel features such as the emergence of a continuous U(1) symmetry at the vortex cores and a multipolar charge (re-)distribution that become universal in these regions. These inner features are expected to bring forth an additional degree of functionality to these topological defects.

DF 15.4 Wed 16:00 WIL B321

Modeling domain wall dynamics in multiferroic hexagonal manganites — Xiaoyu Wu[1], Urko Petralanda[2], Lu Zheng[1], Yuan Ren[1], Rongwei Hu[3], Sang-Wook Cheong[3], •Sergey Artyukhin[2], and Keji Lai[1] — [1]Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA — [2]Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova, Italy — [3]Rutgers Center for Emergent Materials and Department of physics and Astronomy, Rutgers University, Piscataway, NJ 08854

Multiferroic materials with coexisting magnetic and ferroelectric orders hold promise for the manipulation of magnetism by applied electric fields. These effects were demonstrated [1] to be controlled by the dynamics of strongly interacting domain walls of different types. We report on modeling the electric field - driven dynamics of ferroelectric domain walls in hexagonal manganites, where ferroelectric polarization is produced due to condensation of a trimerization mode [2]. The dynamics is studied using a tight-binding model with parameters derived from first-principles calculations.

[1] Y. Tokunaga et al. Nature Materials 8, 558 (2009) [2] S. Artyukhin, K.T. Delaney, N.A. Spaldin, and M. Mostovoy, Nature Materials 13, 42 (2014) [3] C. J. Fennie and K. M. Rabe, Phys. Rev. B 72, 100103(R) (2005)

15 min. break

DF 15.5 Wed 16:30 WIL B321

A numerical approach to optical second harmonic generation imaging of multiferroic domains — •Thomas Lottermoser, Christoph Wetli, Amadé Bortis, and Manfred Fiebig — Department of Materials, ETH Zürich, Zürich, Switzerland

Due to its direct coupling to symmetry optical second harmonic generation (SHG) has been established as a versatile tool for the investigation of magnetoelectric multiferroics. As the only method it allows a non-invasive and simultaneous access to both, the electric and magnetic order of a multiferroic in a single experiment. It not only gives access to the often complex and interlinked interactions of the related order parameters on a macroscopic level, but also spatially resolved on the level of domains. Nevertheless, as any optical imaging method also SHG imaging is limited by the optical resolution of about one micron. Here we present a numerical model based on a statistical analysis of the domain imaging to overcome this limitation and to reveal information of the domain topology and their size distribution even several orders of magnitude below the resolution limit. The model is tested numerically against different domain topologies like the well known antiferromagnetic and ferroelectric domain structures that occur in the multiferroic hexagonal manganites. We can distinguish these different structures by the respective intensity of the SHG response, even if their domains are of equal lateral size.

DF 15.6 Wed 16:45 WIL B321

Local structure and structural coherence across the ferroelectric phase transition of h-$YMnO_3$ — •Sandra Helen Skjaervø[1], Quintin Meier[2], Emil Božin[3], Simon Billinge[3,4], Mikhail Feygenson[5], Nicola Spaldin[2], and Sverre Selbach[1] — [1]Dept. Mat. Sci. Eng, NTNU, Norway — [2]Dept. Mat., ETH Zürich, Switzerland — [3]Brookhaven Natl. Lab., Condensed Matter Phys. & Mat. Sci. Dept., Upton, USA — [4]Columbia Univ, Dept. Appl. Phys. & Appl. Math., New York, USA — [5]Forschungszentrum Jülich, JCNS

We use pair distribution function (PDF) analysis to investigate the nature of the high-temperature (∼1270 K) structural phase transition in multiferroic hexagonal $YMnO_3$. Upon the phase transition, the unit cell is known to triple as the Mn-O_5 polyhedra tilt in trimers and the Y atoms alternatively displace along the tilt axis, with a ferroelectric polarization arising from a coupling to a secondary Y displacement. Whether the polarization emerges simultaneously with the high-temperature structural distortion or a many hundred degrees

lower remains controversial [1,2]. We have measured high-temperature neutron total scattering data at Oak Ridge Natl. Lab. We analyse the data as PDFs to investigate the short range order and structural coherence. We see that the transition shows both displacive and order-disorder character, and we explain the short range mechanisms behind the ferroelectric transition. [1] Lilienblum, M. et al. "Ferroelectricity in the multiferroic hexagonal manganites". Nature Physics, 11, 2015. [2] Nénert, G. et al., "Experimental evidence for an intermediate phase in the multiferroic $YMnO_3$". J. Phys.: Condensed Matter 19, no. 46, 2007.

DF 15.7 Wed 17:00 WIL B321

Kibble-Zurek mechanism in $RMnO_3$ — •Quintin Meier[1], Andres Cano[1,2], Martin Lilienblum[1], Manfred Fiebig[1], and Nicola A. Spaldin[1] — [1]ETH Zürich, Department of Materials, Zürich, Switzerland — [2]CNRS, Univ. Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

We use density functional and Landau-Ginzburg theories to investigate the role of critical fluctuations on the structural phase transition in the ferroelectric hexagonal manganites $RMnO_3$ (R = Y or a element of the rare-earth series). These multiferroic materials are of interest because their improper ferroelectricity leads to an unusual domain structure that has been interpreted in terms of the Kibble-Zurek mechanism in the fluctuation dominated Ginzburg regime [1]. We discuss the effect of critical fluctuations and their influence on the Kibble-Zurek mechanism by studying trends in the domain-formation behavior across the series by comparing with new experimental data.

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

DF 15.8 Wed 17:15 WIL B321

Interstitial oxygen as a source of p-type conductivity in $RMnO_3$ hexagonal manganites — Sandra H. Skjaervø, Espen T. Wefring, Silje K. Nesdal, Nikolai H. Gaukås, Gerhard H. Olsen, Julia Glaum, Thomas Tybell, and •Sverre M. Selbach — NTNU Norwegian University of Science and Technology, 7491 Trondheim, Norway

We use a combination of experiments and first principles electronic structure calculations to elucidate the effect of interstitial oxygen anions, Oi, on the electrical and structural properties of h-$YMnO_3$. Hexagonal manganites, h-$RMnO_3$ (R = Sc, Y, Ho-Lu) have been intensively studied for their multiferroic properties and magnetoelectric coupling, topological defects and electrically conducting domain walls. Although point defects strongly affect the conductivity of transition metal oxides, the defect chemistry of h-$RMnO_3$ has received little attention. Enthalpy stabilized interstitial oxygen anions are here shown to be the main source of p-type electronic conductivity, without reducing the spontaneous ferroelectric polarization [1]. A low energy barrier interstitialcy mechanism is inferred from Density Functional Theory calculations to be the microscopic migration path of Oi. Since the Oi content governs the concentration of charge carrier holes, controlling the thermal and atmospheric history provides a simple and fully reversible way of tuning the electrical properties of h-$RMnO_3$.

[1] S. H. Skjaervø, E. T. Wefring, S. K. Nesdal, N. H. Gaukås, G. H. Olsen, J. Glaum, T. Tybell, S. M. Selbach, Nat. Commun. 7, 13745 (2016).

DF 16: Crystallography - Poster Session (KR with DF)

Time: Wednesday 18:00–20:00 Location: P4

DF 16.1 Wed 18:00 P4

Structural and magneto-electric investigations of Erythrosiderites — •Tobias Fröhlich[1], Daniel Brüning[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

Most erythrosiderites of the form $A_2[FeX_5(H_2O)]$ are magneto-electric without multiferroicity. However, in 2013 it was found that the compound $(NH_4)_2[FeCl_5(H_2O)]$ is multiferroic. A comparison of macroscopic and microscopic properties of different compounds of this family reveals interesting insights into the structural order and magnetic coupling. While the crystal structures of most erythrosiderites can be described with space group *Pnma*, $Cs_2[FeCl_5(H_2O)]$ has space group *Cmcm*. In contrast to the other compounds [1, 2], its magnetic structure is not yet directly determined. However, there are investigations of macroscopic quantities, which allow to predict the magnetic structure [3]. We present a neutron study of the magnetic structure of $Cs_2[FeCl_5(H_2O)]$, which perfectly explains these measurements. Furthermore, $Cs_2[FeCl_5(H_2O)]$ exhibits a structural phase transition which was discovered in 1987 [4]. By single crystal X-ray diffraction, we solved the structural distortion associated with this transition, which involves a slight monoclinic distortion into space group $C2/c$.

[1] M. Gabás et al. (1995), J. Phys. Condens. Matter **7** 4725-4738 [2] J. Rodrígues-Velamazán, et al. (2015), arXiv [3] M. Ackermann et al. (2014), J. Phys. Condens. Matter **26** 506002 [4] J. Chadwick et al. (1987), J. Phys. C: Solid State Phys. **20** 3979-3983

DF 16.2 Wed 18:00 P4

Investigation of new phases in the Ba-Si phase diagram under high pressure by ab initio structural search — •Jingming Shi[1], Wenwen Cui[1], José Flores-Livas[2], Alfonso San-Miguel[1], Silvana Botti[3,1], and Miguel Marques[4,1] — [1]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne Cedex, France — [2]Department of Physics, Universität Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [4]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Barium silicides are versatile materials that have attracted attention for a variety of applications in electronics and optoelectronics. Using an unbiased structural search based on a particle-swarm optimization algorithm combined with density functional theory calculations, we investigate systematically the ground-state phase stability and structural diversity of Ba–Si binaries under high pressure. The phase diagram turns out to be quite intricate, with several compositions stabilizing/destabilizing as a function of pressure. In particular, we identify novel phases of BaSi, $BaSi_2$, $BaSi_3$, and $BaSi_5$ that might be synthesizable experimentally over a wide range of pressures. Our results not only clarify and complete the previously known structural phase diagram, but also provide new insights for understanding the Ba–Si binary system.

DF 16.3 Wed 18:00 P4

Watching the Verwey transition of Magnetite by Timeresolved X-Ray diffraction — •Alexander von Reppert[1], Jan-Etienne Pudell[1], Flavio Zamponi[1], Azize Koc[2], Stephan Geprägs[3], Jose Emilio Lorenzo[4], Luc Ortega[5], Matthias Reinhardt[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht Str. 24-25, 14476 Potsdam, Germany — [2]Helmholtz-Zentrum Berlin BESSY II, Albert-Einstein Str. 15, 12489 Berlin, Germany — [3]Walther-Meißner-Institut, Bayerische Akademie d. Wissenschaften, 85748 Garching, Germany — [4]Institut Nèel, CNRS & Univ. Grenoble Alpes, 38042 Grenoble, France — [5]Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France

We present timeresolved X-Ray diffraction from a 300 nm thin Magnetite(Fe3O4) film that is driven across the Verwey transition by fs-laser excitation. The prototypical insulator to metal transition at 123 K is accompanied by a peak intensity increase and peak width decrease of structural Bragg peaks, which we attribute to the destruction of trimerons that lead to inhomogeneous lattice strain in the low T phase. Our systematic investigations of the lattice dynamics yield two timescales: An ultrafast peak width drop - probably due to electronic processes - which is subsequently enhanced by transport and equilibration of the excitations. Complementary to our lab-based Plasma X-Ray source we conducted measurements at the XPP beamline at the synchrotron BESSY II where we observe that the recovery timescale depends crucially on the proximity to the transition temperature.

DF 16.4 Wed 18:00 P4

Detection of pressure and density waves (acustic waves) in liquid crystal near the phase transition temperature by gold nano particle — •Ricardo Rose, Andre Heber und Frank Ci-

CHOS — Universität Leipzig Fakultät für Physik und Geowissenschaften, Leipzig, Germany

Recent studies have shown, that the intensity of a polarized laser beam can be modulated by a second heating laser beam, which excites plasmons on gold nanoparticles (AuNp) positioned in liquid crystal (LC). The exited AuNp dissipate the energy as heat into the LC. If the LC is near below the phase transition point from nematic phase to isotropic phase, the dissipated heat will suffice to build an isotropic bubble around the AuNp. The size of the bubble can be controlled by the amount of supplied energy. While the polarization within the nematic phase is rotated due to different refractive indices for the ordinary and extraordinary axis similar to a $\lambda/2$ - plate, the polarization will be conserved within the isotropic phase. If an analyzer is placed behind the LC, the intensity of the probe laser beam can be modulated by the optical path length within the nematic phase and their disturbance within the isotropic bubble around the laser heated AuNp. In this study we investigate, if the deformation of the isotropic bubble by acoustical waves and the linked modulation of the probe laser beam intensity at constant, unmodulated power of the heating laser will be clearly detectable, while the ambient temperature is near the phase transition temperature. If that can be proven, we will able to design a microphone at nano size.

DF 16.5 Wed 18:00 P4

Ga^{3+} Substitution in the Brownmillerite-Type Phase $Ca_2Fe_2O_5$: Structural and Spectroscopic Investigations — •QUIRIN STAHL[1,2], ANDREAS REYER[1], REINHARD WAGNER[1], GEROLD TIPPELT[1], and GÜNTHER J. REDHAMMER[1] — [1]Department Chemistry and Physics of Materials, University of Salzburg, Austria — [2]Institute of Structural Physics, Technische Universität Dresden

Brownmillerite-type compounds with the general formula $A_2B'_{2-x}B_xO_5$, where A = alkaline earth metals and B'/B = group III or transition-metal atoms, are among the most frequently studied oxygen-deficient perovskites. 61 synthetic single-crystal samples of $Ca_2Fe_{2-x}Ga_xO_5$ with $0.00 \leq x \leq 1.328$ have been investigated by single-crystal X-ray diffraction at RT. We find that pure $Ca_2Fe_2O_5$ and samples up to x = 0.989 have space group *Pnma*, Z = 4, whereas samples with x > 0.989 show $I2mb$ symmetry, Z = 4. We also performed a detailed Raman study of Ga^{3+} and Al^{3+} doped $Ca_2Fe_2O_5$. The polarized Raman measurements of $Ca_2Fe_{2-x}Ga_xO_5$ single-crystals enable us to assign eleven of the thirteen theoretically predicted A_g modes. Furthermore the change from *Pnma* to $I2mb$ space group symmetry is reflected by a significant change of two Raman modes below 150 cm^{-1}. These Raman modes are obviously linked to changes of the Ca-O bond lengths at the phase transition. To complete the study of the $Ca_2Fe_{2-x}Ga_xO_5$ series, we have performed a detailed Mössbauer spectroscopic study as a function of the chemical composition, mainly to fix site occupation number by a second, independent method beside XRD.

DF 16.6 Wed 18:00 P4

Synthesis and controlled growth of α-RuCl3 crystals on the nanoscale via chemical vapour transport (CVT) — •MARTIN GRÖNKE, MIHAI-IONUT STURZA, BARBARA EICHLER, SANDRA SCHIEMENZ, VICTORIA ECKERT, SILKE HAMPEL, and BERND BÜCHNER — IFW Dresden

Crystal growth of different transition metal halogenides representing a very up to date research topic in solid state chemistry surface physics. Among the interest for materials with strong anisotropic bonding-dependent interactions, resulting frustration effects could stabilize new patterns of cooperative magnetic interactions, or even a spin-liquid-state. One candidate to realize a Kitaev spin model is the layered honeycomb magnet α-Rutheniumchloride (α-RuCl3) with strongly frustrated, anisotropic interactions between spin-orbit entangled jeff = 1/2 Ru3+ magnetic moments.

Physical properties in nanoscale systems may differ from the respective bulk phase and could even lead to novel physical properties. Herein we present to our knowledge the first approach to synthesize phase pure α-RuCl3 crystals on the nanoscale via chemical vapour transport (CVT). To understand the growth mechanisms and to optimize the synthesis we performed thermodynamic modelling with the program Tragmin. We obtained very thin single crystals by CVT with heights around 40 nm. The crystal habit is characterized by means of SEM, TEM and AFM. Furthermore EDX, WDX, XRD, micro-RAMAN and SQUID-VSM measurements proving composition, phase-purity and predicted magnetic properties.

DF 17: Ferroics - Domains, Domain Walls and Skyrmions IV

Chairs: Claude Ederer and Petro Maksymovych

Time: Thursday 9:30–13:30 Location: WIL B321

Topical Talk DF 17.1 Thu 9:30 WIL B321

Magnetic and orbital excitations in the multiferroic skyrmion host GaV_4S_8 — DIETER EHLERS[1], ZHE WANG[1], HANS-ALBRECHT KRUG VON NIDDA[1], VLADIMIR TSURKAN[1], PETER LUNKENHEIMER[1], ISTVAN KÉZSMÁRKI[2], IOANNIS STASINOPOULOS[3], DIRK GRUNDLER[4], and •ALOIS LOIDL[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Department of Physics, Budapest University of Technology, Hungary — [3]Lehrstuhl für Physik funktionaler Schichtsysteme, Physik Department, TUM, Munich, Germany — [4]EPFL, Institut des matériaux, Lausanne, Switzerland

The lacunar spinel GaV_4S_8 exhibits a complex magnetic phase diagram, including ferromagnetic, cycloidal and Néel-type skyrmion phases [1,2]. Orbital ordering induces ferroelectricity [3] and spin-driven excess polarizations emerge in all magnetic phases, including skyrmions with ferroelectric polarization [2]. We present a detailed discussion on orbital and skyrmion excitations using THz and coplanar waveguide (CPW) absorption spectroscopy. At THz frequencies dipolar relaxations are strongly coupled to the orbital dynamics, establishing an orbitally-driven ferroelectric phase [3]. Using broadband CPW absorption spectroscopy we study the temperature and frequency dependence of skyrmion excitations [4].

[1] I. Kézsmárki *et al.*, Nature Materials **14**, 1116 (2015).
[2] E. Ruff *et al.*, Science Advances **1**, E1500916 (2015).
[3] Zhe Wang *et al.*, Phys. Rev. Lett. **115**, 207601 (2015).
[4] D. Ehlers *et al.*, Phys. Rev. B **94**, 014406 (2016).

DF 17.2 Thu 10:00 WIL B321

Investigating the structural phase transition of GaV_4S_8 — •JONATHAN DÖRING[1], ÁDÁM BUTYKAI[2], ISTVAN KÉZSMÁRKI[2], PETER MILDE[1], SUSANNE C. KEHR[1], and LUKAS M. ENG[1] — [1]Technische Universität Dresden, Institut für Angewandte Physik — [2]MTA-BME Lendület Magneto-optical Spectroscopy Research Group

GaV_4S_8 (GVS) is a lacunar spinel. As most materials of this group, it features several magnetic phases at low temperatures, most notably a skyrmion lattice (SkL) phase between 9 K and 13 K under low magnetic fields [1]. Upon cooling below $T = 42$K, GVS exhibits a Jahn-Teller phase transition, changing the crystal structure from paraelectric cubic to ferroelectric rhombohedral. The multiferroic nature of the skyrmions offers interesting application perspectives in magnetoelectronics.

We study GVS by means of low-temperature piezoresponse force microscopy (LT-PFM) [2] and low-temperature scattering scanning near-field optical microscopy (LT-s-SNOM) [3] in order to characterize the ferroelectric domain configurations on the nanometer length scale. LT-PFM measurements are performed at temperatures both below and above the Jahn-Teller phase transition on as-grown (100) and (111) surfaces of single crystalline GVS. We observe several types of domain configurations in the rhombohedral phase. Applying LT-s-SNOM shows an enhanced response at wavelengths around $\lambda = 31.5\ \mu m$ close to a GVS phonon mode, enabling IR-imaging of the crystal anisotropy.

[1] Kezsmarki, I. et al., Nature Materials 14, 1116-1122 (2015)
[2] Butykai, A. et al., submitted
[3] Döring, J. et al., Applied Physics Letters 105, 053109 (2014)

DF 17.3 Thu 10:15 WIL B321

Searching for prospective multiferroic compounds hosting skyrmion lattices — •ERIK NEUBER[1], PETER MILDE[1], ISTVAN KÉZSMÁRKI[2], and LUKAS ENG[1] — [1]Institut für Angewandte Physik, TU Dresden, D-01069 Dresden, Germany — [2]Dep. of Physics, Bu-

dapest Univ. of Technol. and Econ. and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, Hungary

Following earlier predictions, skyrmion lattices (SkL), i.e. non-collinear periodic arrays of (chiral) spin vortices, are now reported to exist in various magnetic crystals of mostly chiral structure [1]. Nevertheless, also non-chiral but polar materials possessing the C_{nv} symmetry have been identified as ideal SkL-supporting hosts. GaV_4S_8 (GVS), a multiferroic polar magnetic semiconductor with rhombohedral (C_{3v}) symmetry, constitutes the first such candidate that has thoroughly been investigated [2]. GVS not only shows easy axis anisotropy that firmly pins SkL vortices even under external magnetic fields, but, furthermore, surprises with an unusally-broad temperature range that exhibits SkL ordering. Motivated by this great success, more such unusual SkL-materials with multiferroic properties must exist, even in the family of lacunar spinels [3]. In this contribution, we will briefly review on the real-space exploitation of such SkLs in GVS by scanning probe techniques, and report on our fascinating search for further such materials exhibiting a similar behavior to GVS.

[1] P. Milde et al., Science **340**, 1076 (2013). [2] I. Kézsmárki et al., Nat. Mater. **14**, 1116 (2015). [3] H.-S. Kim et al., Nat. Commun. **5**, 3988 (2014).

15 min. break

DF 17.4 Thu 10:45 WIL B321

Dielectric properties of organic charge-transfer salts — •Jonas K. H. Fischer[1], Peter Lunkenheimer[1], Rudra Manna[2], Harald Schubert[3], Michael Lang[3], Jens Müller[3], Stephan Krohns[1], John A. Schlueter[4], Cecile Mézière[5], Patrick Batail[5], and Alois Loidl[1] — [1]Experimental Physics V, EKM, University of Augsburg, Augsburg, Germany — [2]Experimental Physics VI, EKM, University of Augsburg, Augsburg, Germany — [3]Phys. Inst. Univ. Frankfurt, SFB/TR 49, Frankfurt, Germany — [4]Materials Research, National Science Foundation, Arlington, Virginia, United States — [5]Laboratoire MOLTECH, UMR 6200 CNRS-Université d'Angers, Bt. K, UFR Sciences, Angers, France

The EDT-TTF-based charge-transfer salts have attracted considerable attention due to their intriguing dielectric properties [1]. An example is κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, which exhibits multiferroicity [2]. Its polar moment was suggested to arise from molecular dimerization, combined with charge order. Other interesting recent examples include α-(BEDT-TTF)$_2$I$_3$, which shows the signature of relaxor-ferroelectric behavior [1]. Here, we will present an overview of the dielectric properties of the above systems and provide new results on κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl, which also seems to show ferroelectric behavior in its charge-ordered state. In addition, we present measurements of δ-(EDT-TTF-CONMe$_2$)$_2$Br. This compound lacks dimerization, but exhibits charge order already at room temperature.

[1] P. Lunkenheimer and A. Loidl, J. Phys.: Condens. Matter **27**, 373001 (2015). [2] P. Lunkenheimer *et al.*, Nat. Mater. **11**, 755 (2012).

DF 17.5 Thu 11:00 WIL B321

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

Multiferroic $Dy_{0.7}Tb_{0.3}FeO_3$ is reported to host a magnetically-driven spontaneous polarization below 2.65 K. This polarization emerges as a result of exchange interaction between Fe^{3+} spins and rare-earth moments. At about 2 K the polarization vanishes due to the change in the magnetic phase of iron (ferromagnetic to antiferromagnetic). Some models have been proposed on the magnetoelectric coupling in this material but a profound experimental study is yet to be done. Here we investigate the magnetic and electric order at the level of domains using spatially resolved techniques. We employ optical Faraday effect and second harmonic generation (SHG) to investigate the magnetic and electric order respectively. Our results reveal that the transition at 2 K is not sharp and the two types of ordering for the Fe^{3+} spins coexist simultaneously from which only one (ferromagnetic phase) contributes to the spontaneous polarization. The volume ratio of these two phases, and hence the amplitude of the ferroelectric polarization, can be controlled via an external magnetic field.

DF 17.6 Thu 11:15 WIL B321

Strong magnetoelectric coupling within ceramic core-shell structures — •Leonard Henrichs[1], Torsten Scherer[1], James Benett[2], Andrew Bell[2], Oscar Cespedes[2], and Christian Kübel[1] — [1]Karlsruhe Insitute of Technology, Karlsruhe, Germany — [2]University of Leeds, Leeds, United Kingdom

In perovskite ceramics of the composition $BiFe_{0.9}Co_{0.1}O_3)_{0.4} - Bi_{1/2}K_{1/2}TiO_3)_{0.6}$, novel nano-sized regions called multiferroic clusters (MFC) were recently discovered. These MFC belong to so-called core-shell structures as known from other relaxor ferroelectrics, where $BiFe_{1-x}Co_xO_3$-rich cores are surrounded by a $Bi_{1/2}K_{1/2}TiO_3$-rich shell within one grain. The MFC exhibit exceptionally large direct and converse local ME coupling. The observed electric-field induced switching of magnetization is especially interesting in terms of applications, since it enables in principle electrically driven magnetic memory, one of the 'holy grails' in information technology research. It is assumed that the strong magnetism stems from ferrimagnetic order of Fe and Co in MFC, which requires a superstructure of Fe and Co on the B lattice site. The main unsolved question in this system is, why the exceptional multiferroic properties occur in the $BiFe_{1-x}Co_xO_3$-rich Cores, but have never been observed in pure $BiFe_{1-x}Co_xO_3$ compounds. An explanation might be epitaxial strain originating from the core-shell structure. It is anticipated, that deeper understanding of the MFC might give valuable insights for the design e.g. of a thin-film material with similar multiferroic properties like the MFC.

DF 17.7 Thu 11:30 WIL B321

Nuclear magnetic and electric interactions in multiferroic $Ba_2CoGe_2O_7$ — •Martina Schädler[1], Titusz Fehér[2], Norbert Büttgen[1], Vilmos Kocsis[2], Yoshinori Tokura[3], Yasujiro Taguchi[3], Alois Loidl[1], and István Kézsmárki[2] — [1]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Hungary — [3]RIKEN Center for Emergent Matter Science, Wako 351-0198, Japan

In the multiferroic compound $Ba_2CoGe_2O_7$ the electric polarization is induced magnetically by the spin-dependent hybridization mechanism. As a result the polarization arises locally inside the CoO_4 tetrahedra and is dependent on the orientation of the external magnetic field H. Nuclear Magnetic Resonance (NMR) allows access to the local electric field gradient (EFG) via the nuclear quadrupole moment. We performed ^{59}Co NMR measurements on $Ba_2CoGe_2O_7$ for various orientations of the applied field in order to determine the local microscopic properties of magnetic spin order and electric polarization at the cobalt site: (1) we were able to model the local hyperfine field at the two magnetically inequivalent cobalt sites and (2) observed the displacement of the surrounding ions by the NMR quadrupolar effect.

DF 17.8 Thu 11:45 WIL B321

The effect of strain on the magnetic and ferroelectric properties of orthorhombic $TbMnO_3$ — •Amadé Bortis[1], Natalya Fedorova[2], Alessandro Vindigni[3], Andrea Scaramucci[2], and Nicola Spaldin[2] — [1]Laboratory for Multifunctional Ferroic Materials (M. Fiebig), Departement of Materials, ETH Zurich, Switzerland — [2]Materials Theory, Departement of Materials, ETH Zurich, Switzerland — [3]Microstructure Research, Departement of Physics, ETH Zurich, Switzerland

We model the effect of strain on magnetic and ferroelectric properties of orthorhombic $TbMnO_3$ using ab initio electronic structure calculations and Monte-Carlo simulations. $TbMnO_3$ is a magnetoelectric multiferroic, where the ferroelectricity is triggered by the magnetic ordering, which allows manipulating the electric polarization by a change in the magnetic order. It was shown experimentally that bulk samples of $TbMnO_3$, at low temperature, show a spiral magnetic order, which drives a weak polarization. Recent experiments showed that by applying strain one can change the magnetic order to E-AFM, which leads to a higher polarization. In order to understand the transition from spiral to E-AFM order, we perform ab initio calculations to extract the relevant exchange couplings for a bulk and strained sample, and we use these couplings to perform Monte-Carlo simulations to find the corresponding ground state spin configuration. This allows the determination of the magnetic order and the investigation of its effect on the polarization. We found that applying strain can drive the transition

from spiral to E-AFM ordering and can enhance the polarization.

15 min. break

Topical Talk DF 17.9 Thu 12:15 WIL B321

Role of charged defects on conduction and dynamics of domain walls in $BiFeO_3$ — •Tadej Rojac[1], Andreja Bencan[2], Goran Drazic[2], Naonori Sakomoto[2], Hana Ursic[2], Bostian Jancar[2], Gasper Tavcar[2], Maja Makarovic[2], Julian Walker[2], Barbara Malic[2], and Dragan Damjanovic[2] — [1]Electronic Ceramics Department, Jozef Stefan Institute, 1000 Ljubljana, Slovenia — [2]See author list of the paper in Nature Materials

Domain walls in ferroelectrics tend to interact with charged point defects, such as oxygen vacancies, resulting in pinning effects. In practice, this "hardening" mechanism represents one of the most important ways of controlling properties in ferroelectrics. For example, doping $Pb(Zr,Ti)O_3$ or $BaTiO_3$ with an acceptor will create oxygen vacancies which by forming re-orientable defect complexes act as pinning sites for domain walls, affecting profoundly the switching behavior and piezoelectric response. It is widely accepted that oxygen vacancies play the major role in pinning effects and hardening. It has been recently established that undoped polycrystalline $BiFeO_3$ behaves as a "hard" ferroelectric. Using atomic-scale structural and chemical analysis, we will show that, in contrast to the usually assumed oxygen vacancies, the dominant defects in $BiFeO_3$ mainly responsible for the pinning effect are electron holes, associated with the presence of Fe^{4+}, and bismuth vacancies. Direct identification of these charged defects using Cs-corrected microscopy also showed that they have a tendency to accumulate in the domain wall region, revealing the p-type hopping conduction at domain walls associated with Fe4+ defects. Discussion will be provided on how this local conductivity affects domain-wall dynamics and thus the piezoelectric response of $BiFeO_3$.

Rojac, Tadej, et al. "Domain-wall conduction in ferroelectric $BiFeO_3$ controlled by accumulation of charged defects." Nature Materials (2016)

DF 17.10 Thu 12:45 WIL B321

Mechanically soft domain walls in hard ferroelectrics — •Neus Domingo, Kumara Cordero-Edwards, James Zapata, and Gustau Catalan — Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Instituteof Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain

All ferroic materials can display regions (domains) with different polarity of the order parameter. The boundaries between domains are known as domain walls. Domain walls may possess functional properties not existent in the host material, such as conductivity in the walls of insulators, ferromagnetism in the walls of antiferromagnets, or polarization in the walls of ferroelastics. This could potentially be used to make new electronic devices at an unprecedented small scale, where the "active ingredient" are not the domains but the domain walls.

Among the many properties of domain walls, mechanical response appears to have been largely neglected, and there are very few, if any, studies specifically aimed at determining the local mechanical properties of domain walls.

In this presentation, we will show our first experimental measurements of the stiffness of domain walls in ferroelectric lithium niobate and related perovskite ferroelectrics, as measured by atomic force microscopy using a mechanical resonance spectroscopy mode. The key result is that even purely ferroelectric (non-ferroelastic) 180 degree domain walls in uniaxial ferroelectrics are considerably softer than the domains they separate.

DF 17.11 Thu 13:00 WIL B321

Reversibly tuning the domain wall conductivity in lithium niobate: from insulating to metallic-like and back again — •Christian Godau, Alexander Haussmann, and Lukas Eng — Institute of Applied Physics, Technische Universität Dresden, D-01062 Dresden, Germany

Ferroelectric domain walls (DWs) have become a central topic of research. Especially their tunable electronic properties stay in focus for the last couple of years, reporting domain wall conductivity (DWC) in both thin films [1] and single crystals [2]. Our recent research established DWC in lithium niobate (LNO) as promising building blocks for prospective electronic devices [3]; as theoretically predicted [4], DWs in fact become more conductive the larger their inclination angle is rendered. We will present here protocols how to fabricate such highly-conductive transport channels. In fact, our high-voltage treatment allows reversibly switching the conductive channels on and off, i.e. varying the inclination angle on will. This allows to fabricate a variety of novel nanoelectronic devices, for instance memory devices based on resistive switching [5] of DWC, or unidirectional / bidirectional diode/Ohmic-like 2-dimensional transport channels across wide band-gap semiconductors.

[1] J. Seidel et al., Nat. Mater. 8, 229 (2009) [2] T. Sluka et al., Nat. Comm. 4, 1808 (2013) [3] C. Godau et al., (2016) submitted [4] E. A. Eliseev et al., Phys. Rev. B 83, 235313 (2011) [5] R. Waser et al., Adv. Mater. 21, 2632 (2009)

DF 17.12 Thu 13:15 WIL B321

Imaging of multiferroic domains at the optical resolution limit — •Stefan Günther, Martin Lilienblum, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zürich, Zürich, Switzerland

Multiferroics accommodate strongly coupled electric and magnetic ordering. In a fundamental work on the hexagonal manganites (h-$RMnO_3$) from 2002, it was shown, that this coupling can extend to the electric and magnetic domain structure [1]. However, in those measurements the coupling was not resolved down to the archetypal ferroelectric vortex domain structure that was established for this system a decade later. In this talk, both type of domains (ferroelectric and antiferromagnetic) are resolved with second harmonic generation (SHG) in multiferroic h-$ErMnO_3$. As verified by piezo-response force microscopy the compound shows ferroelectric as-grown domains in the few μm-size and can thus be imaged with SHG close to the optical resolution limit. The measurements show the ferroelectric vortex domain structure, a partial coupling of magnetic and electric domain walls and give significantly new insights in the fine structure of antiferromagnetic domain walls. In particular, they demonstrate a thermally induced instability of these walls.

[1] M. Fiebig et al., Nature **419**, 818 (2002)

DF 18: Multiferroics (DF and MA)

Chair: Joachim Hemberger

Time: Thursday 15:00–17:15 Location: WIL B321

DF 18.1 Thu 15:00 WIL B321

THz study of the magnon spectra of $BiFeO_3$ — •Dániel Gergely Farkas[1], Sándor Bordács[1], Dávid Szaller[1], Laur Peedu[2], Johan Viirok[2], Urmas Nagel[2], Toomas Rõõm[2], and István Kézsmárki[1] — [1]Department of Physics, Budapest University of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, Hungary — [2]National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia

Multiferroic materials with coexisting and strongly coupled magnetic and ferroelectric orders have attracted much interest due to the novel phenomena they possess, such as magnetoelectric effect [1] and directional dichroism [2]. Among these compounds $BiFeO_3$ has received special attention as it is one of the few known room-temperature multiferroics [3], which puts its technical applications within reach. Here we present an experimental study of the magnon excitations in single crystal samples of $BiFeO_3$. Using THz spectroscopy magnetic field dependence of the spin-wave frequencies are measured along all three high-symmetry axis up to 33T. This systematic study also allowed us to determine the electric and magnetic dipole strengths, i.e. the selection rules. In contrast to the previous theoretical models we found that the (111) plane of $BiFeO_3$ is isotropic and the magnetic field dependence of the excitation frequencies have hysteresis. References: [1] M. Tokunaga, et al., Nat. Commun. 6, 5878 (2015). [2] I. Kézsmárki,

et al., Phys. Rev. Lett. 106, 057403 (2011). [3] J. Moreau, et al., J. Phys. Chem. Solids 32, 1315 (1971).

DF 18.2 Thu 15:15 WIL B321

Strain and electric-field mediated tuning of magnetism in self-assembled iron oxide nanoparticle - $BaTiO_3$ composites — •Liming Wang[1], Oleg Petracic[1], Emmanuel Kentzinger[1], Ulrich Rücker[1], Alexandros Koutsioumpas[2], Stefan Mattauch[2], Markus Schmitz[1], and Thomas Brückel[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich — [2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85748 Garching, Germany

We report about the manipulation of magnetism of self-assembled iron oxide nanoparticle (NP) monolayers on top of $BaTiO_3$ (BTO) single crystals. Magnetoelectric coupling (MEC) as shown in both the magnetization and magneto-electric ac susceptibility (MEACS) measurements is observed. Both the magnetization and MEACS as function of temperature show abrupt jumps at the BTO phase transitions temperatures, which is attributed to strain-mediated MEC from the BTO onto the NPs. We find that a Ti sticking layer and an Au embedding layer play a crucial role to maximize the MEC effect. Moreover, using polarized neutron reflectivity (PNR) we observe a change of the in-depth magnetic scattering length density upon changing an applied electric field. Grazing incident small angle X-ray scattering (GISAXS) and scanning electron microscopy (SEM) confirm a hexagonal close-packed supercrystalline order of the NPs.

DF 18.3 Thu 15:30 WIL B321

Single domain multiferroic $BiFeO_3$ films — •Chang-Yang Kuo[1], Zhiwei Hu[1], Jan-Chi Yang[1], Tun-Wen Pi[2], Stefano Agrestini[1], Kai Chen[3], Philippe Ohresser[3], Arata Tanaka[4], Liu Hao Tjeng[1], and Ying-Hao Chu[5] — [1]MPI-CPfS, Dresden, Germany — [2]NSRRC, Taiwan — [3]Synchrotron SOLEIL, France — [4]Hiroshima University, Japan — [5]National Chiao Tung University, Taiwan

The strong coupling between antiferromagnetism and ferroelectricity at room temperature found in $BiFeO_3$ generates high expectations for the design of technological devices. However, the multi-domain nature of the material tends to nullify the properties of interest and complicates the thorough understanding of the mechanisms involved. Here we report the realization of a $BiFeO_3$ thin film which shows single domain behavior in both its magnetism and ferroelectricity: the entire film has its antiferromagnetic axis aligned along the crystallographic b-axis and its ferroelectric polarization along the c-axis. This allows us to reveal that the canted and net ferromagnetic moment due to the Dzyaloshinskii-Moriya interaction is parallel to the a-axis. Furthermore, by making a Co/$BiFeO_3$ heterostructure, we successfully demonstrate that the ferromagnetic moment of the Co metal film couples directly to the canted ferromagnetic moment of $BiFeO_3$. The realization of the single-domain multiferroic $BiFeO_3$ films thus provides new insights into the fundamental interactions in this functional material and opens a promising path for the engineering of novel functional devices[1]. [1]C.Y. Kuo *et al.* Nature Communications, 7, 12712 (2016).

DF 18.4 Thu 15:45 WIL B321

New multiferroic materials - oxyhalides & orthotellurates — •A. C. Komarek[1], L. Zhao[1], H. Guo[1], M. T. Fernández-Díaz[2], W. Schmidt[3], and L. H. Tjeng[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, F-38042 Grenoble Cedex 9, France — [3]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at ILL, 71 avenue des Martyrs, F-38042 Grenoble Cedex 9, France

Magnetoelectric multiferroics have attracted considerable attention in the past years due to their possible application in future devices. Especially certain spiral magnetic structures are often responsible for the cross-coupling between magnetism and ferroelectricity in these materials. So far multiferroicity has been found mainly in oxide materials. Here, we report the observation of multiferroicity in two other interesting classes of transition metal compounds: First, we found spin-induced multiferroicity with high critical temperature in a transition metal oxyhalide (Cu_2OCl_2 [1]), and second, we also observed multiferroic properties in a transition metal orthotellurate with a complex magnetic structure (Mn_3TeO_6 [1]).

—**References**— [1] L. Zhao, M. T. Fernández-Díaz, L. H. Tjeng and A. C. Komarek, Science Advances, **2**, e1600353 (2016). [2] L. Zhao, Z. Hu, C.-Y. Kuo, T.-W. Pi, M.-K. Wu, L. H. Tjeng and A. C. Komarek, Phys. Status Solidi RRL **9**, 730 (2015).

15 min. break

DF 18.5 Thu 16:15 WIL B321

Magneto-optic and electro-optic effects in multiferroic thin films — •Simon Wisotzki, Liane Brandt, Diana Rata, and Georg Woltersdorf — Martin Luther University Halle-Wittenberg, Institute of Physics, Von-Danckelmann-Platz 3, 06120 Halle (Saale)

Jia *et al.* [1] proposed a magneto-electric coupling effect for ferromagnetic (FM)/ferroelectric(FE) composites. This phenomenon is purely charge-mediated and accompanied by the build-up of an interfacial spiral spin density. Depending on the FE polarization state in a FM/FE composite, the surface spiral spin density induced in the FM layer should change direction. For a suitable sample geometry, one can expect the reversal of the out-of-plane component of the magnetization at the FM/FE interface, with this effect decaying across the spin diffusion length. We utilize a setup that is sensitive to minute changes ($<10^{-6}$ rad) of the polarization state of reflected light from the multiferroic composite. In our experiments, magneto-optic effects (reflection on FM surface) as well as electro-optic effects (caused by the FE layer) may contribute to the measured change of the polarization state upon reflection. In a series of experiments on thin film multiferroic capacitors consisting of FM/FE/FM, we try to distinguish between the two effects and identify a possible magneto-electric contribution as suggested in [1]. The investigated samples include epitaxial LSMO/PZT/LSMO and LSMO/PZT structures with polycrystalline FM top electrodes.

[1] C.-L. Jia *et al.*, *Phys. Rev. B* **90**, 054423 (2014)

DF 18.6 Thu 16:30 WIL B321

Collective spin excitations in polar ferrimagnet $(Fe,Zn)_2Mo_3O_8$ — •Krisztián Szász[1], Dávid Szaller[1], Urmas Nagel[2], Toomas Rõõm[2], Sándor Bordács[1], and István Kézsmárki[1] — [1]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary — [2]National Institute of Chemical Physics and Biophysics, 12618 Tallinn, Estonia

In this work the magnetic excitations are investigated in Zn-doped hexagonal polar $Fe_2Mo_3O_8$ crystal using terahertz spectroscopy. This material is a promising candidate in realizing new generation electronic devices utilizing its giant magnetoelectric effect, i.e. high jump is observed in the polarization when the antiferromagnetic-ferrimagnetic spin-flop transition occurs. The different magnetic phases can be controlled by doping without losing the huge magnetoelectric effect. Microscopically, the Zn-doping fills the tetrahedral Fe sublattice while the octahedral Fe sites remain intact.

Our purpose is to understand the magnetic ground state which is still unclear. Furthermore, from the magnetic field dependence of the magnon modes we aim to deduce the most important exchange and anisotropy parameters to construct a spin model of $Fe_2Mo_3O_8$.

DF 18.7 Thu 16:45 WIL B321

Magnetic excitations in multiferroic $GdMn_2O_5$ — •Sergey Poghosyan and Sergey Artykhin — Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy

RMn_2O_5 compounds recently attracted attention due to non-collinear states and unconventional excitations. YMn_2O_5 with non-magnetic rare earth (RE) shows incommensurate spiral state with spins in the neighbouring chains aligned at 90-degrees to each other [1]. RE ions with unquenched angular momentum enable the control of polarization by magnetic field in the multiferroic materials, such as $TbMn_2O_5$ [2]. $GdMn_2O_5$ with magnetic rare earth in S=7/2, L=0 state, exhibits a spiral state below 40 K, that concedes to a commensurate state below $\sim$ 30K. The latter hosts large magnetically-induced polarization of 3600 μC/m^2 induced via Heisenberg exchange striction mechanism. This polarization changes by 5000 μC/m^2 under the external magnetic field [3]. Here we corroborate THz magnetoabsorption data with the microscopic modelling. The magnetic excitations are calculated using model Hamiltonian with parameters extracted from ab-initio simulations. The resultant magnon spectrum is rather counterintuitive and complex, thus providing new insights on design principles for materials with strong magnetoelectric couplings.

[1] J.-H. Kim et al., Phys. Rev. Lett. **107**, 097401 (2011).
[2] N. Hur et al., Nature **429**, 392 (2004).
[3] N. Lee et al., Phys. Rev. Lett. **110**, 137203 (2013).

DF 18.8 Thu 17:00 WIL B321

Simulation and investigation of polarization kinetics in polycrystalline ferroelectrics. — •Ruben Khachaturyan — Technische Universität Darmstadt, Department of Materials Modeling, 64295 Darmstadt, Stephanstr. 5

The understanding of polarization dynamics over a wide time scale plays a crucial role in a vast range of applications, from non-volatile memories (FeRAM) and sensors to fuel injection applications.

It was established that polarization process under applied voltage develops simultaneously in different parts of a material with different switching times [1]. As switching time is strongly field dependent [2] it was suggested that local switching time distribution is caused by local electrical field distribution [3-5].

There is currently no statistical concept that accounts for spatial correlations of local polarizations and fields during polarization switching in a ferroelectric polycrystalline material.

The main purpose of the work is to simulate dynamics of polarization switching in a polycrystalline material under applied electric field. The data extracted from the simulations, such as field and polarization distributions and their correlations at different times, provide necessary information to study influence of the local field distribution on local switching processes.

DF 19: Glasses and Glass Transition (CPP with DF)

Time: Friday 10:00–12:30 Location: ZEU 118

DF 19.1 Fri 10:00 ZEU 118

Molecular Dynamics Simulations of Aqueous Mixtures in Bulk and Nano-Confinement — •Niels Müller, Rebecca Schmitz, and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt

Binary mixtures of glass forming liquids have complex dynamical properties, leading to shifted time scales of the dynamics or changed temperature dependence compared to the respective behavior of the pure liquids. We performed MD simulations of ethylene-glycol water mixtures in silica-pores, which show unmixing near the pore wall and a change from non-Arrhenius to Arrhenius like temperature dependence. To single out the origin of these unusual behaviors we use binary mixtures composed of two water-like molecules with different polarity as a model system. These systems avoid steric effects from molecules of different size and have the characteristic tetrahedral order of water, but form hydrogen bonds of different strength. Through simulations in a wide temperature range we probe unmixing transitions of these systems. In addition, we confine these model mixtures by walls formed by fixed molecules of one of the water-like species. In this way, we systematically study the effect of the polarity of the confinement on mixtures of hydrogen-bonded liquids. Performing spatially resolved analyses or selecting a subset of the system we can gather detailed insights into the effects of confinement on the dynamics of these systems.

DF 19.2 Fri 10:15 ZEU 118

The glass transition as a mixture of random organization and athermal jamming — Moumita Maiti and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We explore the properties of the glass transition by employing a model system for a mixture of athermal jamming and random organization. We start with random configurations of soft repulsive spheres. While athermal jamming is realized by heading for the local minimum of the overlap energy without crossing energy barriers, random organization is obtained if we displace overlapping particles randomly in each step [1]. When mixing these protocols, we obtain a transition which is in the universality class of a directed percolation transition in time. Furthermore, we reveal that the limit of a small but nonzero probability of random steps differs from the case without random steps. This limit corresponds to the glass transition at small but non-zero temperatures. As a consequence the glass transition is a directed percolation transition and is fundamentally different from the athermal jamming transition. Finally, we explore the relation to spatial percolation transitions.

[1] L. Milz and M. Schmiedeberg, Connecting the random organization transition and jamming within a unifying model system, Phys. Rev. E 88, 062308 (2013).

DF 19.3 Fri 10:30 ZEU 118

NMR and BDS Experiments on Water confined in MCM-41 — •Edda Klotz, Matthias Sattig, Christina Lederle, and Michael Vogel — TU Darmstadt Solid State Physics, Darmstadt, Germany

The investigation of the dynamics of water in confinement is relevant for various fields of interest, from biological applications to geological ones. It is well established that confined water undergoes a dynamic crossover upon supercooling. However, the origin of the crossover is controversially discussed. To further study this issue, we focus on water im MCM-41 silica nanopores and use por diameters for which well defined partial freezing occurs. Calorimetric studies are performed to characterize this freezing behavior. Moreover, nuclear magnetic resonance (NMR) and broadband dielectric spectroscopy (BDS) are applied to ascertain the dynamics of the non-freezing water fraction cross the freezing transition. The dielectric spectra exhibit several processes that are sensitive to an appearance of a solid water fraction. ^{2}H-NMR allows us to show that one of the processes can be identified with the rotational motion of water, exhibiting a kink in the temperature depenence at the freezing-transition. Moreover, ^{1}H static field gradient NMR yields self-diffusion coefficients of water, which can be linked to freezing-affected polarization processes in BDS. Thus, these combined studies clearly show a dynamic crossover due to formation of a solid water fraction.

DF 19.4 Fri 10:45 ZEU 118

Water Dynamics in Mesoporous Silica Confinement — •Max Schäfer, Edda Klotz, Alexander Hariri, and Michael Vogel — Institut für Festkörperphysik, TU-Darmstadt, Germany

Confinement effects on the dynamics of water are examined using mesoporous silica MCM-41 with various pore diameters. Additionally the size of these pores are systematically modified by atomic layer deposition with Al2O3. To explore rotational motion, we combine different 2H NMR technics that are sensitive to molecular reorientations. Applying spin-lattice-relaxation, line shape analyzes and stimulated echo experiments, we cover the dynamical range down to very slow dynamics in a deeply supercooled temperature regime. 1H diffusion measurements in an ultra high static field gradient were performed also. These experiments were supplemented by broadband dielectric spectroscopy and differential scanning calorimetry. We find that the temperature dependence of the structural alpha-relaxation exhibits a kink, which is strongly related to the pore size. We show that this kink is not associated to a proposed liquid-liquid phase transition of water, but to partial freezing. Furthermore we study confinement effects on dynamics and phase behavior in binary mixtures of water and glycerol for various concentrations. The properties of the hydrogen bond network and an eventually phase separation initiated by the confinement are of great interest. Glycerol dynamics for confined mixtures show an Arrhenius behavior at low temperatures in contrast to bulk mixtures and to pure glycerol confined in MCM-41. The similarity to water dynamics in confinement suggests a cooperative motion of water and glycerol.

DF 19.5 Fri 11:00 ZEU 118

Dynamical coexistence in a polydisperse hard-sphere liquid — •Matteo Campo[1,2], Christopher Patrick Royall[3], and Thomas Speck[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Germany — [3]H.H. Wills Physics Laboratory, University of Bristol, United Kingdom

The glass transition is a long-standing challenge of condensed matter physics. One of the problems is that no significant change in the global structure seems to arise upon vitrification [1]. Recent studies however have recovered the old idea of Frank according to which geometric motifs which minimise the local free energy, so-called locally favoured

structures (LFS), would grow in correlation with the slow regions of the glass and thus play an important role in the transition [2]. Among the key insights is the identification of a non-equilibrium phase transition in trajectory space, which implies phase coexistence between a slow phase rich in LFS and the normal supercooled liquid. Here we present a study of a polydisperse hard-sphere model glassformer and its LFS properties upon crystallization [3] and vitrification. We combine our numerical simulations with experimental observations that support the picture of the non-equilibrium phase transition in trajectory space.

[1] Ludovic Berthier and Giulio Biroli. REV MOD PHYS, 2011.
[2] C Patrick Royall and Stephen R Williams. PHYS REP, 2015.
[3] Matteo Campo and Thomas Speck. JSTAT, 2016.

15 min. break

DF 19.6 Fri 11:30 ZEU 118

Electro-diffusion versus chemical diffusion in alkali calcium phosphate glasses - implication of structural changes — •Anneli Hein, Johannes Martin, Martin Schäfer, and Karl-Michael Weitzel — Philipps-Universität Marburg

A long term transport experiment has been performed on a bioactive calcium phosphate glass of the molar composition 30 CaO *25 NaO *45 P2O5 using the technique of bombardment induced ion transport (BIIT) with potassium as foreign bombarder ion. Ion transport due to gradients of the electrical potential and the concentration lead to incorporation of K+ and depletion of both Na+ and Ca++ by electro-diffusion in forward direction. The resulting concentration profile has been quantitatively analyzed by ToF-SIMS. Further analysis of the P+ and POx+ signals (x = 1-4) shows characteristic changes of the structure of the local glass network. Since the concentration profiles imprinted by the BIIT constitute pronounced concentration gradients, these depletion profiles further evolve on a much longer time scale due to chemical diffusion (absence of electric potential gradients). The former depletion zone is partially refilled by chemical diffusion. At the same time the structural changes of the glass network are demonstrated to be reversible. Numerical simulations on the basis of the coupled Nernst-Planck-Poisson equations allow deriving the diffusion coefficients of sodium, potassium and calcium for both cases, i.e. electro-diffusion and chemical diffusion. The two experiments are sensitive to different aspects of the diffusion coefficients and thus are complementary.

DF 19.7 Fri 11:45 ZEU 118

Confinement effects on the correlation of plasticity in amorphous solids — •Muhammad Hassani, Philipp Engels, and Fathollah Varnik — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr Universität, Bochum, Germany

In amorphous solids, spatio-temporal correlations of plastic deformation are known to be mediated by the elastic medium [1]. Solid walls may strongly alter this elastic propagator and are thus expected to also influence these correlations. We study this issue via large scale molecular dynamics (MD) simulations. Spatial correlations of plastic activity are found to decay more slowly when approaching a wall. This observation is paralleled by a similar trend in the case of the strain field around a spherical inclusion placed at various distances from a wall. Results obtained from MD simulations are in quantitative agreement with numerical solution of continuum mechanics equations in the presence of an inclusion [2,3].

[1] F. Varnik, S. Mandal, V. Chikkadi, D. Denisov, P. Olsson, D. Vagberg, D. Raabe, and P. Schall, Correlations of plasticity in sheared glasses, Phys. Rev. E 89, 040301 (2014)
[2] A. Nicolas and J.-L. Barrat, A mesoscopic model for the rheology of soft amorphous solids, with application to microchannel flows, Faraday Discuss. 167, 567 (2013)
[3] M. Hassani, P. Engels, and F. Varnik, Confinement effects on the correlation of plasticity in amorphous solids (in preparation

DF 19.8 Fri 12:00 ZEU 118

Glass transitions, semiconductor-metal (SC-M) transitions and fragilities in Ge-V-Te (V=As, or Sb) liquid alloys: the difference one element can make — •Shuai Wei[1], Garrett Coleman[2], Pierre Lucas[2], and C.Austen Angell[1] — [1]Arizona State University — [2]University of Arizona

Glass transition temperatures (Tg) and liquid fragilities are measured along a line of constant Ge content in the system Ge-As-Te, and contrasted with the lack of glass-forming ability in the twin system Ge-Sb-Te at the same Ge content. The one composition established as free of crystal contamination in the latter system shows a behavior opposite to that of more covalent system. Comparison of Tg vs bond density in the three systems Ge-As-chalcogen differing in chalcogen i.e. S, Se, or Te, shows that as the chalcogen becomes more metallic, the bond density effect on Tg becomes systematically weaker, with a crossover at <r> = 2.3. When the more metallic Sb replaces As at <r> greater than 2.3, incipient metallicity rather than directional bond covalency apparently gains control of the physics. This leads us to an examination of the electronic conductivity and, then, semiconductor-to-metal (SC-M) transitions, with their associated thermodynamic manifestations, in relevant liquid alloys. The thermodynamic components control liquid fragility and cause fragile-to-strong transitions during cooling. We tentatively conclude that liquid state behavior in phase change materials (PCMs) is controlled by liquid state SC-M transitions that have become submerged below the liquidus surface. The analogy to supercooled water phenomenology is highlighted.

DF 19.9 Fri 12:15 ZEU 118

Glass structure and quantum efficiency of luminescent borate glass — •A. Charlotte Rimbach[1], Bernd Ahrens[1,2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Luebecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Luebecker Ring 2, 59494 Soest

Luminescent glasses have gained more importance in the last decades, in particular for lasers, optical fibres, and optical amplifiers. For optical applications, borate glass is very versatile in shape and a suitable host for luminescent lanthanide ions due to its good lanthanide ion solubility. The borate glass system possesses a high transparency, low melting point as well as high mechanical, chemical, and thermal stability. Various luminescent borate glasses using boron oxide as network former and lithium oxide as network modifier are prepared. Here, the ratio between network former and network modifier determines the mechanical and chemical properties of the glass. An important parameter for the evaluation of luminescent materials is the absolute photoluminescence quantum efficiency (QE), i.e. the ratio of emitted to absorbed photons. While the ratio between network former and network modifier affects the QE only slightly, additional doping with aluminium oxide to reduce hygroscopicity results in a significant decrease in QE. Raman and Fourier transform infrared spectroscopy are used to analyze the structure of the glass network; the results are correlated with the QE measurements.