Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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

Overview of Invited Talks and Sessions

(Lecture rooms: GER 37 and WIL B321; Posters: P1)

Invited Talks

DF 1.1	Mon	9:30–10:15	GER 37	**Optics with neutrons using holographic gratings** — •Martin Fally, Jürgen Klepp, Christian Pruner, Yasuo Tomita
DF 5.1	Tue	9:30–10:15	GER 37	**Understanding the puzzling behavior of $LiNbO_3$ surfaces form *first-principles*** — •Simone Sanna
DF 7.1	Tue	12:00–12:45	GER 37	**Defects in functional polar oxide materials - Detection and influence on electrical properties** — •Torsten Granzow, Nina Balke, Julia Glaum, Silke Schaab
DF 11.1	Wed	10:30–11:15	GER 37	**Two-dimensional Oxide Quasicrystals: A new class of materials?** — •Stefan Förster, Klaus Meinel, Rene Hammer, Martin Trautmann, Wolf Widdra
DF 17.1	Wed	15:00–15:45	GER 37	**Smart multiferroic thin films for cognitive computing** — •Heidemarie Schmidt
DF 19.1	Thu	9:30–10:15	GER 37	**Analyzing electronic defect states at perovskite oxide interfaces by surface photovoltage spectroscopy** — •Elke Beyreuther, Lukas Eng

Invited talks of the joint symposium SYCM

See SYCM for the full program of the symposium.

SYCM 1.1	Mon	15:00–15:30	HSZ 02	**Complexity on Compression: The Crystallography of High-Density Matter** — •Malcolm McMahon
SYCM 1.2	Mon	15:30–16:00	HSZ 02	**X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy** — •Christian G. Schroer
SYCM 1.3	Mon	16:00–16:30	HSZ 02	**Modulated martensite: A scale bridging Lego game for crystallographers and physicists** — •Sebastian Fähler
SYCM 1.4	Mon	16:45–17:15	HSZ 02	**Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity** — •Michel Kenzelmann
SYCM 1.5	Mon	17:15–17:45	HSZ 02	**The key role of magnetic neutron diffraction in materials science** — •Laurent C. Chapon

Sessions

DF 1.1–1.1	Mon	9:30–10:15	GER 37	**Invited Talk - Martin Fally (Joint Session with CPP, TT, KR)**
DF 2.1–2.8	Mon	10:30–13:10	GER 37	**Optical and nonlinear optical properties, photonic**
DF 3.1–3.5	Mon	15:00–17:45	HSZ 02	**SYCM - Crystallography in Materials Science (Joint Session with KR)**
DF 4.1–4.9	Mon	15:00–17:30	ZEU 146	**Glasses (Joint Session with DY and CPP)**
DF 5.1–5.1	Tue	9:30–10:15	GER 37	**Invited Talk - Simone Sanna**
DF 6.1–6.4	Tue	10:30–11:50	GER 37	**High- and low-k-dielectrics (Joint Session with DS)**
DF 7.1–7.1	Tue	12:00–12:45	GER 37	**Invited Talk - Thorsten Granzow**

DF 8.1–8.12	Tue	9:30–12:45	BEY 118	**Multiferroics I (Joint Session with MA, DS, KR, TT)**
DF 9.1–9.16	Tue	18:30–20:00	P1	**Poster Session DF**
DF 10.1–10.3	Wed	9:30–10:30	GER 37	**Dielectric surfaces and interfaces**
DF 11.1–11.1	Wed	10:30–11:15	GER 37	**Invited Talk - Stefan Förster (Joint Session with O, DS, KR, MM)**
DF 12.1–12.1	Wed	11:30–11:50	GER 37	**Electrical and mechanical properties**
DF 13.1–13.2	Wed	11:50–12:30	GER 37	**Applications of dielectric solids**
DF 14.1–14.1	Wed	12:30–12:50	GER 37	**Nanostructured oxide thermoelectrics**
DF 15.1–15.13	Wed	9:30–13:00	HSZ 04	**Multiferroics II (Joint Session with MA, DS, KR, TT)**
DF 16.1–16.3	Wed	11:45–12:45	WIL B321	**Glasses (Joint Session with CPP and CY)**
DF 17.1–17.1	Wed	15:00–15:45	GER 37	**Invited Talk - Heidemarie Schmidt (Joint Session with MA, HL, DS, KR)**
DF 18.1–18.7	Wed	16:00–18:20	GER 37	**Dielectric and ferroelectric thin films**
DF 19.1–19.1	Thu	9:30–10:15	GER 37	**Invited Talk - Elke Beyreuther**
DF 20.1–20.4	Thu	10:30–11:50	GER 37	**Nonlinear dielectics, phase transitions, relaxors**
DF 21.1–21.2	Thu	12:00–12:40	GER 37	**Nano- and microstructured dielectrics (Joint Session with KR)**
DF 22.1–22.9	Thu	9:30–12:30	HÜL 186	**Slow Dynamics in Glasses and Granular Matter I (Joint Focus Session with DY and CPP)**
DF 23.1–23.3	Thu	11:45–12:45	ZEU 114	**Glasses and Glass Transition I (Joint Session with CPP and DY)**
DF 24.1–24.8	Thu	15:00–17:30	CHE 184	**Crystallography in Materials Science (Joint Session with KR)**
DF 25.1–25.7	Thu	15:00–17:30	ZEU 114	**Glasses and Glass Transition II (Joint Session with CPP and DY)**
DF 26.1–26.10	Thu	9:30–13:00	POT 251	**Metamorphic structures: Bringing together incompatible materials I (Joint Focus Session with HL and DS)**
DF 27.1–27.5	Thu	15:00–16:30	POT 251	**Metamorphic structures: Bringing together incompatible materials II (Joint Focus Session with HL and DS)**
DF 28.1–28.8	Fri	9:30–12:15	HÜL 186	**Slow Dynamics in Glasses and Granular Matter II (Joint Focus Session with DY and CPP)**

Annual General Meeting of the Dielectric Solids Division

Dienstag 15:30–16:15 GER 37

- Bericht
- Verschiedenes

DF 1: Invited Talk - Martin Fally (Joint Session with CPP, TT, KR)

Time: Monday 9:30–10:15 Location: GER 37

Invited Talk DF 1.1 Mon 9:30 GER 37

Optics with neutrons using holographic gratings — •Martin Fally[1], Jürgen Klepp[1], Christian Pruner[2], and Yasuo Tomita[3] — [1]Faculty of Physics, Uni Wien, Austria — [2]Department of Materials Science and Physics, Uni Salzburg, Austria — [3]University of Electro-Communications, Tokyo, Japan

All neutron-optical phenomena are governed by the neutron-optical potential or, equivalently, the neutron refractive-index. Thus, an important task in the design of neutron-optical elements is to efficiently pattern the neutron refractive-index of materials. For this purpose we use light-sensitive materials and employ holographic techniques to produce diffraction gratings for neutrons.

After an introduction to the basics of neutron optics and the challenges as compared to light optics I will discuss our recent experiments, where we successfully demonstrated the power of this approach. Two- and three-port beam-splitters as well as free-standing film mirrors for cold and very-cold neutrons were set up by exploiting the Pendellösung interference effect. Another intriguing possibility is offered by holographic gratings containing superparamagnetic nanoparticles to produce business card-size neutron polarizers working in comparably low external magnetic induction. Such devices are being developed at present. Finally, I will give an outlook on novel neutron-scattering instrumentation and techniques which are expected from those advancements.

In collaboration with: I. Drevensek-Olenik, S. Gyergyek, J. Kohlbrecher, P. Geltenbort, R. A. Rupp

DF 2: Optical and nonlinear optical properties, photonic

Time: Monday 10:30–13:10 Location: GER 37

DF 2.1 Mon 10:30 GER 37

Domain contrast in photoluminescence at Mg doped LiNbO3 and LiTaO3 single crystals — •Philipp Reichenbach[1], Thomas Kämpfe[1], Andreas Thiessen[1], Mathias Schröder[1], Alexander Haussmann[1], Theo Woike[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany — [2]Institut für Strukturphysik, Technische Universität Dresden, Zellescher Weg 16, 01069 Dresden, Germany

We investigated multiphoton photoluminescence (PL) occurring in Mg doped $LiNbO_3$ (LNO) and $LiTaO_3$ (LTO) single crystals under a focused 100-fs laser beam at 790 nm. The PL signal always allows differentiating between switched domains and the virgin substrate due to the presence of a PL domain contrast of about 3% and 20% for the LNO and LTO substrates, respectively. This contrast shows a physical difference between original and switched state that originates from defect states in the crystals.
When annealing the sample above 100°C the domain contrast shows an exponential decay. Arrhenius plots of the decay times vs. the annealing temperatures show an activation energy of about 1 eV for both LNO and LTO. This value indicates that the contrast reduction is related with the motion of lithium or hydrogen within the crystal.

DF 2.2 Mon 10:50 GER 37

THz Polarization Pulse Shaping by Birefringence in $LiInS_2$ Crystal — •Qijun Liang[1], Shanpeng Wang[2], Xutang Tao[2], and Thomas Dekorsy[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany — [2]State Key Lab. of Crystal Materials, Shandong University, 250100 Jinan, China

The birefringence of $LiInS_2$ crystal in the THz frequency region is investigated by THz time-domain spectroscopy. $LiInS_2$ is a novel nonlinear biaxial crystal with high optical qualities such as large birefringence and low absorption in the THz frequency region. The optical properties of $LiInS_2$ are quantitatively determined. A pronounced sharp absorption caused by a TO-phonon resonance is observed at around 1.70 THz when Z-axis is parallel to the polarization of the incident THz wave. A temporal separation of the transmitted THz pulses with different polarization components is realized by changing the orientation of the $LiInS_2$ crystal with respect to the polarization of the incident THz pulses. By controlling the relative phase and amplitude of the temporally separated THz pulses, THz polarization pulse shaping caused by birefringence in $LiInS_2$ crystal is demonstrated.

DF 2.3 Mon 11:10 GER 37

Optical Modes in Photonic Molecules from Whispering-Gallery-Mode Microcavities — •Tobias Siegle[1], Sarah Wiegele[1], Carolin Klusmann[1], Tobias Grossmann[1,2], Tobias Wienhold[2], Uwe Bog[2], Sebastian Köber[2,3], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [3]Institute of Photonics and Quantum Electronics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Optical modes in photonic molecules consisting of microresonators are classified in analogy to quantum mechanics of chemical molecules. Closely approaching two microcavities leads to a photon exchange and subsequent formation of supermodes extending over the entire cavity system.

We used dye (pyrromethene 597)-doped polymeric microresonators to form active photonic molecules. To vary the inter-cavity gap and therefore the photon tunneling rate we developed a setup for flexible arrangement of two cavities, which must inevitably be substrate-overhanging after the manufacturing process. Spatially resolved spectroscopy of two coupled active microdisks and micorgoblets showed the localization of supermodes and a reduction of the number of lasing modes in size-mismatched cavities (Vernier effect) both proving efficient optical coupling.

DF 2.4 Mon 11:30 GER 37

Boson peak in overdoped manganites $La_{1-x}Ca_xMnO_3$ — •F. Fischgrabe[1], E. Zhukova[2,3,5], B Gorshunov[2,3,5], V. I. Torgashev[4], L. S. Kadyrov[2,3], E. A. Motovilova[2,3,5], T. Zhang[6], R. Kremer[7], U.S. Pracht[5], S. Zapf[5], V. V. Moshnyaga[1], and M. Dressel[5] — [1]I. Physikalisches Institut, Universität Göttingen, Germany — [2]A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, Russia — [3]Moscow Institute of Physics and Technology (State University), Russia — [4]Faculty of Physics, Southern Federal University, Russia — [5]1. Physikalisches Institut, Universitat Stuttgart, Germany — [6]Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, PRC — [7]Max-Planck-Institut für Festkörperforschung, Germany

In the charge-ordered phase of strongly doped manganites $La_{1-x}Ca_xMnO_3 (x \geq 0.5)$ absorption lines appear in the terahertz spectral range for commensurate x values right below the charge-ordering temperature. They are connected to acoustic phonons that become optically active by folding of the Brillouin zone. At lower temperatures a strongly asymmetric extra absorption band develops at frequencies corresponding to the position of the lowest-energy van Hove singularity in the reduced Brillouin zone. The band is assigned to the boson peak, i.e., to the excess of lattice vibrational states over the standard Debye contribution. The folded phonons and the boson peak do not show up for incommensurate calcium contents when no distinct Brillouin zone folding exists. Polycrystals are compared with freestanding films to determine if there are differences in the IR response.

DF 2.5 Mon 11:50 GER 37

Optical phonons and dielectric properties of $LiNb_xTa_{(1-x)}O_3$ — •Michael Rüsing[1], Christopher Buchholz[1], Gerhard Berth[1,2], Huajin Zhang[3], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany — [3]State Key Lab of Crystal Materials, Shandong

University, Jinan 250100, China

Recently Lithium-Niobate-Tantalate mixed crystals have drawn particular attention due to the possibility to tune the optical birefringence while sustaining its ferroelectric properties. A composition with zero birefringence at room temperature is of particular interest, as it represents an optical isotropic, but yet electrically polar material, which is unique in the class of ferroelectric materials.
Despite the unique properties only very few is known about the mixed crystals. Within this work Lithium-Niobate-Tantalate mixed crystals have been studied by polarization dependent μ-Raman spectroscopy. Furthermore the dielectric properties have been characterized via the Lyddane-Sachs-Teller-Relation. Here, all phonon modes exhibit a Vegard-like behaviour. In contrast to recent theoretical work on mixed crystals some phonons show a nonlinear shifting-behaviour, while all around a linear behaviour has been suggested. This also affects the dielectric properties.

DF 2.6 Mon 12:10 GER 37

Vibrational properties and directional dispersion of KTP — •Peter Mackwitz[1], Michael Rüsing[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Potassium titanyl phosphate (KTP) is a commonly used ferroelectric material with outstanding characteristics for applications in integrated optics. These properties include large electro-optical coefficients, high nonlinear coefficients and high damage threshold compared to other ferroelectrics. Particularly the spontaneous polarization enables the fabrication of periodically poled KTP (PPKTP) in order to achieve highly efficient frequency conversion processes by quasi phase-matching.
Although the material is commercially available a better understanding of its properties is inevitable for further advancement application of KTP. In this work polarization-dependent μ-Raman-spectroscopy has been applied in order to study the vibrational properties of KTP. Furthermore the directional dispersion of the phonon modes has been recorded. Our measurements concur well with previous work on KTP. In detail we have assigned the most intense Raman-bands with fundamental vibrations in octahedral and tetrahedral molecules.

DF 2.7 Mon 12:30 GER 37

Visualization of domain gratings in potassium titanyl phosphate by nonlinear microscopy — •Moritz Grothe[1], Christopher Buchholz[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

The nonlinear microscopy combines the high spatial resolution of a confocal operating microscope with the additional information of polarization-dependent second harmonic generation allowing structure-adjusted characterization of the ferroelectric domain structure. In our study we address the nonlinear signatures of specific ferroelectric domain structures in potassium titanyl phosphate (KTP). Here the nonlinear response exhibit specific signatures, which are linked to the domain structure. A direct correlation with the nonlinear susceptibility tensor can be expected. A detailed nonlinear analysis of the transition area of contrarily poled domains reveals specific signal sequences subject to the polarity. Furthermore a functional dependence on depth of such se-quences was observed. Here an influence of surface charge and inner electric field distribution can be assumed.

DF 2.8 Mon 12:50 GER 37

Determination of the nonlinear susceptibility of $LiNbO_3$-$LiTaO_3$ mixed crystals — •Christopher Buchholz[1], Merlin Meise[1], Gerhard Berth[1,2], Huajin Zhang[3], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany — [3]State Key Lab of Crystal Materials, Shandong University, Jinan 250100, China

Varying the composition of mixed crystals allows for the tuning of their specific physical proper-ties. In this context Lithium niobate-tantalate (LNT), one of the simplest ferroelectric mixed crystals, is of particular interest due to its multifunctional characteristics. It shows piezoelectrical, particularly electrooptical and optical nonlinear effects. Furthermore the existence of a com-position with zero birefringence at room temperature is unique in ferroelectric nonlinear-optical materials. In particular we have analyzed the second-order nonlinear optical response for $LiNb_{(1-x)}Ta_xO_3$ over a wide composition range using nonlinear microscopy. The experimentally determined tensor coefficients of the nonlinear susceptibility for different compositions show a linear behavior. Here each tensor coefficient decreases linearly with increasing Ta content. The observed behavior was compered to theoretical calculations, whereby the measured values and those from literature are in good agreement.

DF 3: SYCM - Crystallography in Materials Science (Joint Session with KR)

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

Invited Talk DF 3.1 Mon 15:00 HSZ 02

Complexity on Compression: The Crystallography of High-Density Matter — •Malcolm McMahon — School of Physics and Astronomy, The University of Edinburgh, Edinburgh, UK.

The crystal structure of iron was determined at *normal* conditions as long ago as 1917. But what is the structure of iron within *Super-Earth* exoplanets where core conditions approach 10 million atmospheres (1 TPa) and 10,000 K, and where carbon exists as either diamond, or as an exotic metallic form.

Until the early 1990s, the consensus was that at high pressures, all materials would become metallic, and assume high-symmetry, close-packed crystal structures. But the advent of modern crystallographic methods on synchrotron sources in the early 1990s revealed completely different behavior: even the simplest materials underwent phase transition to complex, frequently incommensurate, forms, while metals became semiconductors or insulators. This complexity is thought to arise from the constraints placed on the electronic wave functions due to the Pauli exclusion principle, the need to orthogonalise the wave functions of both core and valence electrons, and the reduction in the available interstitial space at high compression

In this talk I will present results from recent diffraction studies of elemental metallic systems showing some of the extreme complexity observed at high pressures. I will also look at the new opportunities in extreme conditions crystallography offered by x-ray lasers such as the LCLS in the Stanford, and XFEL in Hamburg.

Invited Talk DF 3.2 Mon 15:30 HSZ 02

X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy — •Christian G. Schroer — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

Hard x-ray microscopy has greatly benefited from the high brilliance of modern synchrotron radiation sources and x-ray free-electron lasers (XFELs). Today, the spatial resolution of conventional x-ray microscopes is limited by the x-ray optics to a few tens of nanometers. Scanning coherent diffraction microscopy, also known as ptychography, can overcome this limitation. In ptychography, the sample is scanned through a confined coherent beam, recording at each location of the scan a far-field diffraction pattern. From these data, the complex transmission function (projected complex refractive index) of the sample and the illuminating complex wave field can be reconstructed with a spatial resolution that clearly exceeds the lateral size of the illuminating beam. The spatial resolution in a ptychogram is shown to depend on the shape (structure factor) of a feature and can vary for different features in the object. In addition, the resolution and contrast depend on the coherent fluence on the sample. For an optimal ptychographic x-ray microscope, this implies a source with highest possible brilliance and an x-ray optic with a large numerical aperture to generate the optimal probe beam. Ptychography closes the gap between real space imaging and reciprocal space structure determination and merges these two fields.

[1] A. Schropp, et al., Appl. Phys. Lett. **100**, 253112 (2012).

Invited Talk DF 3.3 Mon 16:00 HSZ 02

Modulated martensite: A scale bridging Lego game for crystallographers and physicists — •Sebastian Fähler — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Physics, D-09107 Chemnitz, Germany

Among various materials exhibiting reversible phase transformations structures with low crystal symmetry, so-called modulated phases, exhibit the best ferroelectric, magnetocaloric or magnetic shape memory properties. Here it is describe how modulated martensite can be built in a kind of Lego game from simple tetragonal building blocks. It's complex crystallographic (micro-) structure is determined by the boundary conditions during the nucleation process. Though this building principle can be describe in terms of continuum mechanics, it is consistent with first principle calculations. Supported by SPP 1239 and SPP 1599.

15 min break

Invited Talk DF 3.4 Mon 16:45 HSZ 02

Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity — •Michel Kenzelmann — Paul Scherrer Institut

The interplay of magnetic and charge fluctuations can lead to novel quantum phases with exceptional electronic properties. Magnetic order in such quantum phases can fundamentally affect the underlying symmetry and generate new physical properties. Importantly, it has been predicted that spin-density wave (SDW) order in a singlet d-wave superconductor is coupled to triplet superconductivity. We performed neutron diffraction studies of the Q-phase SDW [1] in $CeCoIn_5$, and we make two important observations [2]. We observe a complete and extremely sharp SDW domain switching that is unexplained by current microscopic theories for $CeCoIn_5$. Using representational theory, we interpret our experimental results as evidence for the presence of p-wave superconductivity that coexists with d-wave superconductivity and SDW order. The triplet component is of p-wave symmetry, similar to that found in the A-phase of superfluid ^{3}He, and is modulated as a Cooper pair density wave. Our findings identify the Q-phase as a unique quantum phase where d-wave and modulated p-wave superconductivity are coupled to SDW order, and which emerges in a magneto-superconducting quantum critical point [2].

[1] M. Kenzelmann et al, Science 321, 1652 (2008). [2] S. Gerber et al, submitted to Nature Physics (2013).

Invited Talk DF 3.5 Mon 17:15 HSZ 02

The key role of magnetic neutron diffraction in materials science — •Laurent C. Chapon — Institut Laue-Langevin, Grenoble, France

Since the 1950s, neutron scattering, and more specifically diffraction, has been a tool of choice for studying magnetism at the atomic scale. From the very first experimental proof of antiferromagnetism, a phenomenon predicted by Louis Néel, to unveiling how complex multiferroic materials work, the technique has always offered information of crucial importance to build the physical models that are required to explain macroscopic properties of materials. I will review briefly the historical development of magnetic neutron scattering and present key neutron diffraction experiments in recent areas of interest for condensed matter physicists, in particular highlighting the use of the technique for multiferroics and frustrated magnetic systems.

DF 4: Glasses (Joint Session with DY and CPP)

Time: Monday 15:00–17:30 Location: ZEU 146

DF 4.1 Mon 15:00 ZEU 146

Dynamic Crossover and Stepwise Solidification of Confined Water — •Matthias Sattig and Michael Vogel — Hochschulstraße 6, D-64289 Darmstadt

The dynamical behaviour of water in the regime of the supercooled liquid is still a topic of large interest. In particular, the existence of a fragile-to-strong transition (FST) at around 225K induced by a liquid-liquid phase transition (LL) is controversially discussed [1]. The proposed temperature range of the FST is hardly accessible in bulk water.

Our ^{2}H NMR investigation reveals two dynamic crossovers of supercooled water in nanoscopic (nm) confinement. A dynamic crossover of liquid water at ca. 225K is accompanied by a formation of a fraction of solid water. Therefore, this effect can not be attributed to the LL, but rather to a change from liquid-like to interface-dominated dynamics. Moreover, the ^{2}H NMR data yield evidence that the α process and β process are observed in experiments above and below this temperature, respectively. Upon cooling through a dynamic crossover at ca. 175K, the dynamics of the liquid fraction becomes anisotropic and localized, implying solidification of the corresponding water network, most probably, during a confinement-affected glass transition.

[1] Mishima; Nature, Vol. 396, 329(1998)

DF 4.2 Mon 15:15 ZEU 146

Understanding the nonlinear mobility of single driven particles in supercooled liquids — •Carsten F. E. Schroer[1,2] and Andreas Heuer[1,2] — [1]WWU Münster, Münster, Germany — [2]Graduate School of Chemistry, Münster, Germany

We perform MD simulations of a binary Lennard-Jones mixture where a single particle is pulled by an external field through the liquid. Herein, we are specifically interested in the range of intermediate and strong forces when nonlinear effects occur in the single particle dynamics.

It is known from experimental and simulation studies, that the steady-state velocity $\overline{v}$ follows in the limit of low forces a linear response relation $\overline{v} = \mu F$ where the force F is connected to the dynamical response via the constant mobility $\mu_0 = \frac{D_0}{k_B T}$. For large forces, however, one finds a dramatic increase of $\overline{v}$ with increasing F, indicating a nonlinear force-dependence of the mobility, i.e. $\mu_0 \to \mu(F)$.

To gain a deeper understanding of this behavior, we studied the underlying potential energy landscape of the system by computing the minima the system has resided in during its time-evolution. This immediately allows us to discuss the nonlinear mobility in terms of thermodynamical (distribution of energies) and kinetic (escape rates out of single minima) quantities. Most interestingly it turns out, that both effects are of major importance for the nonlinearity of the system, so that there is no single nonlinear effect but an interplay of two independent which contributes to the dynamical responses of the driven particles.

DF 4.3 Mon 15:30 ZEU 146

Simulation of Borate glasses — •Christoph Scherer[1,2], Friederike Schmid[1], Martin Letz[2], and Jürgen Horbach[3] — [1]Johannes Gutenberg-Universität, Mainz — [2]Schott AG, Mainz — [3]Heinrich-Heine-Universität, Düsseldorf

The model glass former B2O3 is studied as an example for generating accurate glass structures on the computer. B2O3 is an important component for the simulation of oxide glasses since boron can form triangular planar structures, as well as tetrahedral nearest neighbor structures and also boroxol rings. In one approach, configurations of a few hundred atoms are equilibrated at high temperature, well above the glass transition temperature, with a classical molecular dynamics simulation (MD). After a quench down to 0K, they are structurally relaxed by means of an ab inito (DFT) calculation. The structural and vibrational properties are compared to the results of a full ab inito quench to 0K and to experimental results. The dependence of the glass structure and the liquid properties on the classical force field is examined. Therefore, a set of classical force fields is generated by means of a structural fitting procedure. The parameters are fitted in a way that the structure, namely the radial distribution functions and the angular distributions, of a classical MD run matches as closely as possible the structure of an ab initio (DFT) run at the same temperature. Parameter fits are carried out according to an ab initio trajectory at high temperature, where the system is in the liquid state. This sets the basis for the next steps: The development of a classical force field for sodium-borate glasses by the same methodology.

DF 4.4 Mon 15:45 ZEU 146

Mixing random organization and jamming — •Michael

Schmiedeberg — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

The random organization and the athermal jamming transition can both be studied in a unifying model system. We study the mixture of the protocols of the two transitions and argue that such a mixture can be interpreted as the glass transition at small but non-zero temperatures.

In our model system, first particles are randomly distributed and then in each step overlapping particles are displaced. In case of displacements in random directions the so-called random organization transition is observed. For purely deterministic displacements the jamming transition is realized. While the jamming protocol match with a quench of a soft sphere system from infinite to zero temperature without crossing energy barriers, the random displacements of the random organization protocol correspond to thermally activated rearrangements of particles. If in a mixed protocol the probability of random displacements is small but non-zero we find that the transition differs significantly from the purely deterministic jamming transition. We believe that our model system can help to understand why there is a difference between the glass transition at small but non-zero temperatures and the athermal jamming transition.

DF 4.5 Mon 16:00 ZEU 146

Existence of glass-form factors — •Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, A-6020 Innsbruck, Austria

A hallmark of the glass transition is the slow structural relaxation of a quasi-arrested structure. As an idealization the dynamics is considered to become non-ergodic directly at the glass transition such that all auto-correlation function coupling to the structural relaxation exhibit finite non-trivial long-time limits often referred to as glass-form factors or nonergodicity parameters. Simultaneously, the theory of stochastic processes in the framework of probability theory imposes quite stringent conditions on the class of correlation functions. The existence of a finite limit at long times is then connected to the properties of the associated spectral measure, and in general correlation functions can either oscillate forever, display quasi-periodic behavior, or even intermittent behavior. While for purely relaxation dynamics, e.g. Brownian dynamics, the existence of a long-time limit is trivial, the situation for the case of Newtonian dynamics has been elusive so far.

In this talk I elaborate conditions covering a broad class of theoretical approaches that guarantee the existence of a long-time limit. As a special case I show that the mode-coupling theory of the glass transition belongs to that class. As an outlook I briefly discuss the case of multiple decay channels relevant for molecular or confined systems.

15 min break

DF 4.6 Mon 16:30 ZEU 146

Spin freezing in geometrically frustrated magnets — Jorge Rehn[1], Arnab Sen[1,2], •Alexei Andreanov[1], Antonello Scardicchio[3], Kedar Damle[4], and Roderick Moessner[1] — [1]Max-Planck Institut fur Physik komplexer Systeme, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India — [3]The Abdus Salam ICTP, Trieste, Italy — [4]The Tata Institute, Mumbai, India

Materials which are believed to be faithfully represented by classical frustrated magnets with macroscopically degenerate groundstates, often exhibit spin-freezing. The latter is a transition to a spin-glass phase. Explaining the mechanism of such freezing is not always a simple task, since conventional ingredients, like randomness of the interactions, is not always present in the systems under study. We present a model, where dilution alone generates frustrating interaction between certain spins in the systems and leads to their freezing. The effective model deals with antiferromagnetically coupled Heisenberg spins in 2D. Both the long-range nature of the interaction and its dependence on the distance are crucial for the existence of the glass phase. We confirm our predictions by performing Monte-Carlo simulation of the effective model.

DF 4.7 Mon 16:45 ZEU 146

Glasses of binary colloidal mixtures in the quiescent state and under shear — •Tatjana Sentjabrskaja, Marco Laurati, and Stefan Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine Universität Düsseldorf, D-40225 Düsseldorf, Germany

We investigate mixing effects on the glass state of binary colloidal hard sphere mixtures with large size asymmetry (size ratio 1:5). Increasing the amount of small spheres in a system of large ones, a glass-glass transition is observed, where the large particles, initially caged by the large spheres, become localised in a cage of small spheres [1]. During the transition, the dynamics accelerate and a strong reduction of the yield strain as a result of the shift of random close packing is observed[2].

The results of rheology are compared to measurements of the dynamics of particles under shear. The super-diffusion typically associated with stress overshoots [3] becomes more pronounced for mixtures in which the dynamics are increasingly arrested. Moreover, we observe different degrees of shear-induced constriction depending on mixing ratio, which closely follow changes in the magnitude of the stress overshoot.

[1] T.Sentjabrskaja et al., AIP Conf.Proc., 1518, 206, 2013.
[2] T.Sentjabrskaja et al., Soft Matter, 9(17), 4524- 4533, 2013.
[3] M.Laurati et al., J. Phys.: Condens. Matter, 24, 464104, 2012.

DF 4.8 Mon 17:00 ZEU 146

Microscopic theory for sheared colloidal glasses and gels — •Christian Amann and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We use mode coupling theory (MCT) to calculate in three dimensions (3D) transient density autocorrelators in start-up shear flow. It is thus possible to quantitatively predict flow curves and distorted structure of colloidal glasses and gels under shear flow. We investigate the transient, non-linear, non-monotonous stress response to strain and structure-factor distortion in 3D as well as steady-state flow curves (cf. [1] for 2D calculations). Density correlators, stress response, and structure-factor distortions are in good qualitative agreement with experiments [2], while the quantitative errors of the theory can be identified. A close connection between the time-evolution of symmetries of structure-factor distortions and non-monotonous stress response (i.e. stress overshoot) can be observed. We use as input a structure factor calculated with analytical Percus Yevick closure, which allows to approximate a hard sphere repulsion as well as augmenting a short range square-well attraction [3]. Hence, implications of a gel-glass to repulsive-glass transition on the transient rheology can be studied.

[1] Amann, C.P. et al. *J. Rheol.* **57**, 149 (2013); Henrich O. et al. *Phil. Trans. R. Soc. A* **367**, 5033 (2009)
[2] Denisov, D. et al. *Sci. Rep.* **3**, 1631 (2013)
[3] Dawson K. et al. *PRE* **63**, 011401 (2000)

DF 4.9 Mon 17:15 ZEU 146

An efficient Monte Carlo algorithm to study structural relaxation in network forming materials — •Richard Vink — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Germany

Network forming materials are ubiquitous in nature, common examples being semiconductors such as silicon and silica, as well as fluids that can form hydrogen bonds. What these materials have in common is that their topology on short length scales is governed by certain rules. For example, in amorphous silicon, most atoms are 4-fold coordinated, the preferred Si-Si bond length being $\approx$ 2.35 Å, and the preferred Si-Si-Si bond angle being the tetrahedral angle. This complicates molecular dynamics simulations of these materials, where the particles spend most of their time thermally fluctuating about their equilibrium positions, while large structural changes in the network topology are rare. To overcome this problem, Wooten, Winer, and Weaire (WWW) introduced a special Monte Carlo move consisting of bond switching Monte Carlo moves which turned out to be very efficient at structurally relaxing networks of amorphous silicon and silica [Phys. Rev. Lett. **54** 1392 (1985)]. Unfortunately, the algorithm is only correct when used at zero temperature. In order to also address finite temperature, I propose a modification to the original WWW algorithm such that the Boltzmann distribution is faithfully sampled at any given temperature. The resulting algorithm is used to study the melting transition of a two-dimensional three-fold coordinated network.

DF 5: Invited Talk - Simone Sanna

Time: Tuesday 9:30–10:15 Location: GER 37

Invited Talk DF 5.1 Tue 9:30 GER 37

Understanding the puzzling behavior of $LiNbO_3$ surfaces form *first-principles* — •Simone Sanna — Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The hallmark of ferroelectric surfaces is the possibility to switch their surface chemistry and physics by switching the bulk polarization. This is a unique feature, successfully exploited in modern applications, such as molecular self-assembly or molecular detectors. At the same time, however, the polarization charge gives rise to many exciting surface phenomena such as reconstructions and relaxations, which are not fully understood. Striking differences in the evaporation rates, work functions, chemical reactivity, etching rates and water freezing temperatures at differently polarized $LiNbO_3$ (0001) surfaces are further puzzling examples of a peculiar behavior, whose origin is still unclear. Unfortunately, the atomic structure of the $LiNbO_3$ surfaces remained for a long time experimentally inaccessible, as the unscreened surface charges hinder atomic force microscopy (AFM). In this work we present theoretical models of the technologically relevant (0001) and $(2\overline{1}\overline{1}0)$ lithium niobate surfaces, commonly referred to as Z-cut and X-cut. In a first step, the microscopic structure of the stable surface terminations is determined by ab initio thermodynamics. In a second step, the outcome of available experiments is explained on the basis of our density functional theory models. Particular emphasis is given to the interpretation of available AFM-images and to the explanation of several uncommon properties.

DF 6: High- and low-k-dielectrics (Joint Session with DS)

Time: Tuesday 10:30–11:50 Location: GER 37

DF 6.1 Tue 10:30 GER 37

Magnetoelectric effect in $FeCr_2S_4$ — •Martin Wohlauer, Stephan Krohns, Joachim Deisenhofer, Vladimir Tsurkan, and Alois Loidl — Universität Augsburg, Lehrstuhl für Experimentalphysik V, Universitätsstraße 1, 86150 Augsburg

The substance $FeCr_2S_4$ is a well investigated ferrimagnetic[1] spinel-type halfmetal[2]. Despite many publications describing effects in this compound over the last 50 years, the complex interactions of its many physical features leave many unanswered questions until today. Especially its magnetic and dielectric properties still show unreported effects. In this talk I'll present new measurements of dielectric constants under the influence of magnetic fields up to 7 Tesla, showing a magneto-electric coupling below 10 K. Kalvius *et al.*[3] presented evidence for a noncollinear spin structure below 40 K. The change of ϵ' by a magnetic field indicates a lowered crystal symmetry which may be caused by a helical spin configuration.

[1] G. Haacke *et al.*. *J. Phys. Chem. Solids*, **28**:1699 – 1704 (1967).
[2] M. S. Park *et al.*. *Phys. Rev. B*, **59**:10018 – 10024 (1999).
[3] G. M. Kalvius *et al.*. *J. Phys.: Condens. Matter*, **22**:052205(2010).

DF 6.2 Tue 10:50 GER 37

Barium silicate (Ba_2SiO_4) as high-k dielectric material — •Shariful Islam[1], Karl Hofmann[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik (ATMOS), leibniz universität hannover — [2]Inst. f. Bauelemente der Mikroelektronik, leibniz universität hannover

In search of an alternative gate oxide, the structural and electronic properties of mixed Ba/Sr silicates on Si(001) were investigated. In order to specify the stoichiometry and band gap of these oxides we used X-ray Photoelectron Spectroscopy (XPS) and Electron Energy Loss Spectroscopy (EELS) respectively. Crystal structures were investigated by Spot Profile Analysis-Low Energy Electron Diffraction (SPA-LEED). Electrical characterization was done by CV and IV measurements.

Characteristics of high-k dielectric $(Ba_{0.8}Sr_{0.2})_2SiO_4$ and Ba_2SiO_4 were studied both on structured and unstructured samples. Both oxides are stable at high temperature and at ambient atmosphere. Crystalline $(Ba_{0.8}Sr_{0.2})_2SiO4$ has dielectric constant, $\varepsilon = 18 \pm 2$. The band gap was found to be 6.0 eV, with band offsets $>$ 2eV both for valence and conduction band. The thick crystalline layers of pure $(Ba_{0.8}Sr_{0.2})_2SiO_4$ were also grown. An $\varepsilon = 19.6 \pm 0.4$, a small reduction of bandgap to 5.7 ± 0.1 eV and band offsets comparable to $(Ba_{0.8}Sr_{0.2})_2SiO_4$ were found. Due to our growth procedure (diffusion of Si into oxide) leakage currents are still comparatively high (0.1 A/cm^2 at 1V). Further electrical and structural properties of Ba_2SiO_4 will also be presented.

DF 6.3 Tue 11:10 GER 37

Comparison of different gate dielectrics for GaN based high electron mobility transistors — •Annett Freese[1], Stefan Schmult[2], Andre Wachowiak[1], and Thomas Mikolajick[1,2] — [1]NaMLab gGmbH, Nöthnitzer Str. 64, D-01187 Dresden — [2]TU Dresden, Institute of Semiconductor and Microsystems (IHM), Nöthnitzer Str. 64, D-01187 Dresden

The wide-bandgap and high electron mobility make gallium nitride (GaN) based heterostructures particularly interesting for future high-power switching applications. However, conventional GaN heterostructure field effect transistors (HFET) use a simple Schottky gate contact. Thus, they suffer from undesired high gate leakage currents and current collapse. To eliminate these challenges, a dielectric material can be placed between the gate electrode and the semiconductor. Aluminium oxide (Al2O3), hafnium oxide (HfO2), and zirconium dioxide (ZrO2) are potential candidates for such a gate dielectric material due to their high dielectric constant as well as their high conduction band offset to GaN. Learning from silicon processing technology, a successful integration of a suitable dielectric does not only depend on its material properties, but also relies heavily on the nature of the interfaces to the top and bottom electrodes. In this work we investigated Al2O3, HfO2 and ZrO2 with respects to their structural and electrical properties on GaN. The influence of the deposition methods, Molecular Beam Deposition (MBD) and Atomic Layer Deposition (ALD), on the film quality was studied.

DF 6.4 Tue 11:30 GER 37

Effect of different precursor for Atomic Layer growth of Ga2O3 using H2O as the oxygen source — •Sakeb Hasan Choudhury, Massimo Tallarida, Chittaranjan Das, and Dieter Schmeisser — Brandenburg University of Technology, Applied Physics-Sensors technology, Konrad-Wacshmann-Allee, 17, 03046 Cottbus, Germany

Atomic Layer deposition as a technique provides appropriate thickness control, conformality and Homogeneity. However, the contribution of Precursor and Substrate in the growth process is worth exploring and cannot be avoided as previously seen in case of Trimethyl Gallium. Ga2O3 is a member of group *Transparent Conducting Oxides*, hence possess immense potential in numerous applications. In this work, we would like to report about the growth of Ga2O3 using Tris-(dimethylamino)-gallium dimer and H2O as metal and oxygen precursors, respectively. Unlike Trimethylgallium, Ga2O3 films can be produced between temperature 200-300°C using Tris-(dimethylamino)-gallium dimer and it seems to be well compatible with H2O. These films were characterized by Synchrotron X-ray photoemission spectroscopy at BESSY/HZB, Berlin and subsequent analysis reveals stable film growth and absence of growth terminating phenomenon*s.

DF 7: Invited Talk - Thorsten Granzow

Time: Tuesday 12:00–12:45 Location: GER 37

Invited Talk DF 7.1 Tue 12:00 GER 37

Defects in functional polar oxide materials - Detection and influence on electrical properties — •Torsten Granzow[1], Nina Balke[2], Julia Glaum[3], and Silke Schaab[4] — [1]CRP - Gabriel Lippmann, Belvaux, Luxembourg — [2]ORNL, Oak Ridge, USA — [3]UNSW, Sydney, Australia — [4]TU Darmstadt, Darmstadt, Germany

All properties of functional polar oxide materials are critically influenced by defects, both charged and uncharged, in the crystal structure. This gives the possibility to systematically tune properties relevant for application by doping, but also carries the risk of deteriorating performance under different conditions. This presentation takes a look at both sides. It first addresses the question of electrical fatigue and aging in bulk piezoelectric ceramics on the example of doped lead zirconate titanate (PZT). A comparison of large- and small-signal properties shows phenomenological similarities between fatigue - deterioration of properties under cyclic electric loading - and aging - deterioration with time without load. It is shown in how far both effects can be explained by the same cause, migration of charge carriers to grain boundaries. After that, the possibilities to influence phase stability and relaxor behavior in lanthanum-modified lead zirconate titanate (PLZT) are investigated. Here, the defects are modified by annealing in different reducing atmospheres. A combination of optical and electrical measurements reveals that the final defect structure and the resulting electrical properties depend on the type of reducing agent just as much as on the oxygen partial pressure. The results are discussed and contrasted to commonly used relaxor models.

DF 8: Multiferroics I (Joint Session with MA, DS, KR, TT)

Time: Tuesday 9:30–12:45 Location: BEY 118

DF 8.1 Tue 9:30 BEY 118

***Ab initio* study of electronic transport in the Co/PZT-based tunnel junctions** — •Vladislav Borisov[1], Sergey Ostanin[1], Igor Maznichenko[2], Arthur Ernst[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Magnetoelectric coupling at the multiferroic interfaces FM/FE (FM=Co,Fe, FE=$PbTiO_3$,PZT) was studied from first principles. The magnetic interfacial effect, which is controlled by the FE polarization, originates from the charge transfer and *d*-orbital redistribution of Co/Fe and Ti mediated by the *p*-states of interfacial oxygens. In PZT, the presence of Zr dopants may locally enhance the effect. We analysed also the spin polarization of tunneling electrons in Co/PTO/Co and Fe/PTO/Co junctions, in which the calculated four-state conductance can account for the ferroelectrically switchable TMR signal observed recently in LSMO/PZT/Co [1].

[1] D. Pantel *et al.*, *NATURE MATERIALS* **11**, 289 (2012).

DF 8.2 Tue 9:45 BEY 118

Tunneling transport and memristive effects in PbTiO3- based multiferroic tunnel junctions — •Andy Quindeau, Marin Alexe, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

A gradually tunable resistance effect based on the tunnel electroresistance (TER) of multiferroic tunnel junctions is investigated. The ferroelectric tunnel barrier comprises, a PbTiO3 layer of a few nm thickness, is embedded between two different ferromagnetic layers, viz. La0.7Sr0.3MnO3 and cobalt. In this capacitor geometry an electric bias, applied perpendicularly to the films, results in a direct tunneling current flowing between the two electrodes. The tunnel resistance is dependent on the polarization of the ferroelectric, which is switchable via relatively high voltage pulses. Due to the variation of the pulse parameters a variety of non-volatile resistance states can easily be achieved. These gradually tunable resistance states, characteristic for a memristor device, can be explained by a ferroelectric domain distribution inside the ferroelectric film: Domains with different polarities can coexist inside one capacitor after partial polarization switching and act as parallel connected tunnel barriers with different tunnel resistances. Temperature dependent measurements show the influence of different electron transport mechanisms, which will be discussed. The impact of the memristive states on the tunnel magnetoresistance (TMR) can be shown.

DF 8.3 Tue 10:00 BEY 118

Lattice and polarizability mediated spin activity in EuTiO3 — •Annette Bussmann-Holder[1], Kevin Caslin[1,2], Patrick Reuvenkamp[1], Zurab Guguchia[3], Hugo Keller[3], Reinhard Kremer[1], and Jürgen Köhler[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr.1, D-70569 Stuttgart, Germany — [2]Brock University, 500 Glenridge Ave., St. Catharines L2S-3A1, Ontario, Canada — [3]Physik-Institut der Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich, Switzerland

EuTiO3 is shown to exhibit novel strong spin-charge-lattice coupling deep in the paramagnetic phase. Its existence is evidenced by an, until now, unknown response of the paramagnetic susceptibility at temperatures exceeding the structural phase transition temperature TS=282K. The extra features in the susceptibility follow the rotational soft zone boundary mode temperature dependence above and below TS. In addition, novel magnetostriction experiments and dielectric constant measurements have been performed which both reveal giant anomalies related to the antiferromagnetic phase transition at TN=5.7K and the structural phase transition at TS. The theoretical modeling consistently reproduces these anomalies and provides evidence that EuTiO3 has considerable analogies to SrTiO3 but also substantial differences stemming from the Eu 4f spins which are lattice activated at high temperatures far above TN.

DF 8.4 Tue 10:15 BEY 118

Magnetoelectric coupling in a composite multiferroic structure revealed by Ferromagnetic Resonance — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle/Saale, GERMANY — [2]Centro de Investigacion Materiales Avazados, S.C. (CIMAV), Chihuahua/Monterrey, MEXICO — [3]Lanzhou University, Lanzhou, CHINA

We theoretically study [1] a thin multiferroic junction related to a barium titanate (tetragonal or rhombohedral phase) layer in contact with an iron layer. Depending on the type of the magnetoelectric coupling at the interface - either due to screening charge or due to an epitaxial strain resulting in a strong magnetoelastic coupling - we present a detailed analysis of the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance as a function of the applied electric field.

[1] A. Sukhov, P.P. Horley, C.-L. Jia, J. Berakdar, J. Appl. Phys. **113**, 013908 (2013).

DF 8.5 Tue 10:30 BEY 118

Magnetoelectric monopoles in bulk periodic solids — •Michael Fechner[1], Eric Bousquet[1], Alexander Balatsky[2], Nicoal A. Spaldin[1], and Lars Nordström[3] — [1]ETH Zürich, Department for Materials Theory, Zürich, Switzerland — [2]NORDITA, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Sweden

The magnetoelectric (ME) response is described by a second rank tensor that can be decomposed into irreducible isotropic diagonal, antisymmetric and trace-free part. Here we show that the former component can be identified with a ferroic ordering of magnetoelectric monopoles[1]. We further develop a scheme to calculate the ME monopole in bulk periodic solids, by exploiting similarities to the ferroelectric polarization. Finally, as an example we present results for the series of lithium transition metal phosphate compounds ($LiMPO_4$, with M = Co, Fe and Ni), which include both ferromonopolar and

antiferromonopolar ordered cases. We predict for the latter case a q-dependent diagonal ME effect.

[1] N . A. Spaldin et al., PRB 88, 094429 (2013)

DF 8.6 Tue 10:45 BEY 118

Different routes for enhanced control of ferroelectric polarization by magnetic field — •I. Fina[1,2], V. Skumryev[3,4], D. O'Flynn[5], G. Balakrishnan[5], N. Dix[2], J. M. Rebled[2,6], P. Gemeiner[7], X. Marti[8], F. Peiró[6], B. Dkhil[7], F. Sánchez[2], L. Fàbrega[2], and J. Fontcuberta[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institut de Ciència de Materials de Barcelona, Catalonia, Spain — [3]Institució Catalana de Recerca i Estudis Avançats (ICREA), Catalonia, Spain — [4]Universitat Autònoma de Barcelona, Barcelona, Spain — [5]University of Warwick, Coventry, United Kingdom — [6]LENS - MIND/IN2UB, Barcelona, Spain — [7]Propriétés et Modélisation des Solides, Paris, France — [8]Faculty of Mathematics and Physics, Praha, The Czech Republic

I will focus on the direct magnetoelectric effect, control of polarization vector by magnetic field, in single-phase and composite multiferroic materials in thin film form.

In single-phase multiferroic materials, cycloidal magnet, we will see that strong coexistence of polar and non-polar regions allow large susceptibilities leading to a full control of the polarization vector by means of magnetic field [1]. In composite materials, ferromagnetic-ferroelectric heterostructures, the limiting factor is the substrate clamping effect. We will show that we can overcome this undesired effect, enhancing the presence of some small quantity of defects. These defects store the needed elastic energy, enhancing the magnetoelectric coupling, which result in huge effects near room temperature [2].

[1] I. Fina, et al., Phys. Rev. B 88, 100403(R) (2013). [2] I. Fina, et al., Nanoscale 5, 8037 (2013).

15 min. break

DF 8.7 Tue 11:15 BEY 118

Investigation of A-site Bismuth based double perovskites as potential room-temperature multiferroics — •Vikas Shabadi, Mehran VafaeeKhanjani, Mehrdad BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

A-site Bismuth based double perovskites ($Bi_2BB'O_6$), where ferroelectricity arises from the stereochemically active $6s^2$ lone pair of electrons on the Bi^{3+} cations, provide a vital test bed to engineer room temperature multiferroicity. Here, different combinations of 3d-3d or 3d-5d cations may be introduced at the B-site in order to obtain an effective ferri/ferromagnetic moment. The 3d-3d compound Bi_2FeCrO_6 (BFCO) has drawn a heightened interest due to its large experimentally reported ferroelectricity and divergent observations of its magnetic properties. We report epitaxial BFCO thin films grown by pulsed laser deposition on single crystal $SrTiO_3(100)$ substrates. Detailed structural characterization was performed by X-ray Diffraction and the magnetic properties were studied with a SQUID magnetometer. We show that BFCO adopts a superstructure with the same unit cell as the chemically ordered double perovskite. The magnetization is a function of chemical but not of structural order.

DF 8.8 Tue 11:30 BEY 118

Room temperature magnetism and ferroelectricity in eps-Fe2O3 thin films — •I. Fina[1], M. Gich[2], A. Morelli[1], F. Sánchez[2], M. Alexe[1], J. Fontcuberta[2], and A. Roig[2] — [1]Max Planck Institute of Microstructure Physics D-06120 Hallle/Salle, Germany — [2]Institut de Ciència de Materials de Barcelona ICMAB, Consejo Superior de Investigaciones Científicas CSIC, Campus UAB 08193 Bellaterra, Catalonia, Spain

The quest for magnetoelectric multiferroics is driven by the promise of a novel generation of devices combining the best characteristics of ferromagnetic and ferroelectric materials. These cherished applications require materials displaying a substantial magnetization and electric polarization which are coupled and coexist well above room temperature. These properties are not commonly fulfilled by single phase materials and firm candidates for the development of these technologies are still sought.

In this contribution, we will report on epitaxial eps-Fe2O3 thin films grown by Pulsed Laser Deposition on (111) SrTiO3 and present recent data on its structural, magnetic and dielectric characterization. The films are ferromagnetic and ferroelectric at room temperature and display magnetization and polarization values at remanence of about 50 emu/cm3 and 1 uC/cm2 with a long retention. A magnetocapacitive response has also been detected indicating that the films present coupling between both ferroic orders.

DF 8.9 Tue 11:45 BEY 118

Time-resolved analysis of switching in spiral multiferroics — •Jonas Stein[1], Tobias Cronert[1], Jeannis Leist[2], Karin Schmalzl[3], A Agung Nugroho[4], Alexander C Komarek[5], 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]Institut Teknologi Bandung, Indonesia — [5]MPI für chemische Physik fester Stoffe

Multiferroic crystals are promising materials for future memory devices with extremely low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spiral spin multiferroic $TbMnO_3$. Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an external electric field. Using the stroboscopic technique we can follow the reversion of chiral domains in the timescale of a few 100 microseconds to hours. In $TbMnO_3$ we find a clear logarithmic relation between the rise time and temperature that is fulfilled over 5 decades.

DF 8.10 Tue 12:00 BEY 118

Thermodynamic properties of the new multiferroic material $(NH_4)_2[FeCl_5(H_2O)]$ — •Matthias Ackermann[1], Daniel Brüning[2], Thomas Lorenz[2], Petra Becker[1], and Ladislav Bohatý[1] — [1]Institut für Kristallographie, Universität zu Köln, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

Multiferroic materials with coupled ferroelectric and (anti-)ferromagnetic order in the same phase have attracted considerable interest during the last decade. The search for new multiferroic materials is an important issue to further improve the understanding of the underlying coupling mechanisms. Here, we present a detailed investigation of the new multiferroic compound $(NH_4)_2[FeCl_5(H_2O)]$ [1]. Our measurements of pyroelectric currents reveal, that the electric polarization occuring in the antiferromagnetically ordered phase can drastically be influenced by applying magnetic fields. Based on the results of these dielectric investigations, together with measurements of thermal expansion, magnetostriction and specific heat, detailed magnetic field versus temperature phase diagrams are derived. Depending on the direction of the magnetic field up to three different multiferroic phases are identified, which are separated from the paramagnetic phase by a magnetically ordered, but non-ferroelectric phase.

This work was supported through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] Ackermann M et al. 2013 *New J. Phys.* (in press, arXiv:1308.0285)

DF 8.11 Tue 12:15 BEY 118

Stoichiometric Effects on Crystal Quality in $LuFe_2O_4$ and $YbFe_2O_4$ — •Hailey Williamson[1,2], Geetha Balakrisnan[2], and Manuel Angst[1] — [1]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany. — [2]Department of Physics, The University of Warwick, CV4 7AL, Coventry, UK

The multiferroic rhombohedral $LnFe_2O_4$ (Ln=Lu, Y, Yb, Tm, Ho and Er) system, which can be described as stacked hexagonal Fe bilayers separated by Lu monolayers, has been in focus since the discovery of interesting magnetic and electrical characteristics in $LuFe_2O_4$. The specific CO configuration within the Fe bilayers was initially thought to produce a ferroelectricity through cross polarization of the two layers of the bilayer. However our recent investigations indicate that the CO configuration is actually non-polar. Extensive research highlighted a large sensitivity to oxygen stoichiometry, where crystals grown in an excess/deficient oxygen partial pressure environment exhibit smeared glassy magnetic transitions and diffuse CO. Through fine tuning of the atmospheric conditions, crystals exhibiting 3D CO and magnetism were produced. Interest then spread to isostructural $YbFe_2O_4$, which has currently few detailed investigations. Single crystals of $YbFe_2O_4$ were grown in four different partial pressure atmospheres to view the effects of oxygen stoichiometry on the magnetism and CO. A series of macroscopic and microscopic measurements provided a detailed look into the effects of oxygen stoichiometry on the intrinsic characteristics as well as a comparison to that of its predecessor $LuFe_2O_4$.

DF 8.12 Tue 12:30 BEY 118

Multiferroicity in Cu_2OSeO_3? — •Eugen Ruff[1], Stephan Krohns[1], Helmuth Berger[2], Peter Lunkenheimer[1], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Institute of Physics of Complex Matter, École Polytechnique Fédérale de Lausanne

Skyrmions are topologically stable vortex-like objects, for the first time detected in the B20 alloy MnSi [1]. Their electrical controllability via small currents qualifies skyrmions for applications in high-density magnetic storage devices. The recent discovery of magnetoelectric skyrmions in the insulating chiral magnet Cu_2OSeO_3 leads to another promising route to electrical control [2]. This system is suggested to carry a local electrical dipole, which implies that the skyrmions should be controllable by an external electrical field without losses due to Joule heating. Here we provide a thorough analysis of the magnetic and polar phases of this material, using SQUID and pyrocurrent measurements. In order to investigate the possible ferroelectric properties of Cu_2OSeO_3, we have performed dielectric spectroscopy in various magnetic fields in a broad frequency range below 70 K. Combining all these different techniques, we address the question whether Cu_2OSeO_3 is magnetoelectric or multiferroic. [1] S.Mühlbauer *et al.*, Science **323**, 915 (2009). [2] S.Seki *et al.*, Science **336**, 198 (2012).

DF 9: Poster Session DF

Time: Tuesday 18:30–20:00 Location: P1

DF 9.1 Tue 18:30 P1

A comprehensive surface photovoltage investigation of the $SrTiO_3$ surface — •Elke Beyreuther, Andreas Thiessen, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

In the past, surface photovoltage (SPV) analysis has been successfully applied to derive the electronic defect status of a number of wide-bandgap semiconductor surfaces. Here, the method is applied to the model perovskite strontium titanate, whose SPV phenomena are comprehensively studied over seven decades of excitation-light intensity. The SPV was recorded by a Kelvin probe setup as a function of wavelength in order to extract the energetic positions of electronic surface states within the bandgap. At selected wavelengths addressing distinct surface states, SPV transients were measured as a function of light intensity and temperature. Several models known from the literature were used to estimate and cross check surface state parameters such as surface state densities, capture cross sections for photons and electrons, and the surface band bending in the dark and under illumination. In contrast to other wide-bandgap materials, SPV transients of SrTiO3 exhibit highly complex shapes, i.e. they (i) show signatures of multiple carrier transitions, (ii) mixtures of surface and bulk contributions, as well as (iii) both ex- and intrinsic SPV processes.

[E. Beyreuther et al., Surf. Sci. 612, 1–9 (2013)]

DF 9.2 Tue 18:30 P1

Lithium Niobate (0001) Surfaces in Thermodynamic Equilibrium with Ambient Conditions — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — University of Paderborn

$LiNbO_3$ (LN) is a frequently used material for optical and acoustic applications due to its strong piezoelectric, pyroelectric, and photorefractive properties. As for other ferroelectric materials, the (0001) surface reactivity can be manipulated by polarization reversal. This opens the possibility for the realization of devices such as molecular detectors[1].

In contrast to the popularity of the material, few is known about the microscopic structure of the (0001) surfaces. Recently the surface structure in liquid solution has been demonstrated by a joint AFM and DFT investigation[2]. At relatively dry conditions only the value for the surface charge is available[3].

As a further step towards the simulation of realistic surfaces, the adsorption of the most important components of dry air (N_2, O_2, CO_2, CH_4, H_2, N_2O, CO) is simulated and the adsorption energies and geometries are determined. We present phase diagrams in dependence of temperature and pressure for every component and in presence of different amounts of water. From these phase diagrams we can extract the desorption temperatures. Additionally the influence of the adsorbed molecules on the surface charge is estimated.

[1] D. Li, M. H. Zhao, et al., *Nat. Mat.* **7**, 473 (2008)
[2] S. Rode, R. Hölscher, et al., *Phys. Rev. B* **86**, 075568 (2012)
[3] F. Johann and E. Soergel, *Apl. Phys. Let.* **95**, 232906 (2009)

DF 9.3 Tue 18:30 P1

Studying interaction between mineral particles by atomic force spectroscopy — •Stefan Klima[1,2], Monika Mirkowska[1,2], Markus Kratzer[2], Helmut Flachberger[1], and Christian Teichert[2] — [1]Chair of Mineral Processing, Department Mineral Resources and Petroleum Engineering, Montanuniversität Leoben, Austria — [2]Institute of Physics, Montanuniversität Leoben, Austria

The processes taking place when two mineral particles come into contact are most important for the industrial applied triboelectrostatic separation (TS). During TS, charge is transferred between touching particles yielding positive/negative net charges on the particles. Subsequently, the particles are separated in an electric field. However, the mechanism of charge transfer is not yet completely understood. As a model system, we investigated the charging behaviour of a single micrometer-size mineral particle touching an insulator single crystal surface. For this purpose, atomic force microscopy (AFM) was employed and force-to-distance (F-x) curves with a mineral particle attached to the free end of an AFM cantilever have been recorded. An attempt was made to evaluate changes in the F-x-curves induced by the electrostatic particle-surface interaction. As a reference, we used the interactions between the single crystal surface and the commercial, unmodified AFM cantilever. Experiments were carried out under various conditions.

DF 9.4 Tue 18:30 P1

Vibrational properties of lithium niobate from density-functional perturbation theory — •Michael Friedrich, Arthur Riefer, Simone Sanna, Wolf Gero Schmidt, and Arno Schindlmayr — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

Lithium niobate ($LiNbO_3$) is a dielectric crystal with outstanding electro-optical properties. It is characterized by a ferroelectric-paraelectric structural phase transition at 1480 K, which has been studied both theoretically and experimentally. Despite these investigations, the mechanisms of the phase transition are far from being understood. Although the phonon modes in relation to the ferroelectric instability are believed to play a crucial role, our actual knowledge of the phonon spectrum is limited to the center of the Brillouin zone. In order to shed light on the lattice dynamics leading to the ferroelectric transition, we have modeled the vibrational properties of $LiNbO_3$ within the density-functional perturbation theory. In this work we present the full phonon dispersion of both the ferroelectric and the paraelectric phases.

DF 9.5 Tue 18:30 P1

Quantum dots and lanthanides as cw-emitters in polymeric microresonators — •Carolin Klusmann[1], Sarah Wiegele[1], Tobias Siegele[1], Tobias Wienhold[2], Sebastian Köber[2,3], and Christian Koos[2,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Institute of Photonics and Quantum Electronics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Polymeric whispering gallery mode (WGM) microresonators are considered to be very auspicious candidates for the label-free detection and characterization of individual nanoscale objects due to their high quality factor and small modal volume. So far, we utilized laser dyes embedded in a polymeric host matrix as active medium for the resonators. However, resonators doped with dyes should be operated with pulsed excitation sources to reduce bleaching effects. Thus, we are looking into emitters which allow the use of a continuous pump source. Quantum dots are considered to be promising candidates for this approach due to their high quantum yield, narrow and tunable emission in combination with broad absorption spectra, higher stability and lower photobleaching rates compared to organic fluorophores. Furthermore, lanthanides with fluorescence stemming from atomic transitions are appropriate

emitters for our application because of their high photostability, sharp emission profile and large Stokes Shift. Using cw-emitters as active medium opens the possibility to observe mode-splitting by using a heterodyne detection system.

DF 9.6 Tue 18:30 P1

Monte Carlo Simulations of the Electrocaloric Effect in Relaxor Ferroelectrics — •Constanze Kalcher, Alexander Stukowski, and Karsten Albe — Institut für Materialwissenschaft, TU Darmstadt, Germany

Relaxor ferroelectrics (RFEs) are a promising material class for cooling devices based on the electrocaloric effect.

It is widely accepted, that polar nanoregions and quenched random fields arising from disorder in the atomic structure are inherent features of RFEs. However, their interplay is not yet fully understood.

Here we present the results of lattice based Monte Carlo simulations. We model a relaxor ferroelectric with a Random-Bond-Random-Field Ising model and study its behavior in an electric field using Wang-Landau sampling and a demon algorithm after Creutz. This allows us to predict the electrocaloric effect in the model material. Finally the results of the direct methods are compared with the indirect approach via the Maxwell equation.

DF 9.7 Tue 18:30 P1

Kerr gating efficiency of tellurite glasses as a function of their composition — •Christian Karras, Kay Schuster, Stephan Grimm, Wolfgang Paa, and Herbert Stafast — Institut für Photonische Technologien, Albert - Einstein - Straße 9, 07745 Jena

Tellurite glasses were announced to be a promising material for optical Kerr gating (OKG) [1]. We investigated the applicability of tellurite glasses as OKG switching material as function of its composition. Therefore we used a dual frequency Kerr gating setup where the material was pumped at 800 nm and the transient Kerr signal was observed at 530 nm. Four different composite tellurite glasses with varying ratios of TeO_2 and K_2O or ZnO were investigated with respect to the optimum gating efficiency, the optimum pump power, and the temporal resolution. Especially the gating efficiency strongly depended on the material composition. For materials with a high TeO_2 concentration gating efficiencies above 50% could be achieved at moderate pump intensities below 1 TW/cm^2. We compared the switching behavior of the tellurites glasses with other promising materials for OKG, such as fused silica, zinc sulfide and Schott SF56, a heavy flint glass. All tellurites showed superior behavior in terms of efficiency but had a significantly extended minimum gating time compared to fused silica. We considered dispersion to be a major reason for the latter effect. Therefore we applied an easy pulse propagation model in order to estimate the signal broadening due to dispersion.

[1] Z. Hang et al., Journal of Optics, 14(6), 065201 (2012).

DF 9.8 Tue 18:30 P1

Optical properties of Ti indiffused LiNbO3 from first principles — •Arthur Riefer, Simone Sanna, Arno Schindlmayr, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn, Germany

Lithium niobate (LN) is one of the most important ferroelectric materials and the most important nonlinear optical material. Recently, the linear and nonlinear optical properties of highly ordered stoichiometric as well as of congruent LN have been investigated theoretically[1,2,3]. However, many applications, such as waveguides for signal processing or sensor systems, are based on Ti indiffused LiNbO3, whereby the Ti doping modifies in particular the refractive index[4]. In the present work, we investigate the electronic and optical properties of Ti indiffused LN from first-principles. Different concentrations of Ti are simulated by substitutions of Li or Nb atoms with Ti atoms. Based on this approach the electronic properties are calculated within DFT-GGA. The optical response is determined at the level of independent particles.

[1] W. G. Schmidt *et al.*, Phys. Rev. B **77**, 035106 (2008)
[2] Riefer *et al.*, IEEE Trans. on Ultrasonics, Ferroelectrics and Frequency Control **59**, 1929 (2012).
[3] Riefer *et al.*, Phys. Rev. B **87**, 195208 (2013)
[4] G. Singh *et al.*, "Ti indiffused Lithium Niobate ..", in "New Advanced Technologies" (2010), ISBN: 978-953-307-067-4

DF 9.9 Tue 18:30 P1

Magnetization dynamics and chirality control in the Cu_2OSeO_3 skyrmion compound — •Rolf Versteeg, Matteo Montagnese, and Paul Van Loosdrecht — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77

Skyrmions are 2D-topologically protected magnetic structures which appear as screw-like nanostructures. The combination of different magnetic interactions gives rise to these intriguing structures with sizes generally between 20-90nm. Skyrmions promise to be of great technological value in the form of nano-sized, easily writeable and readable bits. Apart from the technological interest these magnetic structures also open new avenues in fundamental research in light-matter interaction, magnetization dynamics and chirality. Our ideas and recent efforts to study Skyrmion dynamics and their formation in the multiferroic insulator Cu_2OSeO_3 by means of different optical techniques will be presented.

DF 9.10 Tue 18:30 P1

Selective preparation and detection of phonon polariton wavepackets by stimulated Raman scattering — •Jan-Etienne Pudell[1], Jewgeni Goldshteyn[2], Andre Bojahr[1], Peter Gaal[2], Daniel Schick[1], and Matias Bargheer[1,2] — [1]Institut für Physik & Astronomie, Potsdam, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany

Wavevector-selective impulsive excitation of phonon-polaritons by a spectrally broad femtosecond transient gratings produces wavepackets propagating in opposite directions. The photons in spectrally narrow probe pulses are scattered from these elementary excitations in Lithium Niobate (LiNbO3). Both elastically and inelastically scattered photons are simultaneously detected in a spectrometer. The Stokes- and anti-Stokes shifted probe pulses uniquely determine the propagation direction of the detected polariton wavepacket component and correspond to creation and annihilation of phonon-polaritons, respectively. This experiment with spectrally broad pump and spectrally narrow probe pulses allows dissecting the four-wave-mixing process into two sequential stimulated Raman scattering events. Based on this analysis, we selectively prepare phonon-polariton wavepackets propagating only in one direction according to a spectrally assymmetric excitation by two light pulses.

DF 9.11 Tue 18:30 P1

Modified differential scanning calorimeter setup for the measurement of the electrocaloric effect in relaxor ceramics — •Mehmet Sanlialp, Vladimir Shvartsman, and Doru C. Lupascu — Institute for Materials Science, University Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany

Demand for energy-efficient refrigeration technologies with a reduced environmental impact has stimulated interest to materials that exhibit the electrocaloric (EC) effect. The EC effect is a change of temperature or entropy of a dielectric material under an applied electric field at adiabatic or isothermal conditions, respectively. In spite of intensive studies of EC materials during the last 5 years, reliable direct measurements of the EC effect still remain a challenge. In this presentation we report on the development of an experimental setup based on a differential scanning calorimeter for EC measurements of bulk samples at quasi-isothermal conditions in the temperature range 150-500 K at applied electric fields up to 100 kV/cm. We performed EC measurements in several lead-containing and lead-free ceramics:

(1-x)$PbMg_{1/3}Nb_{2/3}O_3$-x$PbTiO_3$, $(Pb_xLa_{1-x})(Zr_yTi_{1-y})O_3$,
and(1-x)$Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$.

Effects of temperature, electric field magnitude as well as a degree of relaxor behavior on the measured EC effect are discussed. Furthermore we compare the results of direct EC measurements with indirect EC estimations based on the Maxwell relations to judge the compatibility of these two measurement methods.

DF 9.12 Tue 18:30 P1

Influence of leakage current in $BaTiO_3$-capacitors on stored energy — •Tino Band[1], Martin Diestelhorst[1], Sebastian Lemm[1], Mandy Zenkner[2], and Albrecht Rost[3] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, D-06099 Halle, Germany — [2]Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, D-06099 Halle, Germany — [3]University of Applied Sciences Merseburg, 06217 Merseburg, Germany

The development of dielectric energy storage is of prime importance. Our investigations are motivated by the expectation to realize higher power densities and much more load/reload cycles compared to electrochemical energy storages. Up to now the high energy densities of electrochemical storage batteries could not be achieved by dielectric

materials. Therefore the aim is to raise the energy density of capacitors by finding dielectrics with high permittivities ε. At first glance ferroelectrics fulfil these requirements, because of their relatively high values of ε. We use modified $BaTiO_3$ ceramic capacitors for our research. It is well known that ceramic capacitors show a non negligible leakage current. Based on the equivalent circuit of real capacitors we discuss the influence of leakage currents on hysteresis measurements and the stored energy. As a result we present comparisons of our calculation and compensated hysteresis measurements.

DF 9.13 Tue 18:30 P1

Electrical and optical defect spectroscopy on high-k materials — •Patrick Scharf, Alexander Schmid, and Johannes Heitmann — Institute of Applied Physics, TU Bergakademie Freiberg, 09599 Freiberg

Temperature dependent electrical and optical defect spectroscopy on high-k materials, especially on Al_2O_3 and ZrO_2 was performed. High-k layers of varying thickness were realized by atomic layer deposition (ALD). The samples were prepared as MIS (metal-insulator-semiconductor) or MIM (metal-insulator-metal) structures on a silicon substrate. The electric contact to the top electrode was established by ball bonding of a 25 μm thick gold wire on Ti/Al/Ti/Au contact pads. For the MIM samples a 12 nm thick TiN layer was used as bottom electrode.

The samples were characterized by current voltage measurements. Therefore investigations were carried out in the range of room temperature down to 25 K. The current voltage characteristics were found to be strongly temperature dependent. For further investigation of defects in the high-k material and at the high-k/silicon interface, a laser-assisted current voltage method is presented. By optical excitation with an infrared laser and measurement of the resulting current with respect to the incident wavelength, defect states in the band gap of the dielectric can be characterized.

DF 9.14 Tue 18:30 P1

Frequency Dispersions of Accumulation Capacitances of Metal/n-VO2/SiO2/p-Si Capacitors — Varun John[1], •Lei Zhang[1], Danilo Bürger[1], Ilona Skorupa[2], Oliver Schmidt[3], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [3]Institute for Integrative Nanosciences, IFW Dresden

Admittance measurements have been performed on Al/n-VO_2/SiO_2/p-Si capacitors with different VO_2 thicknesses and on Al/SiO_2/p-Si reference MOS capacitors. The MOS capacitor with an extra VO_2 layer shows an anomalous frequency dependent capacitance for -7V accumulation bias due to bulk traps introduced to the SiO_2 layer during the growth of VO_2 by PLD[1]. The accumulation capacitance varies from a large value at the low AC test bias frequency of 1kHz to a value of 0.05 μF at the frequency of 1MHz which corresponds to the capacitance of the 80nm thick SiO_2 layer. The accumulation capacitance has a direct relation to the VO_2 layer thickness. The capacitance vs frequency curves of the Al/n-VO_2/SiO_2/p-Si capacitors are modeled using a distributed circuit model taking into account the admittance arising from the change in occupancy of bulk traps in SiO_2[2]. The position dependent density and the time constant of the traps have been obtained from the best fit parameters in the simulations. [1] György J. Kovács, et al., Appl. Phys. 109, 063708 (2011). [2] Y. Yuan, et al., IEEE Trans. on Electron Devices, 59, 2100-06 (2012).

DF 9.15 Tue 18:30 P1

Thermoelectric oxides in glass-ceramic materials — •Julian Lingner[1,2], Gerhard Jakob[1], and Martin Letz[2] — [1]Johannes Gutenberg-Universität Mainz — [2]Schott AG Mainz

Energy demand worldwide is a central topic which motivates the research in the field of conversion materials. Within this area, thermoelectric materials have received wide attention in the last 20 years and some major improvements have been made in order to tune their efficiency. Material classes like silicides, half-heusler compunds or oxides are currently under investigation with individual advantages and disadvantages. Materials that withstand high temperatures above 500°C are especially in great demand since the thermoelectric conversion efficiency is proportional to the applied temperature difference so that the potential fields of application are extended. Due to the requirement paired with environmental regulations it is very important to find materials which operate in these temperature regions while at the same time being naturally abundant and non-toxic. This presentation shows two unconventional glass-ceramic systems which contain thermoelectric active crystalline regions. Starting from a base glass system, a thermoelectric crystal structure is embedded in the glass-matrix via a controlled thermal treatment. This leads to many new properties of the material. Especially the possibility to induce small crystallites, the pore-free surface combined with the high-temperature durability of this material class support this approach. The preparation and results of thermoelectric measurements on different glass-ceramic systems are presented.

DF 9.16 Tue 18:30 P1

Ferroelectric Domains at the Phase Transition in Bariumtitanate — •Thorsten Limböck and Elisabeth Soergel — Institute of Physics, University of Bonn, Nussallée 12, 53115 Bonn, Germany

The classical example of a perovskite crystal, Bariumtitanate, exhibits several phase transitions, namely from rhombohedral to orthorhombic (at -90°C)to tetragonal (at +7°C) to cubic (at +120°C). In order to investigate the behave of the ferroelectric domain patterns at the phase transition occurring at +7°C we upgraded our scanning force microscope with a Peltier cooler/heating stage allowing for operation in a temperature range between -80°C and +120°C. Piezoresponse force microscopy (PFM) images, directly mapping the ferroelectric domain configuration, can be acquired either at fixed temperature or, when using a custom-designed script, during temperature ramps linked to the scanning process. We can thereby record the emergence of the domains at high temperatures but also the change of the domain patterns across the orthorhombic to tetragonal phase transition.

DF 10: Dielectric surfaces and interfaces

Time: Wednesday 9:30–10:30 Location: GER 37

DF 10.1 Wed 9:30 GER 37

Aligned deposition of λ-DNA on $LiNbO_3$ substrates by means of Ferroelectric Lithography — •Saminathan Ramakrishnan, Alexander Haussmann, and Lukas Eng — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany.

We report on the controlled deposition of λ-DNA to domain walls (DWs) of 5 mol.% Mg doped congruent $LiNbO_3$. Firstly, DWs were photochemically decorated with Au nanoparticles serving as pinning points to graft the DNA molecules [1]. Subsequently,these pin points were functionalized with 1,6-hexanedithiol, thus providing free reactive thiol groups at the Au surface. Incubation of fluorescently (YOYO-1) labeled λ-DNA followed by an intensive washing with a buffer solution that finally resulted in single DNA molecules that bridge the gaps between the aforementioned pin points. The analysis of these multi-component nanostructures and the underlying domain pattern was carried out by means of optical fluorescence microscopy, dynamic mode scanning force microscopy, and piezoresponse microscopy.

[1] A. Haußmann et al., Nano Lett. 9, 763 (2009)

DF 10.2 Wed 9:50 GER 37

Exploring contact charging of single crystalline dielectrics by atomic force microscopy — •Monika Mirkowska[1,2], Markus Kratzer[2], Stefan Klima[1,2], Helmut Flachberger[1], and Christian Teichert[2] — [1]Chair of Mineral Processing, Department Mineral Resources and Petroleum Engineering, Montanuniversität Leoben, Austria — [2]Institute of Physics, Montanuniversität Leoben, Austria

The electrostatic charging of surfaces is successfully applied in the triboelectrostatic separation of mineral particles. However, the knowledge about the charge exchange during the insulator-insulator contact is still limited. Here, we study the electric charging of well-defined dielectric surfaces (quartz and calcite single crystals) upon contact with conventional atomic force microscopy (AFM) probes and with micrometer sized single calcite particles attached to the end of commercially

available AFM cantilevers. We examined the effect of different contact types like static contact, point charging, and rubbing on the charging. A combination of contact mode atomic force microscopy (for charging) and Kelvin probe force microscopy was applied in order to verify the local electrostatic potentials of the surfaces before and after charging. Special attention was put on the influence of humidity (adsorbed water layer), contact time and load force on the charge transfer.

DF 10.3 Wed 10:10 GER 37

Dielectric screening of surface states in a topological insulator — •James LeBlanc[1] and Jules Carbotte[2] — [1]Max-Planck Institute for the Physics of Complex Systems, Dresden DE — [2]McMaster University, Hamilton Canada

Hexagonal warping provides an anisotropy to the dispersion curves of the helical Dirac fermions that exist at the surface of a topological insulator. We show how modifications to the Dirac spectrum by inclusion of hexagonal warping, as well as a Schrödinger and gap term modify the polarization function of the surface states. We derive in the long wavelength limit the plasmon dispersion and show that it obtains a weak dependence on the direction of scattering momentum, q. Further, we show numerically the plasmon dispersions at large q and find considerable directional anisotropy of the plasmon bands in comparison to the pure Dirac plasmons.

DF 11: Invited Talk - Stefan Förster (Joint Session with O, DS, KR, MM)

Time: Wednesday 10:30–11:15 Location: GER 37

Invited Talk DF 11.1 Wed 10:30 GER 37

Two-dimensional Oxide Quasicrystals: A new class of materials? — •Stefan Förster[1], Klaus Meinel[1], Rene Hammer[1], Martin Trautmann[1], and Wolf Widdra[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Two-dimensional materials - like graphene, hexagonal boron nitride, or topological insulators - have recently pioneered a new field of materials science. Their peculiar properties are often related to their specific two-dimensional periodic structure.

Here we report the first observation of a two-dimensional oxide quasicrystal (QC), a new member in the family of 2D materials [1]. The QC is derived from $BaTiO_3$ thin films on a hexagonal Pt(111) substrate. Low-energy electron diffraction (LEED) reveals a twelve-fold rotational symmetry. Scanning tunneling microscopy (STM) at room temperature as well as at low temperatures (80 K) allow to resolve the atomic structure. The aperiodic structure is formed by primitive atomic arrangements in squares, triangles, and rhombi with a universal edge length of 0.69 nm. In addition to this dodecagonal atomic arrangement, building blocks of squares, triangles,and rhombi are also found on $(2+\sqrt{3})$ and $(2+\sqrt{3})^2$ larger scales indicating the characteristic self-similarity of an ordered QC. The observed interface-driven formation of a 2D QC from a perovskite oxide in contact with a hexagonal substrate is expected to be a general phenomenon.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature 502*, 215 (2013).

DF 12: Electrical and mechanical properties

Time: Wednesday 11:30–11:50 Location: GER 37

DF 12.1 Wed 11:30 GER 37

Dielectric spectroscopy on MFU-type metal-organic frameworks — •Pit Sippel[1], Dmytro Denysenko[2], Peter Lunkenheimer[1], Dirk Volkmer[2], and Alois Loidl[1] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Solid State and Material Science, Institute of Physics, University of Augsburg, Germany

Metal-organic frameworks (MOFs) have a broad range of potential applications, e.g., gas storage, electronic devices and clean-energy technologies [1]. This class of coordination polymers with a crystalline periodic structure consists of metal-containing units with organic linkers, leading to permanent porosity. Here we present dielectric spectroscopy data on several MOFs, namely, MFU-2, MFU-3, MFU-4 and Co-substituted MFU-4 [2]. The dielectric measurements of MFU-4 reveal interesting relaxational dynamics of the solvent dimethylformamide, confined in the pores of the host system. Moreover, we find a significant change of the electrical conductivity when replacing Zn by Co due to a modification of the band gap [3]. In MFU-2 and MFU-3, by a variation of the organic linkers a dipolar moment is generated. Its dynamics is monitored by dielectric spectroscopy. The results could be of relevance for the application of MOFs in gas separators, gas storage and even information storage devices.

[1] H. Furukawa *et al.*, Science **341**, 1230444 (2013).
[2] D. Denysenko *et al.*, Chem Commun. **48**, 1236 (2012).
[3] P. Sippel, D. Denysenko, A. Loidl, P. Lunkenheimer, G. Sastre, and D. Volkmer, unpublished.

DF 13: Applications of dielectric solids

Time: Wednesday 11:50–12:30 Location: GER 37

DF 13.1 Wed 11:50 GER 37

Why should one account for dielectric nonlinearities — •Martin Diestelhorst — Martin-Luther-Universität Halle, Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, 06120 Halle, diestelhorst@physik.uni-halle.de

Many applications of dielectrics assume the materials to be linear. That is often legitimated by confining the choice of parameters to ranges, for which that assumption is valid. However for some applications it is necessary to apply such high external fields, that one has to take into account deviations from the linear behaviour. On the one hand these nonlinearities may be harmful for some applications. Otherwise there could arise applications that may be realized only utilizing the nonlinear properties. Especially when using ferroelectric materials one has to be aware of the dielectric nonlinearities. We discuss implications for both cases of applications. As an example for the first case we consider the process of energy storage on a capacitor with ferroelectric material as dielectric, where the stored energy falls short of the amount extrapolated from small signal permittivities to high electric fields assuming linear behaviour. The second example is concerned with a parametric amplifier in a nonlinear series circuit with ferroelectric capacitor. The described effect is observable near period doubling bifurcations which may not be observed in linear circuits.

DF 13.2 Wed 12:10 GER 37

Ultra-thin Al_2O_3 passivation layers for solar cell applications — •Andreas Nägelein[1], Christian Koppka[1], Katja Tonisch[1], and Thomas Hannappel[1,2] — [1]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — [2]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

Thin Al_2O_3-layers have been shown to provide a high quality passivation on p-type surfaces. Especially for nanowire-solar cells surface-passivation plays a major role.
In order to investigate the quality of Al_2O_3 produced by atomic layer deposition (ALD) in an MOCVD reactor, p-type silicon (1-5 Ωcm)

samples were coated on both sides with three different Al_2O_3 layer thicknesses (10 nm, 20 nm and 30 nm). UV/VIS measurements were done to determine the optical properties. XPS and FTIR investigations showed the composition of the layers. Passivation quality was proofed by QSSPC and MWPCD. Optical properties were measured by UV/VIS and obtained a transmission of more than 95% over a large wavelength range. QSSPC lifetime measurements showed a maximum lifetime of 388 μs at 30 nm Al_2O_3. After annealing 30 minutes at 400°C the lifetime increased to 1.25 ms. Comparable results are expected for nanowire applications.

DF 14: Nanostructured oxide thermoelectrics

Time: Wednesday 12:30–12:50 Location: GER 37

DF 14.1 Wed 12:30 GER 37

Application of nanostructures in the removal of contaminants: An experimental and theoretical approach — •Samuel Baltazar[1], Dora Altbir[1], Alejandra Garcia[2], Aldo Romero[3], Maria Rubio[4], and Nicolás Arancibia[4] — [1]Departamento de Física y CEDENNA, Universidad de Santiago de Chile, Chile — [2]Centro de Investigación en Materiales avanzados CIMAV, Monterrey, México. — [3]Max-Planck-Institute für Mikrostrukturphysik, Halle, Germany — [4]Facultad de Química y Biología, CEDENNA, Universidad de Santiago de Chile, Santiago, Chile

The study and application of metallic iron nanoparticles for cleaning contaminated water has been enhanced during the last years in several regions around the world. In particular, we consider the sorption of arsenic and lead from water following the kinetic process of the nanoparticles. Characterization of the material before and after the sorption process is considered in order to identify the new structures as a function of pH, and specific details of the nanoparticles such as the sorption capacity or the surface area. A Theoretical approach is also considered in order to identify the interactions between Arsenic compounds and iron nanoparticles performing ab initio calculations based on density functional theory.

DF 15: Multiferroics II (Joint Session with MA, DS, KR, TT)

Time: Wednesday 9:30–13:00 Location: HSZ 04

DF 15.1 Wed 9:30 HSZ 04

An Engineered Polar Oxide Heterostructure Built from Isosymmetric Magnetically Ordered Components — •Matthew S Dyer[1], Jonathan Alaria[1], Pavel Borisov[1,5], Troy D Manning[1], Serban Lepadatu[2], Markys G Cain[2], Elena D Mishina[3], Natalia E Sherstyuk[3], N A Ilyin[3], Joke Hadermann[4], David Lederman[5], John B Claridge[1], and Matthew J Rosseinsky[1] — [1]University of Liverpool, Liverpool, UK — [2]National Physical Laboratory, Teddington, UK — [3]Moscow State Technical University, Moscow, Russia — [4]University of Antwerp, Antwerp, Belgium — [5]West Virginia University, Morgantown, USA

Theory predicts that certain layered heterostructures consisting of perovskite blocks have non-centrosymmetric structures. The breaking of spatial inversion symmetry arises through a combination of octahedral tilting and A site ordering. Following this prediction, we grow a thin-film of the $[(YFeO_3)_5(LaFeO_3)_5]_{40}$ heterostructure using RHEED monitored pulsed layer deposition. Polar domains are present in the thin-film, as demonstrated by second harmonic generation and piezoelectric force microscopy measurements. We experimentally confirm that the heterostructure is also magnetically ordered at room temperature with a finite magnetization, retaining the magnetic structure of the individual $YFeO_3$ and $LaFeO_3$ components.

DF 15.2 Wed 9:45 HSZ 04

First-principles study of the $BaTiO_3/BaFeO_3$ perovskite interface — •Igor Maznichenko[1], Sergey Ostanin[2], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Epitaxial growth can combine a robust ferroelectric, such as $BaTiO_3$, and strong ferromagnets into the so called composite multiferroic films. The switching properties of artificial multiferroics sandwiched between metallic contacts make them excellent candidates for the room temperature four-state memories.

Regarding the ferromagnetic side of composite multiferroics, we suggest to use the cubic perovskite $BaFeO_3$ whose epitaxial growth has been recently reported. Here, from the basis of *ab-initio* electronic structure calculations, within the Korringa-Kohn-Rostoker method, we study the magnetic properties of bulk $BaFeO_3$. The approach allows us to accurately monitor the evolution of the Curie temperature upon both the tetragonal distortions and presence of oxygen vacancies. Finally, we examine magnetoelectricity at the $BaTiO_3/BaFeO_3$ interface.

DF 15.3 Wed 10:00 HSZ 04

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

$BiFeO_3$ (BFO) is an interesting candidate for multiferroic applications. In this work we focus on the Raman spectroscopic investigation of epitaxially grown thin films of BFO by pulsed laser deposition on different substrates, belonging to the group of scandates ($DyScO_3$, $SmScO_3$, $GdScO_3$). The Raman spectra were recorded using the 442 nm emission line of a He-Cd laser. Some phonon modes show changes in the position, full width at half maximum (FWHM) and intensity depending on the azimuthal angle. We found a 90 degree periodicity of the peak position and of the FWHM for particular modes. For both parallel and crossed polarisation the four maxima in positions correspond to the minima in FWHM. Such a behaviour can be explained considering a twin family of domains with a very well defined orientation to each other. Our results are supported by piezoresponse-force microscopy and X-ray diffraction measurements as well.

DF 15.4 Wed 10:15 HSZ 04

$BiFeO_3/LaFeO_3$: a magnetoelectric multiferroic — •Zeila Zanolli[1,3], Jacek Wojdel[2], Jorge Iniguez[2], and Philippe Ghosez[3] — [1]Forschungszentrum Jülich, PGI and IAS, Jülich, Germany — [2]ICMAB-CSIC, Bellaterra, Spain — [3]Université de Liège, Physics Department, Lieǵe, Belgium

Transition-metal oxides of perovskite structure present a wide variety of physical properties. In particular, there is a strong interest in multiferroic materials that are simultaneously ferroelectric and magnetic (*magnetoelectrics*). Due to the scarcity of natural magnetoelectric multiferroics and thanks to recent advances in epitaxial growth techniques, designing new magnetoelectric multiferroic heterostructures is a promising way to succeed in this quest.

First-principles techniques are used to investigate electric control of the magnetization in the $BiFeO_3/LaFeO_3$ perovskite oxide superlattice (SL) on a (001)-$SrTiO_3$ substrate. Our results [1] show that the $BiFeO_3/LaFeO_3$ SL exhibits a trilinear coupling of a polar mode with two different rotations of the oxygen cages (*hybrid improper ferroelectricity*). Non-collinear spin calculations reveal that the ferroelectric ground state also presents weak ferromagnetism with easy axis along the [1 -1 0] direction. The microscopic mechanism allowing one to manipulate the magnetization with an electric field in such systems is presented and its dependence on strain and chemical substitution is

discussed. The $BiFeO_3/LaFeO_3$ SL is found to be a good candidate to attain electric switching of magnetization at room temperature.

[1] Phys. Rev. B **88**, 060102(R) (2013)

DF 15.5 Wed 10:30 HSZ 04

The influence of strain on the optical properties of pseudo-tetragonal $BiFeO_3$ thin films — •Cameliu Himcinschi[1], Akash Bhatnagar[2], Andreas Talkenberger[1], Dietrich R.T. Zahn[3], Jens Kortus[1], and Marin Alexe[2,4] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [4]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Tetragonally distorted $BiFeO_3$ recently attracted a lot of attention because of its interesting multiferroic properties and the larger spontaneous polarization as compared to its rhombohedral counterpart. Highly strained (when grown on $LaAlO_3$ substrates) and nearly pseudomorphic (when grown on $TbScO_3$ substrates) $BiFeO_3$ films were deposited by pulsed laser deposition. The symmetry of the tetragonally distorted $BiFeO_3$ films is discussed based on polarisation dependent Raman measurements and the comparison with Raman spectra measured for films deposited on $TbScO_3$. The evaluation of ellipsometric spectra reveals that the films deposited on $LaAlO_3$ are optically less dense and the dielectric function is blue-shifted by more than 0.3 eV as compared to the films deposited on $TbScO_3$. By analyzing the absorption edge using a bandgap model, bandgaps of 3.10 eV and 2.75 eV were determined for the films deposited on $LaAlO_3$ and $TbScO_3$, respectively. This work is supported by the German Research Foundation DFG HI 1534/1-1.

DF 15.6 Wed 10:45 HSZ 04

Electrically induced magnetic transiton at the LSMO/BTO interface — •Markus Schmitz, Alexander Weber, Paul Zakalek, Markus Waschk, and Thomas Brückel — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich Germany

The magnetoelectric coupling is one of the most fascinating and active research areas today. The control of the magnetism due to an applied electric field may lead to new device concepts. First principles calculations of $La_{(1-x)}Sr_xMnO_3/BaTiO_3(001)$ interfaces show magnetic reconstructions due to the change of the polarization of BTO by applying an external electric field. The different electron densities influence the equilibrium between super- and double-exchange favoring a ferromagnetic or an antiferromagnetic order at the interface for the two different orientations of the polarization. Here we report on LSMO/BTO, grown with an Oxide Molecular Beam Epitaxy system. The epitaxial layer-by-layer growth was confirmed by in-situ RHEED analysis and the crystalline quality of the surface was investigated by LEED and Atomic Force Microscopy. The structural characterization was carried out by X-ray reflectometry and diffraction. We could prove the possibility to electrically polarize $BaTiO_3$ substrates due to an applied voltage of 400V by optical methods. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. The magnetic formation at the interface with respect to the polarization of the $BaTiO_3$ was investigated by Polarized Neutron reflectometry measurements performed at MARIA (FRM II).

15 min. break

DF 15.7 Wed 11:15 HSZ 04

Growth and structure characterization of double perovskite Sr2FeMoO6 thin films — •Hakan Deniz[1], Dietrich Hesse[1], Marin Alexe[1], Robert Lowndes[2], and Lucian Pintilie[2] — [1]Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle (Saale), Germany — [2]National Institute of Materials Physics, Atomistilor 105bis, Magurele 077125, Romania

The double perovskite Sr2FeMoO6 (SFMO) has drawn considerable attention recently owing to some of its unique features such as high Curie temperature (˜410K) and half-metallic ferrimagnetic nature with a high saturation moment of 4μB. The low-field room temperature magnetoresistance observed in SFMO makes it an attractive candidate for oxide spintronics applications. However, the broad distribution of results reported so far on SFMO films suggests that an optimal structure is attainable only within a narrow window of growth conditions; and magnetic/transport properties are highly akin to Fe and Mo atomic site disorder. Pulsed laser deposition was employed to grow SFMO thin films on vicinal SrTiO3 substrates from a custom-made stoichiometric target using argon as ambient gas. X-ray diffraction data revealed that the SFMO films were grown epitaxially with respect to the substrate, including, however, a small percentage of secondary phases. The morphology of the films shows flat plains with embedded grain- or needle-like structures, which are most likely the result of spurious phases. The nature of these defects and their interfaces with the SFMO matrix are under investigation by transmission electron microscopy. This work is supported by the EU-FP7 project IFOX.

DF 15.8 Wed 11:30 HSZ 04

Magnetic Anisotropy in Multiferroic Lu_2MnCoO_6 — •Martin Lonsky[1], Merlin Pohlit[1], María Antonia Señarís Rodríguez[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Dpto. Química Fundamental U. Coruña, Coruña, Spain

Lu_2MnCoO_6 recently has been introduced as a new type-II multiferroic with ferroelectricity due to charge ordering and magnetostriction related to magnetic Mn^{4+} and Co^{2+} ions which are arranged alternately in the form of Ising chains along the c-axis of the crystal [1]. The magnetic properties, however, remain puzzling, which in particular is due to the lack of measurements on single crystals, that have not yet successfully been synthesized. Here, we present for the first time measurements of the magnetic anisotropy by employing micro-Hall magnetometry on a few micrograins of dimensions $\sim 1\,\mu$m only. Our results reveal a strong dependence of magnetic hysteresis on temperature and the applied field direction. This anisotropy is also reflected in the observation of a variety of unusual effects as for instance wasp-waisted hysteresis loops, sharp jumps in magnetization at about $T = 300\,$mK and an exchange bias, ocurring in each case in only one field direction. Additionally, the observation of a pronounced maximum in the coercive field at $T_{SF} \sim 12\,$K indicates a significant change in the spin dynamics of the system below T_{SF}, similar to the behavior of the related compound $Ca_3Co_{2-x}Mn_xO_6$ ($x \approx 0.95$) [2].

[1] S. Yáñez-Vilar et al., Phys. Rev. B. 84, 134427 (2011).
[2] T. Lancaster et al., Phys. Rev. B 80, 020409 (2009).

DF 15.9 Wed 11:45 HSZ 04

The multiferroic $CuCrO_2$ compound: interlayer exchange and domain population — •Matthias Frontzek — Laboratory for Neutron Scattering, Paul Scherrer Institut, 5232 Villigen-PSI, Switzerland

Multiferroic materials have become of interest for their unusual low-temperature properties in general, and the tunability of the magnetic structure through an electric field and the electric polarization through a magnetic field in particular. The most promising candidates for such controllable multiferroics have been found among the materials with inherent geometric magnetic frustration.

Among these, the delafossite $CuCrO_2$, which crystallizes in the rhombohedral $R\bar{3}m$ space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, thus the magnetic ordering alone breaks the inversion symmetry. The peculiar magnetic structure of $CuCrO_2$ allows the direct quantitative analysis of the domain population.

In our contribution, we present a detailed study on $CuCrO_2$ single crystals using neutron diffraction in applied electric and magnetic fields. With the fields we were able to tune the multiferroic states in $CuCrO_2$ and could directly relate them to the underlying domain physics. Our results allow the re-interpretation of macroscopic measurements and show that the $p-d$ hybridization is the dominant spin-charge coupling mechanism.

DF 15.10 Wed 12:00 HSZ 04

Structure and Magnetic Coupling in $YBaFeCuO_5$ — •Andrea Scaramucci[1], Mickael Morin[2], Ekaterina Pomjakushina[2], Marek Bartkowiak[2], Denis Sheptyakov[2], Lukas Keller[2], Juan Rodriguez-Carvajal[3], Michel Kenzelmann[2], Kazimierz Conder[2], Marisa Medarde[2], and Nicola A. Spaldin[1] — [1]Materials Theory, ETH-Zurich, Zurich, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland — [3]Institute Laue Langevin, Grenoble, France

We theoretically study the structure and exchange couplings in multiferroic $YBaFeCuO_5$ (YBFCO). Using density functional theory we calculate energies of configurations with various Fe^{3+}/Cu^{2+} orderings in the bilayered perovskite structure of YBFCO. We find that configu-

rations with different distribution of Fe^{3+} and Cu^{2+} ions fall into two groups with distinctly different energies. The energies of those in the lowest energy group are close to that of the ground state (relative to the growth temperature) suggesting Fe^{3+} and Cu^{2+} to be disordered in YBFCO. Finally, we calculate exchange coupling constants for all the low energy configurations and show that the magnetic ordering resulting from these couplings is compatible with the experimentally-observed high-temperature magnetic ordering. However, they do not explain the existence of the experimentally observed low-temperature incommensurate magnetic structure.

DF 15.11 Wed 12:15 HSZ 04

Hybrid-functional study of the structural, magnetic and electronic properties of rare-earth nickelates — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Rare-earth nickelates ($ReNiO_3$) are very promising functional perovskite crystalline materials, exhibiting metal-insulator (MI) transition, which can be continuously controlled by composition, bi-axial strain and(or) electric field. Unfortunately, conventional *ab initio* DFT+U results fail to reproduce their magnetic ground state as well as the effect of epitaxial strain on MI transition temperature. We present results of our comprehensive study of structural, magnetic and electronic properties of bulk $ReNiO_3$ (Re=Y, Gd, Eu, Sm, Nd and Pr) and strained $SmNiO_3$ films [1], performed with HSE06 functional. We show correlation between MI transition temperature and structural parameters of bulk and films, which nicely fits known experimental data. We also analyze the difference in the electronic structure obtained in DFT+U and with the hybrid functional and their influence on the resulting magnetic ordering in the ground state.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409, JSC and JARA-HPC.

[1] F.Y. Bruno, K.Z. Rushchanskii, S. Valencia, Y. Dumont, C. Carrétéro, E. Jacquet, R. Abrudan, S. Blügel, M. Ležaić, M. Bibes, and A. Barthélémy, Phys. Rev. B 88, 195108 (2013).

DF 15.12 Wed 12:30 HSZ 04

Magnetic properties of multiferroic $TbMnO_3$ — •Natalya Fedorova, Andrea Scaramucci, Claude Ederer, and Nicola Spaldin — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

We use ab-initio calculations to investigate the magnetic properties of multiferroic $TbMnO_3$.

At low temperatures $TbMnO_3$ demonstrates an incommensurate spiral ordering of Mn spins which is accompanied by appearance of spontaneous electric polarization driven by applied magnetic field [1]. The establishment of such spin ordering is usually described within the framework of a Heisenberg model with competing nearest-neighbor and next-nearest-neighbor exchange interactions. However, our theoretical estimations of these interactions by ab-initio calculations demonstrate a clear deviation from Heisenberg model.

We consider first the coupling between magnetic and orbital orderings as a main source of non-Heisenberg behavior in $TbMnO_3$, but conclude that it does not explain the observed deviation. We find that higher order interactions (biquadratic and four-body spin couplings) should be taken into account for proper treatment of the magnetism in $TbMnO_3$.

[1] T. Kimura et al., Nature 426, 55-58 (2003)

DF 15.13 Wed 12:45 HSZ 04

Coupling of epitaxial strain and point-defect formation in perovskites — •Ulrich Aschauer, Philipp Baumli, and Nicola A. Spaldin — Materials Theory, ETH Zurich, Zürich, Switzerland

Using density functional theory calculations we recently established the existence of a strong coupling between epitaxial strain and the formation energy of oxygen vacancies in the model perovskite $CaMnO_3$ (Phys. Rev. B. 88, 054111, 2013). Here we investigate the generality of this concept for other oxides including metallic perovskites and also investigate the effect of strain on the formation of cation vacancies. We find that in general the response of the defect profile follows the behavior expected from chemical-expansion arguments, with tensile strain favoring oxygen vacancies and compressive strain favoring cation vacancies. We show, however, that material-specific details of the electronic structure can cause deviations from this trend under both tensile and compressive strain.

DF 16: Glasses (Joint Session with CPP and CY)

Time: Wednesday 11:45–12:45 Location: WIL B321

DF 16.1 Wed 11:45 WIL B321

Two-level tunneling systems in amorphous alumina — Alejandro P. Paz[1], •Irina V. Lebedeva[1], Ilya V. Tokatly[1,2], and Angel Rubio[1,3,4] — [1]Nano-bio Spectroscopy Group, Universidad del Pais Vasco, San Sebastian, Spain — [2]IKERBASQUE, Bilbao, Spain — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]European Theoretical Spectroscopy Facility

The decades of research on thermal properties of amorphous solids at temperatures below 1 K suggest that their anomalous behaviour can be related to quantum mechanical tunneling of atoms between two nearly equivalent states that can be described as a two-level system (TLS) [1]. This theory is also supported by recent studies on microwave spectroscopy of superconducting qubits [1]. However, the microscopic nature of TLSs remains unknown. To identify bistable structural motifs in amorphous alumina we have performed extensive classical molecular dynamics simulations. Several motifs with only one or two atoms jumping by considerable distance ~ 0.5 Å were found at temperature 25 K. Accounting for the surrounding environment relaxation was shown to be important up to distances ~ 7 Å. The energy asymmetry and barrier for the detected motifs lied in the ranges 0.5 - 2 meV and 4 - 15 meV, respectively, while their density was about 1 motif per 10000 atoms. Tuning of motif asymmetry by strain was demonstrated with the coupling coefficient below 1 eV. The tunnel splitting for the symmetrized motifs was estimated on the order of 0.1 meV. The properties of the discovered motifs are in good agreement with the available experimental data. [1] G. J. Grabovskij et al. Science 338, 232 (2012).

DF 16.2 Wed 12:05 WIL B321

Resistive Properties of Lithium-Ion Conducting LiSICon Glass Ceramics in Contact with Lithium Metal and Nonaqueous Electrolytes — •Kim Oliver Hofmann[1,2], Meike Schneider[2], Maria-Louisa Reich[2], Miriam Kunze[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt — [2]Schott AG Mainz

Lithium-ion conducting glass ceramics with LiSICon type crystalline phase are promising materials as solid electrolytes in future batteries due to their high ionic conductivity, which is higher than $1x10^{-5}$ S/cm. These materials can not only be applied to solid state lithium batteries but also for lithium-sulfur and lithium-air batteries. For these applications the LiSICon materials need to be stable against metallic Li and battery specific liquid electrolytes.

Lithium contact stability is derived by measuring the impedance Z over a period of seven days. In case the glass ceramic reacts with metallic lithium and reduces the polyvalent ions in the glass ceramic like Ge or Ti, the impedance Z is increasing and the sample turns black, noticeably. Further on the impedance spectroscopy is used to determine the interaction of glass ceramics with different liquid electrolytes. The impedance spectra are additionally analyzed by a distribution of relaxation times, based on a distribution function over infinite serial connected RC elements [1]. The resistance contribution of the glass ceramics in contact with liquid electrolytes can be distinguished in interface, grain boundary and grain core resistance by this method.

[1] H. Schichlein et al., J. Appl. Electrochem., 32 (2002) 875- 882

DF 16.3 Wed 12:25 WIL B321

Optical properties of trivalent rare-earth ions in barium borate glasses — •Sebastian Loos[1], Franziska Steudel[2], Bernd Ahrens[1,2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, 06120 Halle (Saale)

Rare-earth doped glasses gain increasing importance in optical devices, such as fibre lasers or light emitting diodes. Luminescence properties of rare-earth ions are well-known, but absolute photoluminescence quantum efficiencies have been insufficiently studied. In this work, series of Sm^{3+}, Eu^{3+}, and Tb^{3+} doped barium borate glasses are investigated for their potential application as frequency down-converters in solid state lighting and photovoltaics. Photoluminescence quantum efficiencies have been analyzed for rare-earth doping levels up to 5 at.%. The best values of more than 50% are achieved for Eu^{3+} doping. To increase the photoluminescence quantum efficiency even further, the Sm^{3+}-doped samples have been co-doped with a second rare-earth ion, namely Eu^{3+} or Tb^{3+}. Here, energy transfer processes between Sm^{3+} and the second rare-earth ion become important; they are discussed in detail.

DF 17: Invited Talk - Heidemarie Schmidt (Joint Session with MA, HL, DS, KR)

Time: Wednesday 15:00–15:45 Location: GER 37

Invited Talk DF 17.1 Wed 15:00 GER 37

Smart multiferroic thin films for cognitive computing — •Heidemarie Schmidt — Technische Universität Chemnitz, Department of Materials for Nanoelectronics, Reichenhainer Str. 39, 09126 Chemnitz

Cognitive systems promise to penetrate complexity and assist people and organizations in better decision making [1]. We have successfully prepared metal-multiferroic-metal (MMM) structures with the multiferroic material BiFeO3 and BiFeTiO3. All those MMM structures exhibit nonvolatile resistive (meristive) switching. Investigations of memristive switching is driven by promising applications of power-efficient memristive nanostructures including data storage, logic systems, cognitive computing and artificial neural networks. Prominence of work on memristive systems might be visualized by the near-future breakthrough in computing technology, where classical Von Neumann architecture is replaced by cognitive systems. In this talk I present three new functionalities of smart MMM structures including nonvolatile multilevel resistive switching [2], nonvolatile reconfigurable logics and nonvolatile second and higher harmonics generation [3] which are very promising for the development of cognitive computing. [1] J. E. Kelly III, S. Hamm, Smart Machines: IBM*s Watson and the Era of Cognitive Computing, Columbia University Press, 2013 [2] Y. Shuai et al., J. Appl. Phys. 109 (2011); Appl. Phys. Lett. 98 (2011); Appl. Phys. Exp. 4 (2011); 111 (2012); IEEE Electron Device Letters 34 (2013); Scientific Reports 3 (2013) [3] N. Du et al., Rev. Sci. Instr. 84 (2013)

DF 18: Dielectric and ferroelectric thin films

Time: Wednesday 16:00–18:20 Location: GER 37

DF 18.1 Wed 16:00 GER 37

An unexpected depolarization current peak in polyethylene oxide — •Bjoern Martin and Herbert Kliem — Saarland University, Germany

Thin films of polyethylene oxide (PEO) are investigated as model systems for a solid electrolyte. Metal-PEO-metal capacitance structures show a pronounced relaxational behaviour with a thickness dependent effective dielectric permittivity caused by a space charge polarization of mobile ions.

In the experiment it is found that the transient polarization and depolarization currents after application of small field steps follow a power law in the long time range. By using higher fields charge injection during the polarization sets in resulting in nearly constant currents in the long time range. The depolarization currents now show an unexpected maximum in time. The time to the maximum depends on the height of the voltage applied before, the polarization time, the sample thickness, the temperature, and the Li doping.

A discrete three-dimensional model is developed to describe the charge motion. Single charges are regarded. Negative ions can fluctuate thermally activated over energy barriers in a multiwell potential. Positive immobile ions provide charge neutrality. Additionally, electrons can be injected into the system and also be extracted from the dielectric. Interactions of the charges with the electrodes using the method of images and all other electrostatic interactions are considered.

From these simulations it is shown that the appearance of the transient depolarization current maximum is caused by injected electrons.

DF 18.2 Wed 16:20 GER 37

Correlation between structural and ferroelectric properties of epitaxial PMN-PT films — •Michael Mietschke[1,2], Sebastian Fähler[1,3], Ludwig Schultz[1,2], and Ruben Hühne[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden — [2]Technische Universität Dresden — [3]Technische Universität Chemnitz

Ferroelectric materials like lead magnesium niobate-lead titanate (PMN-PT) show an electrocaloric effect induced by an electrical field during a diffusionless phase transition, which might be used for novel solid state cooling devices. However, the interplay between the microstructure and the ferroelectric properties is not completely understood so far. To study this in detail, epitaxial 0.68 $Pb(Mg_{1/3}Nb_{2/3})O_3$-0.32 $PbTiO_3$ films were grown by pulsed laser deposition on (001) single crystalline $SrTiO_3$ (STO) substrates with a miscut angle between 0 and 15 degrees towards the [100] direction. The influences of the deposition parameters and the miscut angle on the PMN-PT structure was studied by x-ray diffraction, atomic force microscopy and scanning electron microscopy. A capacitor like structure was realized by growing the PMN-PT film on a conducting buffer layer with additional Pt-top electrodes on the surface. A nearly pure perovskite phase was found using $La_{0.7}Sr_{0.3}Co_3$ buffer layers on (001) STO substrates and low deposition temperatures. An increasing miscut angle improves the purity of the PMN-PT perovskite phase further. Finally, a correlation of the ferroelectric properties with the phase purity of the PMN-PT film was found.

This work was supported by DFG priority program 1599.

DF 18.3 Wed 16:40 GER 37

First principles study of the electrocaloric effect in strained $BaTiO_3$ — •Madhura Marathe and Claude Ederer — Materials Theory, ETH-Zurich, Switzerland

The electrocaloric (EC) effect – a reversible change in temperature of a material by applying an external electric field – has been known for a very long time [1]. Recently however, the discovery of a "giant electrocaloric effect" [2] has stimulated extensive work on the EC effect, due to its huge potential to increase the efficiency of cooling devices. We have studied how misfit strain affects the EC temperature change in bulk $BaTiO_3$.

We have performed molecular dynamics simulations for an effective Hamiltonian based on first-principles density functional theory [3]. The calculated EC temperature change ΔT reduces when $BaTiO_3$ is only clamped but not strained, but increases again with increasing misfit strain. Further with increasing misfit strain, there is a shift in the ΔT peak towards higher temperatures. Therefore the misfit strain can be utilized in two ways – (i) to enhance the EC temperature change and (ii) to achieve a maximal effect in the temperature range of interest for a given application.

[1] J. F. Scott, Annu. Rev. Mater. Sci. **41**, 229 (2011).
[2] A. S. Mischenko, *et al.*, Science **311**, 1270 (2006).
[3] T. Nishimatsu, *et al.*, Phys. Rev. B **82**, 134106 (2010).

DF 18.4 Wed 17:00 GER 37

Multilayer Thin Films of Ferroelectric VDF-TrFE Copolymer Characterized by Dielectric Nonlinearities — •Danny von Nordheim[1], Andreas Austin[1], K.H. Chew[2], and Bernd Ploss[1] — [1]Department of SciTec, University of Applied Sciences Jena, Carl-Zeiss-Promenade 2, 07745 Jena, Germany — [2]Department of Physics,

University of Malaya, 50603 Kuala Lumpur, Malaysia

Multilayer ferroelectric structures consist of two or more layers, usually thin films, with at least one of them exhibiting ferroelectric properties. Ceramic multilayers and superlatticess have attracted immense attention during the last years due to their unique behaviour and potential applications namely data and energy storage. Organic materials provide a nontoxic, easily processable alternative. As a model system a stack of two ferroelectric P(VDF-TrFE) thin films with a composition of 56/44 mol% and 70/30 mol% and a thicknesses of approx. 200 nm each has been deposited on a glass substrate covered with aluminium electrodes. The single layers and the multilayer have been characterized regarding their nonlinear dielectric properties at different temperatures. The results have been evaluated with reference to phase transitions and remanent polarisation.

DF 18.5 Wed 17:20 GER 37

Photo-electronic processes in $BiFeO_3$ — •Akash Bhatnagar[1], Young Heon Kim[2], Dietrich Hesse[1], and Marin Alexe[1,3] — [1]Max Planck Institute of Microstructure Physics, D-06120 Halle, Germany — [2]Korea Research Institute of Standards and Science, Daejeon 305-304, Rep. of Korea — [3]University of Warwick, Department of Physics, Coventry CV8 2EN, United Kingdom

Recently, reports regarding the observation of above-band gap open-circuit voltages (V_{oc}) in $BiFeO_3$ (BFO) thin films under illumination, i.e. the photovoltaic effect (PV), has attracted much attention in the field of ferroelectric materials. Initial investigations primarily attributed this effect to charge separation at ferroelastic domain walls . Subsequent studies, via localized measurements, revealed the presence of shallow trap levels which might be contributing towards the effect . Thus till now, the origin of this effect has been under some clouds of speculations.

In the present work we have elaborated upon conclusive evidence to determine the actual role of domain walls in the PV effect. Moreover, an analytical model will be presented via which the generation of PV current in different directions can be calculated. By performing temperature dependent and angle resolved measurements we prove that the bulk photo effect, which has been at the origin of the PV effect in other ferroelectric materials, is also responsible in case of BFO. However, the presence of ferroelastic domains and domain walls largely influences its manifestation. Similar measurements performed on strained BFO provide an insight into different conduction mechanisms.

DF 18.6 Wed 17:40 GER 37

Epitaxial PLD growth of strained ferroelectric KxNax-1NbO3 thin films and superlattices — •Jan Sellmann, Jutta Schwarzkopf, Dorothee Braun, Andreas Duk, Albert Kwasniewski, and Martin Schmidbauer — Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin

(K,Na)NbO3 single crystals exhibit excellent ferro-/piezoelectric properties, however, they are less investigated in thin film form. We have deposited KxNa1-xNbO3 single layers and (NaNbO3)n/(KNbO3)m superlattices epitaxially by Pulsed Laser Deposition (PLD) on various lattice mismatched substrates providing compressive and tensile lattice strain. KxNa1-xNbO3 films have been realized by the use of KxNa1-xNbO3 ceramics (x = 0 - 0.75) as PLD targets. Increased K incorporation up to x = 0.5 into the films leads to a significant improvement of both the piezoresponse and to an increased lattice mismatch between film and substrate. In order to obtain higher critical thicknesses for fully strained film growth superlattice structures were grown by the alternating deposition of NaNbO3 and KNbO3 films with individual film thicknesses between 1 to 20 monolayers. While alternating layers with nominal thicknesses of up to three monolayers result in single layers consisting of a KxNa1-xNbO3 solid solution, superlattice structures (NaNbO3)n/(KNbO3)m were successfully deposited with individual layer thicknesses of seven or more monolayers. In particular, high piezoresponse was obtained on films with 5x(NaNbO3)17/(KNbO3)9 superlattice structure. We present a detailed study of different m/n ratios on piezoresponse and local ferroelectric hysteresis curves.

DF 18.7 Wed 18:00 GER 37

Asymmetric oxygen vacancy distribution in $CaTiO_3$ capacitors — •Andreas Krause[1], Walter M. Weber[1], Uwe Schroeder[1], Johannes Heitmann[1,2], and Thomas Mikolajick[1,3] — [1]NaMLab gGmbh, D-01187 Dresden — [2]Institut fuer Angewandte Physik, TU Bergakademie Freiberg — [3]Institut fuer Halbleiter- und Mikroelektronik IHM, TU Dresden

$CaTiO_3$ is a promising material as a high-k dielectric in metal-insulator-metal capacitors, combining a high dielectric constant (k) and relatively low leakage currents. Using various electrodes, $CaTiO_3$ shows intrinsic differences for both top and bottom charge carrier injection in addition to electrode dependent injection. Therefore, the band offset between valence band of the dielectric and the work function of the electrode material is not the only parameter responsible for leakage currents. As previously stated in literature for $SrTiO_3$[1], electrodes induce differences in oxygen vacancy distribution in the dielectric. Here, $CaTiO_3$ exhibits a conduction behavior comparable to $SrTiO_3$ with different electrodes Pt, C, Ru and TiN. This indicates an universal behavior of high-k perovskites and may be crucial for future device integration.

[1]*Kim et al.* Understanding of Trap-Assisted Tunneling Current - Assisted by Oxygen Vacancies in $RuO_x/SrTiO_3$/TiN MIM capacitor for the DRAM application. *Memory Workshop, 2012 4th IEEE International*

DF 19: Invited Talk - Elke Beyreuther

Time: Thursday 9:30–10:15 Location: GER 37

Invited Talk DF 19.1 Thu 9:30 GER 37

Analyzing electronic defect states at perovskite oxide interfaces by surface photovoltage spectroscopy — •Elke Beyreuther and Lukas Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

Surface photovoltage (SPV) spectroscopy, being a versatile method to analyze the energetic distribution of electronic defect states at surfaces and interfaces of wide-bandgap semiconductor (hetero-)structures, is discussed as an alternative approach for studying perovskite oxide surfaces and interfaces [1]. In particular, the method is applied to comparatively investigate prototypical heterostructures made of 5-unit-cell-thick $LaAlO_3$ films grown on either TiO_2- or SrO-terminated $SrTiO_3$. As shown by a number of experimental and theoretical investigations in the past, these two systems exhibit dramatically different interface properties with the first establishing a conducting interface and the second being insulating. The present SPV investigation reveals clearly distinguishable interface defect state distributions for both configurations within the framework of a classical semiconductor band scheme. Furthermore, bare $SrTiO_3$ crystals with TiO_2 or mixed SrO/TiO_2 terminations show similar SPV spectra and transients as the $LaAlO_3$ covered samples with the respective termination of the $SrTiO_3$ substrate [2]. This is in accordance with a number of recent works, which stress the decisive role of the $SrTiO_3$ and the minor role of the $LaAlO_3$ for the electronic properties of the interface.

[1] E. Beyreuther et al., Surf. Sci. 612, 1–9 (2013).
[2] E. Beyreuther et al., arXiv:1311.0491 [cond-mat.mtrl-sci] (2013).

DF 20: Nonlinear dielectics, phase transitions, relaxors

Time: Thursday 10:30–11:50 Location: GER 37

DF 20.1 Thu 10:30 GER 37

Precursor dynamics, incipient ferroelectricity and huge anharmonicity in antiferroelectric lead zirconate PbZrO3 — •Annette Bussmann-Holder[1] and Krystian Roleder[2] — [1]Max Planck Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

To understand better the phase transition mechanism of PbZrO3 (PZO) the lattice dynamics of this antiferroelectric compound are investigated within the polarizability model, with emphasis on the cubic to orthorhombic phase transition. Similarly to ferroelectric phase transitions in ABO3 perovskites, polar dynamical clusters develop and grow in size upon approaching TC from the high temperature side and never form a homogeneous state. Simultaneously, elastic anomalies set in and compete with polar cluster dynamics. These unusual dynamics are responsible for precursor effects that drive the PZO lattice towards an incipient ferroelectric state. Comparison of the model calculations with the temperature dependences of elastic coefficients measured on PZO single crystals reveals striking similarity.

DF 20.2 Thu 10:50 GER 37

Tuning of the electrocaloric effect in $BaTiO_3$ and $PbTiO_3$-based relaxors by molecular dynamics simulations — •Anna Grünebohm[1], Peter Entel[1], Takeshi Nishimatsu[2], and Scott P. Beckman[3] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute for Materials Research (IMR), Tohoku University, Sendai 980-8577, Japan — [3]Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011, United States

The electrocaloric effect is an adiabatic temperature change of a material upon applying an external electrical field. Recently, this effect has been rediscovered as a promising candidate for solid state refrigeration as large temperature changes have been found in experiment and theoretical simulations.[1–3] However, the underlaying mechanisms for the large caloric response as well as possible obstacles are still not well understood. In addition, the effective temperature range in pure ferrolectric materials is narrow. We thus perform molecular dynamics simulations of an ab-initio based effective Hamiltonian as implemented in the feram package[3] in order to study the effect of local fields, defects, and alloying on the electro caloric response and its operation range. Our systematic study will focus on $BaTiO_3$, (Ba,Sr)TiO_3, $PbTiO_3$ and PNM-PT.

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

DF 20.3 Thu 11:10 GER 37

Optically induced switching and bistability of the insulator-metal phase transition in vanadium dioxide nanoclusters — •Thorben Jostmeier[1], Johannes Zimmer[2], Achim Wixforth[2], Helmut Karl[3], Hubert J. Krenner[2], and Markus Betz[1] — [1]Experimentelle Physik 2, TU Dortmund — [2]Lehrstuhl für Experimentalphysik 1 and Augsburg Centre for Innovative Technologies, Universität Augsburg — [3]Lehrstuhl für Experimentalphysik IV, Universität Augsburg

Bulk vanadium dioxide (VO_2) exhibits a insulator-metal phase transition (IMT) at a near ambient temperature of 68°C. Upon heating, VO_2 undergoes a structural and electronic change which is accompanied by a substantial change of the complex dielectric function. More specifically, the metallic phase features a strongly decreased transmission of near-infrared frequencies. A well known effect in nanoscopic VO_2 is a reversible thermal hysteresis of the IMT. Ion beam synthesised $VO_2 : SiO_2$ nanoclusters show a more pronounced thermal hysteresis with an supercooled state at room temperature. Additionally, diffraction gratings formed by site selective ion beam implantation show giant switching contrasts exceeding one order of magnitude.

The IMT can be also controlled using femtosecond near-infrared laser pulses. We for the first time show a broad fully reversible hysteresis/bistability in the *optically* induced phase transition of $VO_2 : SiO_2$ nanoclusters which allows for a permanent but still erasable switching of the IMT. These properties allow for the implementation of applications like ultrafast optical switches and optical storage devices.

DF 20.4 Thu 11:30 GER 37

Study of field induced critical point in relaxor ferroelectric single crystal and ceramics — •Nikola Novak[1,3], Raša Pirc[1], and Zdravko Kutnjak[1,2] — [1]Jožef Stefan Institute, Jamova 39, 1001 Ljubljana, Slovenia — [2]Jožef Stefan International Postgraduate School, Jamova 39, 1001 Ljubljana, Slovenia — [3]Institute of Materials Science, 64287 Darmstadt, Germany

Relaxor ferroelectrics represent a class of disordered ferroelectrics, which are characterized by the absence of long range ferroelectric order in zero applied field at any temperature. The study of the third-order nonlinear dielectric permittivity some time ago predict a first-order phase transition into a ferroelectric state by cooling a relaxor in an electric field E larger than some threshold electric field Ec.

In order to investigate the field-induced phase transition in relaxor ferroelectric a high-resolution calorimetric and polarization measurements were utilized along the Ec(T) transition line. The behavior of the heat capacity as a function of the temperature and electric field as well as the vanishing of the latent heat gives a sharp defined critical point in [110] relaxor ferroelectric single crystal $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN). On the other hand in 9/65/35 PLZT ceramic the heat capacity as a function of electric field shows a crossover from a discontinuous to continuous step, however, the sample temperature change as a consequence of released latent heat does not vanishes completely. The persisting of the sample temperature anomaly at high temperature can be attributed to two effects: i) the anisotropy of the critical point and ii) electrocaloric effect (ECE).

DF 21: Nano- and microstructured dielectrics (Joint Session with KR)

Time: Thursday 12:00–12:40 Location: GER 37

DF 21.1 Thu 12:00 GER 37

Influence of nano crystallites in barium titanate glass ceramics on the ferroelectric phase transition — •Berit Körbitzer, Martun Hovhannisyan, and Martin Letz — Schott AG, Mainz

Dielectrics based on glass ceramics with ferroelectric phases have potential for application as high power capacitors because of their intrinsic pore-free structure. Due to this property glass ceramics reach high dielectric breakdown strengths compared to conventional ceramic materials. In addition the nano cristalline structure broadens the sharp ferroelectric transitions and allows applications up to 200°C. By solid solution type doping and variation of crystallite size one can influence the ferroelectric transition temperature of barium titanate based glass ceramics. The effect of strontium and zirconium doping on the dielectric properties and glass stability of this system is analysed.

DF 21.2 Thu 12:20 GER 37

Polarization-dependent second harmonic analysis of ferroelectric domain structures in z-cut lithium niobate — •Alex Widhalm[1], Moritz Grothe[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Short-periodic domain grids in ferroelectric materials like lithium niobate (LN) are inevitable to achieve quasi phase matching for sophisticated applications in the visible spectral range. A deeper understanding of the physical processes involved in the periodic inversion of the spontaneous dielectric polarization is essential for guaranteeing sufficient quality of these domain structures. Within this work we study the nonlinear signature of the z-cut surface region of periodically poled LN with integrated Ti waveguide structures by means of second harmonic microscopy. In this context, the polarization-dependent SH-analysis has turned out to be an extremely high contrastive method for imaging the ferroelectric domain structure. In addition this technique enables directly the assignment of polarity. All in all, it has been proven that the occurring nonlinear signatures are essentially determined by the polarization and the tailored crystal structure.

DF 22: Slow Dynamics in Glasses and Granular Matter I (Joint Focus Session with DY and CPP)

The transition into an amorphous solid state is typically accompanied by the observation of slow dynamics. The understanding of such transitions from first principles has seen progress in many of its aspects recently, including nonlinear response, residual stresses, and non-affine deformations. The Focus Session provides an overview of common phenomena and of general concepts in the physical picture of disordered materials. (Organizers M. Sperl and A. Zippelius)

Time: Thursday 9:30–12:30 Location: HÜL 186

Invited Talk DF 22.1 Thu 9:30 HÜL 186

The memory of sand — •Matthieu Wyart — New York University

Complex systems are characterized by an abundance of meta-stable states. To describe such systems statistically, one must understand how states are sampled, a difficult task in general when thermal equilibrium does not apply. This problem arises in various fields of science, and here I will focus on a simple example, sand. Sand can flow until one jammed configuration (among the exponentially many possible ones) is reached. I will argue that these dynamically-accessible configurations are atypical, implying that in its solid phase sand "remembers" that it was flowing just before it jammed. As a consequence, it is stable, but barely so. I will argue that this marginal stability answers long-standing questions both on the solids and liquid phase of granular materials, and will discuss tentatively the applicability of this idea to other systems.

Invited Talk DF 22.2 Thu 10:00 HÜL 186

Complex rheology at the jamming transition: shear thickening, shear thinning, shear banding — •Claus Heussinger — Institut für theoretische Physik, Universität Göttingen

The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. The usefulness of such a unifying concept hinges on the presence or absence of phenomena that are in some sense *universal*.

In this contribution, we discuss how certain features in the particle interactions affect the rheological properties of the material. First, we discuss the effect of frictional forces, and show how the jamming phase diagram has to be modified as compared to the frictionless scenario [1,2]. Essential findings are a discontinuous and hysteretic jamming transition, as well as a shear thickening regime where frictionless particles are generically shear thinning.

Secondly, we investigate the role of attractive interactions between the particles [3]. For weakly attractive systems a fragile solid develops which displays self-organization towards a minimal (isostatic) connectivity. Moreover, the measured flow curves have unstable regimes, which lead to persistent shearbanding. These features are rationalized by establishing a link between rheology and inter-particle connectivity, which also provides a minimal theoretical model to describe the flow curves.

[1] CH, PRE (2013). [2] M. Grob. CH, A. Zippelius, arXiv (2013). [3] E. Irani, P. Chaudhuri, CH, arXiv (2013).

DF 22.3 Thu 10:30 HÜL 186

Stress-birefringence information in three-dimensional binary granular packings — •Peidong Yu, Stefan Frank-Richter, and Matthias Sperl — Institut für Material Physik im Weltraum, Köln, Deutschland

We report our newly developed 3D stress-birefringence technique and its application in a binary static packing. We show how we precisely determine the stress state of one single spherical particle from its stress-birefringent response to external contacts. Such particles of two different sizes are used in a dense packing with different packing fractions. Based on the knowledge of one-particle calibration, we are able to define a transition point from the integrated stress-birefringent signal of the whole packing under changing packing fraction. Variations of these transition points with different size ratio and specie number ratio of the two particle species are measured and discussed.

DF 22.4 Thu 10:45 HÜL 186

Jamming of Frictional Particles: a First Order Phase Transition — •Matthias Grob[1], Claus Heussinger[2], and Annette Zippelius[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland — [2]Institut für Theoretische Physik, Universität Göttingen, Göttingen, Deutschland

With numerical simulations, we produce flow curves for dense frictional granular media with features different from the frictionless analog. When the strain rate is controlled and increased, a smooth transition from inertial to plastic flow is observed below a critical volume fraction. Above this packing fraction, the transition becomes discontinuous as a hallmark of friction. Upon an increase of packing fraction, the flow curves show hysteretic behaviour, the emergence of a yield stress and the divergence of the shear viscosity - each at a different packing fraction. All the reported behaviour is reproduced with a simple model for a non-equilibrium first order phase transition. An inherent feature of dense frictional granular rheology is that the transition from flowing to jammed states is reentrant with transient jam-and-flow states in between which are, within the models' framework, metastable flow states.

15 min. break

DF 22.5 Thu 11:15 HÜL 186

Vibrational Masking of Critical Decay in the Early beta-Relaxation Regime of Incoherent Intermediate Scattering Functions in Simulated Glass Forming Ni0.5Zr0.5 — •Helmar Teichler — Institut f. Materialphysik, Univ. Göttingen

Results are presented concerning the origin of discrepancy between mode coupling theory (MCT) prediction for critical decay in the early beta-regime and molecular dynamics (MD) simulation data. The discrepancy is known since long in the literature and is heuristically ascribed to effects of atomic vibrations not fully taken into account in MCT. A proper theoretical treatment is missing so far. Here I present a formally exact framework for analyzing the MD data, which allows deducing the origin of the discrepancy and its quantitative description, and I apply it to MD simulated glass forming Ni0.5Zr0.5. The approach relates incoherent intermediate scattering functions (ISFs) from atomic trajectories, which show the discrepancy, to those from inherent structure (IS), which are in agreement with MCT. Cumulant expansion of the ISFs demonstrates that the discrepancy reflects the vibrational density of states, with minor effect of the Boson peak. The results for Ni0.5Zr0.5 rely on the fact that there are only weak correlations between atomic vibrations and IS relaxation displacements in the beta-regime, and that the essential part of the vibrational displacements distribution acts Gaussian-like.

DF 22.6 Thu 11:30 HÜL 186

Glass Transition of Yukawa Systems: Crossover from Hard Sphere to Soft Sphere Limits — •Anoosheh Yazdi[1], Alexei Ivlev[2], Sergei Khrapak[2], Adam Wysocki[3], Hartmut Löwen[4], and Matthias Sperl[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum fuer Luft- und Raumfahrt, 51147 Köln, Germany — [2]Max-Planck-Institut für extraterrestrische Physik, 85741 Garching, Germany — [3]Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, 85741 Düsseldorf, Germany

The mode-coupling theory for ideal glass transitions (MCT) is applied to the single and double Yukawa potential systems. Glass transition curves are obtained in the full range of two control parameters: the screening parameter κ, which is the inverse screening length, and the interparticle potential strength Γ. With increasing κ along the transition, glass form factors and effective packing fractions undergo a crossover from the one-component plasma (OCP) limit, which resembles a very soft sphere system, to a hard sphere system (HSS). The entire transition diagram can be described by analytical functions. Suprisingly and different from those of other potentials, glass transition curves are found to be shifted but otherwise identical to the melting curves in the control parameter plane.

DF 22.7 Thu 11:45 HÜL 186

rheology near jamming-the influence of lubrication forces — •moumita maiti and Claus Heussinger — Georg-August University of Goettingen, Goettingen, Germany

The talk discusses the role of different dissipation forces on the rheological properties of highly dense non-Brownian suspensions. The focus is on the random close packing limit ("jamming") where particle motion is limited due to steric volume exclusion. We define a simplified lubrication force where we change the dissipation mechanisms by tuning the range of the interaction. Two densities are considered, one is near jamming the other further away. For both densities, a crossover is seen from 'inertia' dominated flow to viscous flow by changing the lubrication range. Interestingly, we observe that velocity fluctuations are independent of the different dissipation mechanisms ("universal")near jamming. Away from jamming this universality is lost and an unexpected non-monotonic dependence is seen. We present an understanding of our findings in terms of geometric constraints of random-close packing and a decoupling of dissipative forces and particle trajectories.

DF 22.8 Thu 12:00 HÜL 186

Lattice Boltzmann Simulations for Glass-Forming Liquids — •Simon Papenkort[1,2] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany — [2]Zukunftskolleg und Fachbereich Physik, Universität Konstanz, Germany

In continuum mechanics, the Navier-Stokes (NS) equation is used to study fluid flows. The Lattice Boltzmann (LB) model is an efficient method to find solutions of the NS equation of Newtonian liquids even for complex flow geometries.

Complex fluids, such as glass formers, colloidal suspensions, or granular media, display a wide range of non-Newtonian flow effects, determined by the interplay between slow structural dynamics on the microscopic scale, and the mesoscopic flow field. Prominent examples are shear thinning and yield stresses, leading to plug flow in channels.

Starting from first principles, mode coupling theory of the glass transition is able to provide constitutive equations that describe the history effects determining the flow of glass-forming fluids. We present results from a new LB scheme that allows to include memory-integral effects in fluid-mechanics simulations.

DF 22.9 Thu 12:15 HÜL 186

Slow convection in densely packed granular mixtures — •Frank Rietz and Ralf Stannarius — University of Magdeburg, Institute of Experimental Physics, Department of Nonlinear Phenomena

Handling of granulate in partly filled rotating containers is a common situation in industrial processes. Contrary to ensembles of loosely packed grains, the container can be filled so dense that fluidization is limited to a shallow surface layer. Then, the deeper layers are in a locked state, only creeping motions on longer time scales are possible.

We study such a situation in a flat rotating container of aspect ratio 1 that is almost completely filled with a bidisperse mixture. Irrespective of the limited mobility of the grains we observe nonuniform segregation patterns accompanied by slow convective motion. Many features of the convection flow amplitude, like regular oscillatory modulations of the convection velocity, cessations and spontaneous reversals of the circulation are comparable to convection in ordinary liquids at high Rayleigh numbers, in geometries with aspect ratio 1.

[1] F. Rietz & R. Stannarius, Phys. Rev. Lett. 108, 118001 (2012).

DF 23: Glasses and Glass Transition I (Joint Session with CPP and DY)

Time: Thursday 11:45–12:45 Location: ZEU 114

Invited Talk DF 23.1 Thu 11:45 ZEU 114

Dynamics and thermodynamics of glassy polymers below the glass transition temperature — •Daniele Cangialosi — Paseo M Lardizabal 5, 20080 San Sebastian, Spain

Glass-forming systems constitute an important class of materials. Among different aspects, the dramatic slowing down of the dynamics when decreasing temperature and the possible connection between such slowing down and the thermodynamics of the glass-former have been intensively studied. It has been speculated that mere extrapolation of the dynamics and thermodynamics to temperatures below the glass transition temperature (T_g) produces a singularity at a finite temperature, with divergent relaxation time and vanishing configurational entropy. Here the dynamics and thermodynamics are studied at temperatures as low as T_g- 40 K by performing enthalpy recovery experiments on glassy polymers for times up to 10^7-10^8 seconds. We find a single stage recovery behavior for temperatures larger than about T_g- 10 K. A double stage recovery is observed for $T < T_g-$ 10 K. The enthalpy recovered after the two-stage decay equals that extrapolated from the melt, whereas partial enthalpy recovery occurs in the first decay. From the analysis of the time to reach each equilibrium it is found that the equilibration time corresponding to the first stage recovery exhibits relatively low activation energy, whereas the second one exhibits activation energy similar to that of the polymer segmental relaxation. These results indicate a complex scenario of the dynamics and thermodynamics below T_g with multiple equilibration steps and leave open the question the finite temperature singularity.

DF 23.2 Thu 12:15 ZEU 114

Excess heat capacity and fictive temperature of polystyrene in a wide range of cooling and heating rates — •Gunnar Schulz[1], Timur Vasilievich Tropin[2], Yeong Zen Chua[1], Jürn W. P. Schmelzer[1], and Christoph Schick[1] — [1]Institut für Physik , AG Polymerphysik, Universität Rostock, Rostock, Germany — [2]Frank Laboratory of Neutron Physics, Joint Institut for Nuclear Research, Dubna, Moscow region, Russia

The physical characteristics of polystyrene allow straightforward and reproducible measurements of heat capacity, C_p, glass transition temperature, T_g, and other properties. The possibility to reuse one sample for numerous cooling and heating cycles permits the investigation of the influence of the cooling and heating rates on C_p and T_g.

In our research, we conduct the cooling phases with various (constant) cooling rates, but the respectively following heating phases with only one heating rate. The comparison of the heat capacities observed after different cooling rates results in an excess C_p, which we also calculate by means of a model.

Our measurements furthermore yield the fictive temperature in the cooling rate range from $10^{-4}\,\mathrm{K\,s^{-1}}$ to $10^{4}\,\mathrm{K\,s^{-1}}$. We compare these results with the dynamic T_g observed by means of temperature-modulated differential scanning calorimetry (TMDSC). The dependence of the fictive T_g on the cooling rate and the dependence of T_g on the modulation frequency turn out to be closely related.

DF 23.3 Thu 12:30 ZEU 114

Glassy dynamics and physical aging in fucose saccharides as studied by Infrared- and Broadband Dielectric Spectroscopy — •Wilhelm Kossack[1], Karolina Adrjanowicz[2], Magdalena Tarnacka[1], Wycliffe Kiprop Kipnusu[1], Mateusz Dulski[2], Emanuel Urandu Mapesa[1], Kamil Kaminski[2], Sebastian Pawlus[2], Marian Paluch[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Linnestr.5, Molekülphysik, 04103 Leipzig, Germany — [2]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

Fourier Transform InfraRed (FTIR) and Broadband Dielectric Spectroscopy (BDS) are combined to study both, the intra- and intermolecular dynamics for two isomers of glass forming fucose, far below and above the calorimetric glass transition temperature, T_g. It is shown, that the various IR-active vibrations exhibit in their spectral position and oscillator strength quite different temperature dependencies, proving their specific signature in the course of densification and glass formation. The coupling between intra- and inter-molecular dynamics is exemplified by distinct changes of IR active ring vibrations far above the calorimetric glass transition temperature at about $1.16T_\mathrm{g}$, where the dynamic glass transition (α relaxation) and the secondary β relaxation merge. — For samples physically annealed below T_G slower isothermal relaxation times than extrapolated from liquid state are observed .

DF 24: Crystallography in Materials Science (Joint Session with KR)

Time: Thursday 15:00–17:30 Location: CHE 184

Invited Talk DF 24.1 Thu 15:00 CHE 184

Crystals: Structure, Properties and Heart of Energy Conversion Devices — •Tilmann Leisegang[1], Juliane Hanzig[2], Erik Mehner[2], Matthias Zschornak[2], Falk Meutzner[2], Tina Nestler[2], Bianca Störr[2], Charaf Cherkouk[2], Ulrike Wunderwald[1], and Dirk C. Meyer[2] — [1]Fraunhofer-THM, Am-St.-Niclas-Schacht 13, 09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg

Crystalline materials are wide spread in our today's life. More than 98 % of the solid fraction of the earth comprises crystalline matter, most of which are oxides. Single-crystals in particular are the basis for many applications - lasers, LEDs, sensors, etc. - and play an important role in fundamental research for instance in superconductivity or magnetic properties. The discipline that elucidates the impact of the crystal structure on the physical properties of particularly crystalline materials - crystallography - is of specific importance for the design of new materials. X-ray and other diffraction methods are of great relevance for the investigation of crystal structures and their peculiarities. Moreover, crystallography can be utilized to establish new concepts and thus may contribute solving today's challenges in science and technology. In this context, the work presented highlights several examples. First, it is demonstrated how composition variations can be used to change the three dimensional crystal structure - including commensurate or incommensurate modulated phases - in order to tune the materials properties. Second, applications of crystals for energy conversion devices are presented.

DF 24.2 Thu 15:30 CHE 184

Clusters in intermetallic compounds: fullerenes and more — •Julia Dshemuchadse and Walter Steurer — Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland

The study of the structure of metals has kept crystallographers busy for the past century: starting with the simplest of structures – sphere packings, such as found in aluminium or copper – up to some of the most complex inorganic structures known to date with more than 20 000 atoms per unit cell [1]. But knowing all the atomic positions does not yet provide us with a deeper understanding of the design of the structure.

Different cluster interpretations of the atomic arrangement in an intermetallic can provide us with recurring motifs in the form of atomic environments, *i.e.* coordination polyhedra, or larger, endohedral clusters, such as dual Frank-Kasper polyhedra and fullerene-like shells (*e.g.*, [2]). These cluster descriptions illustrate common features in structures either within the same intermetallic system or of related structures with entirely different constituents. However, they do not necessarily represent chemical entities and their meaningfulness is usually derived from their repeated occurrence in diverse compounds.

We will present possible ways of structure description for complex intermetallic phases and clues toward their significance.

[1] T. Weber, J. Dshemuchadse, M. Kobas, M. Conrad, B. Harbrecht and W. Steurer, *Acta Cryst. B* 65, 308–317 (2009).

[2] J. Dshemuchadse, S. Bigler, A. Simonov, T. Weber, W. Steurer, *Acta Cryst. B* 69, 238–248 (2013).

DF 24.3 Thu 15:45 CHE 184

Theoretical investigation of the high pressure structure of CaTe — •Oliver Potzel and Gerhard Taubmann — Institute of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany

The majority of the alkaline halides and the alkaline earth chalcogenides undergoes a structural phase transition from the B1 (rock-salt) structure to the B2 (CsCl) structure at elevated pressures [1].

The x-ray diffraction data of CaTe at high pressures (320 - 400 kbar) fit to a simple cubic indexing (B2) except for two reflections near the (110) peak [2]. This indicates the possible existence of an intermediate structure within the transition from the B1 to the B2 structure.

We are currently using the evolutionary algorithms of the USPEX code [3] with the periodic DFT code VASP [4] in order to predict the structure of CaTe at a pressure of 350 kbar.

Preliminary DFT studies without genetic algorithms pointed to an AgO structure. In these calculations, all known (binary) AB structures were taken into account.

The results are to be verified by the comparison of the calculated data to the experimental diffraction data.

[1] O. Potzel, G. Taubmann, J. Solid State Chem. 184, 1079 (2011)
[2] H.G. Zimmer, H. Winzen, K. Syassen, PRB 32, 4066 (1985)
[3] A.R. Oganov , C.W. Glass, J. Chem. Phys. 124, 244704 (2006)
[4] G. Kresse, J. Furthmüller, PRB 54, 11169 (1996)

DF 24.4 Thu 16:00 CHE 184

In-situ ion beam irradiation: X-ray scattering & diffraction experiments — Olga Roshchupkina, Carsten Baehtz, Stefan Facsko, Lothar Bischoff, Matthias Posselt, and •Joerg Grenzer — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden

Ion beam techniques are widely used in semiconductor industry e.g. for introducing dopant atoms into materials. Ion implantation is characterized by fast dynamic processes associated with the evolution of collision cascades resulting in formation of defects such as vacancies, interstitials, etc. As a consequence, typically a strained layer that expands in the direction normal to the substrate surface is formed. This is due to the fact that the bulk material prevents any lateral macroscopic expansion and as a result the thin irradiated layer is subjected to an in-plane biaxial compressive stress. Ion irradiation is a very fast process and it is almost impossible to monitor it in-situ with the present x-ray sources. However, the accumulation of damage and the diffusion of defects are much slower processes and can be studied in-situ by X-rays. An in-situ ion beam implantation experiment was set up at ROBL/MRH at ESRF. Samples were irradiated using 20 keV He^+ ions at room temperature. Reciprocal space maps to investigate the evolution of the strain depending on the accumulation of defects, as well as the conversion of the strained layer into a completely (X-ray) amorphous layer on single crystal Si and Al_2O_3 substrates were measured and discussed.

Coffee break

DF 24.5 Thu 16:30 CHE 184

Focused Ion Beam implantation of Erbium into Y2SiO5 crystals — •Nadezhda Kukharchyk[1], Jasper Rödiger[2], Arne Ludwig[1], Alexey Ustinov[3], Pavel Bushev[4], and Andreas D. Wieck[1] — [1]Ruhr University Bochum, Bochum — [2]RUBION, Bochum — [3]Karlsruhe University, Karlsruhe — [4]University of Saarland, Saarbrücken

In the context of research on quantum computation and information, different systems have been developed and investigated recently. Particular interest is focused on the systems based on the rare earth (RE) elements, which feature semi-shielded 4f-electrons from external crystal fields and therefore possess long optical and microwave coherence time. Among all the REs, exclusively erbium has the transition which falls into Telecom C-Band at 1540 nm. In the present work, we perform Focused Ion Beam (FIB) implantation of Erbium ions into Y2SiO5 substrates. The FIB allows us to have a high control over the implanted pattern and area, as well as the depth and even the choice of the isotopes - which gives high flexibility in the system preparation. Luminescence of the implanted crystals appears to be an effective way to characterize the system. The measurements were performed in the confocal regime with an excitation at 488 nm and detection in the range of 450 nm to 900 nm at room temperature. A marked intensity-to-fluence dependence is observed and compared to the spectra from the grown doped crystals. Additionally the influence of defects and annealing was studied.

DF 24.6 Thu 16:45 CHE 184

White beam synchrotron x-ray topography of sapphire single crystals — •Atefeh Jafari[1,2], Angelica Cecilia[3], Jürgen Härtwig[4], Andreas Danilewsky[5], Dimitrios Bessas[4], Viktor Asadchikov[6], Boris Roschin[6], Denis Zolotov[6], Alexander Deryabin[6], Ilya Sergeev[7], Svetoslav Stankov[3], Tilo Baumbach[3], Pavel Alexeev[1,7], Hans-Christian Wille[7], and Raphaël Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institute PGI, JARA-FIT, Forschungszentrum Jülich, Germany — [2]Faculté des Sciences, Université de Liège, Liège, Belgium — [3]Institute for Photon Science and Synchrotron Radiation, KIT, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France — [5]Crystallographic institute, University of Freiburg,Germany — [6]Shubnikov Institute of Crystallography, RAS, Moscow, Russia — [7]Deutsches Elektronen-Synchrotron, Hamburg, Germany

Sapphire single crystals grown by different techniques have been assessed with white beam and meV-resolution synchrotron x-ray topography at ANKA, KIT and PETRA III, DESY, and ESRF, respectively. Excellent crystal quality is required for the use in backscattering x-ray monochromators for nuclear resonance scattering with resonance energies above 30 keV. X-ray topography reveals defects and dislocations and hints at their origin. Crystals grown by the Kyropoulos method show the lowest dislocation density. Support of the Helmholtz-Russia joint research group HRJRG-402, ANKA, PETRA III and ESRF is acknowledged.

DF 24.7 Thu 17:00 CHE 184

Improving Nanomagnetometry Based on Nitrogen-Vacancy Centers by Coupling to Superparamagnetic Iron Oxide Nanoparticles — •Nikola Sadzak, Janik Wolters, Andreas W. Schell, Sten Wenzel, and Oliver Benson — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, Berlin, Germany

The single negatively charged nitrogen-vacancy (NV) defect center in diamond is known to be a stable solid-state single photon source [1], with an electronic spin showing long coherence times even at room temperature. Furthermore, the optical readout of the spin state and its microwave-assisted manipulation allow this defect to be used either as a qubit register [2] or as a magnetic field sensor [3]. Here, we perform the coupling of individual NV centers in nanodiamond with single-domain superparamagnetic iron oxide nanoparticles. By showing huge magnetic susceptibilities and no hysteresis, the latter can be used as local microwave amplifiers, allowing the achievement of faster Rabi oscillations between the NV center electronic spin sublevels. Moreover, we investigate the effects on the NV- electronic spin dynamics and coherence times and discuss some applications in NV-based nanomagnetometry.

[1] I. Aharonovich et al., Rep. Prog. Phys. 74, 076501 (2011).
[2] L. Robledo et al., Nature 477, 574-578 (2011).
[3] J. R. Maze et al., Nature 455, 644-648 (2008).

DF 24.8 Thu 17:15 CHE 184

Selective preparation of single-crystalline alpha- & beta-phase perylene platelets — •André Pick and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg

Though polarization resolved optical absorption spectroscopy in transmission geometry is a simple method to characterize optoelectronic properties of pi-conjugated molecular crystals their large absorption requires rather thin crystals. Moreover such studies are complicated by the presence of polymorphism and structural defects like twinning. For the case of the polycyclic aromatic hydrocarbon perylene two crystalline phases (alpha and beta) are known which comprise different molecules per unit cell. Both crystalline phases exhibit also characteristic differences in the habitus of single crystals which allows their differentiation. Here, we present a method to selectively prepare thin platelets of both polymorphisms, which are suitable for optical studies of single crystals. In order to get full morphological information, the crystallites were characterized by means of optical microscopy, X-ray diffraction and atomic force microscopy.

DF 25: Glasses and Glass Transition II (Joint Session with CPP and DY)

Time: Thursday 15:00–17:30 Location: ZEU 114

Invited Talk DF 25.1 Thu 15:00 ZEU 114

Microscopic investigation of creep in glasses — Tatjana Sentjabrskaja[1], Pinaki Chaudhuri[2], Wilson Poon[3], Jürgen Horbach[2], Stefan Egelhaaf[1], and •Marco Laurati[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Theoretische Physik II, Heinrich Heine University, Düsseldorf, Germany — [3]SUPA and COSMIC, The University of Edinburgh, United Kingdom

The microscopic origin of the creep rheological response of colloidal glasses is investigated, based on the particle-level dynamics measured by confocal microscopy during application of a step stress. Sub-diffusive single-particle dynamics are the microscopic signature of creep. At a more local scale enhanced dynamic activity is observed at random locations, with the number of active regions following the time-dependence of the macroscopic strain. Instead, diffusive dynamics characterise the flowing system, with a transient super-diffusive regime during the onset of flow. Transient super-diffusion coincides with the appearance of enhanced dynamics in a specific region of the system, which subsequently rapidly expands and finally spans the whole system when the steady state of flow is reached.

Invited Talk DF 25.2 Thu 15:30 ZEU 114

Getting into shape: Jamming of frictional particles. — •Matthias Schröter, Jean-François Métayer, Frank Rietz, and Max Neudecker — MPI for Dynamics and Self-Organization

In recent years the Jamming paradigm has been promoted as a grand unifying theory of particulate soft matter systems like foams, colloids, emulsions, and granular media [1,2]. However, this approach has mostly evolved from simulations of soft, perfect spheres. Real world particulate systems are often "rough" on either a microscopic or a particle scale. In the first case we talk about friction, in the second about non-spherical shapes.

This talk will use 3D imaging techniques such as X-ray tomography to provide insight into the mechanical stability of tetrahedra packings [3], the volume response of sheared granular media, and the first order phase transition occurring at Random Close Packing. We will show that in non of these three examples the underlying physics is adequately described by the Jamming paradigm.

[1] A. Liu and S. Nagel, Ann. Rev. Cond. Mat. Phys. **1**, 347-369 (2010)

[2] M. van Hecke, J. Phys.: Condens. Matter **22**, 033101 (2010)

[3] M. Neudecker, S. Ulrich, S. Herminghaus, and M. Schröter, Phys. Rev. Lett. **111**, 028001 (2013)

DF 25.3 Thu 16:00 ZEU 114

Glassy Dynamics of Collapsed Isolated Polymer Chains — •Martin Tress[1], Emmanuel Urandu Mapesa[1], Manfred Reiche[2], and Friedrich Kremer[1] — [1]Universität Leipzig — [2]MPI für Mikrostrukturphysik, Halle

While structure and conformation of condensed, isolated low molecular weight and polymeric molecules are well explored, knowledge concerning their dynamics, as measured in a broad spectral range and at widely varying temperatures is sparse. To overcome this, Broadband Dielectric Spectroscopy is combined with nano-structured electrodes having 35 nm separation and the dynamics of collopsed isolated poly(2-vinylpyridine) (P2VP) globules is measured. The collapsed globule conformation is revealed by Atomic Force Microscopy scans of the identical samples with an average globule volume corresponding to the estimate for a single chain (using the molecular weight and bulk density). Hence, for the first time the dynamic glass transition of condensed isolated polymer chains is directly measured and found to be bulk-like; only segments close (< 0.5 nm) to the substrate are weakly slowed down. The observation of bulk-like dynamics is in full accord with the length scale on which the dynamic glass transition is to be expected. In contrast, the emersion of new, slower relaxation modes is attributed to attractive interactions of the P2VP segments with the supporting silica surface, a finding which is corroborated by complementary infrared experiments. Our approach paves the way for numerous experiments on the dynamics of isolated molecules.

15 min break

DF 25.4 Thu 16:30 ZEU 114

A direct quantitative measure of surface mobility in a glassy polymer — Yu Chai[1], •Thomas Salez[2], Joshua D. McGraw[3], Michael Benzaquen[2], Kari Dalnoki-Veress[4], Elie Raphaël[2], and James A. Forrest[1] — [1]University of Waterloo, Canada — [2]ESPCI, Paris, France — [3]Saarland University, Saarbrücken, Germany — [4]McMaster University, Hamilton, Canada

The simple geometry of a polymer film on a substrate with a step at the free surface is unfavourable due to the excess interface induced by the step, thus allowing for a new nanoprobe of the melt state rheology. After recalling the experimental technique, we demonstrate how the same theoretical tools enable to understand the surface evolution of thin polymer films below the glass transition temperature T_g. While above T_g the entire volume between the substrate and the free surface participates to the flow, below T_g only a near surface region responds to the excess interfacial energy. In the latter case, the developed thin film theory for flow limited to the free surface region is in excellent agreement with experimental data. Strikingly, the system transitions from whole film flow to surface localized flow over a narrow temperature region near the bulk glass transition temperature. The measurements and model presented provide a quantitative measure of the surface mobility in a sample geometry where the confinement of polymer chains and substrate effects are negligible. Therefore, this study may help to solve further the ongoing controversy around glass transition in polymer films.

DF 25.5 Thu 16:45 ZEU 114

Effects of soft confinement on the glass dynamics of glycerol, studied by deuteron NMR — •Michael Lannert[1], Markus Rosenstihl[1], Thomas Blochowicz[2], Bernd Stühn[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, Hochschulstraße 6, 64289 TU Darmstadt — [2]Institut für Festkörperphysik, Hochschulstraße 8, 64289 TU Darmstadt

The dynamics of glycerol in a microemulsion with droplet diameters ranging from 2nm to 9nm were investigated by deuteron NMR in the temperature range 150K - 330K. While previous studies of liquid dynamics in confinement mostly used solid matrices, microemulsion droplets formed by AOT surfactants and toluol/m-xylol provide a soft confinement. Deuteron NMR longitudinal (T_1) and transversal (T_2) spin relaxation times, solid echo spectra, and two time correlation functions were recorded. High temperature dynamics are independent from droplet diameter and a Vogel-Fulcher-Tamann temperature dependence was observed. The line shape transition occurs at 240K for all studied droplet sizes, but is broader in confinement than in bulk, indicating a broadening of the distribution of correlation times. Time constants obtained from the measured correlation functions exhibit a weaker, Arrhenius temperature dependence. Detailed analysis suggests that the reorientation results from the rotational diffusion of whole droplets rather than individual molecules.

DF 25.6 Thu 17:00 ZEU 114

Single molecule diffusion measurements in highly viscous media — •Dominik Wöll[1,2] and Maren Dill[2] — [1]Zukunftskolleg, Universität Konstanz, D-78457 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz

Single molecule diffusion measurements in highly viscous media require a method which can readily detect very low diffusion coefficients. Single molecule fluorescence tracking typically becomes rather unreliable for diffusion coefficients below 10^{-18} m^2 s^{-1} due to the limited accuracy in determining single molecule positions of a few nanometres and the need for a very high stability of the optical system, even for long-time measurements of several hours. We developed a photocleavable energy transfer dyad which, so far, has allowed us to extend the range of single molecule (pair) diffusion measurements by three orders of magnitude and to determine slow single molecule motion in polymer films in close vicinity to their glass transition temperature. As a FRET pair, we used a perylene and a terrylene diimide derivative, two very efficient and stable fluorophores ideal for single molecule fluorescence spectroscopy. A phenacyl derivative was chosen as the photolabile moiety which could be cleaved with UV light. Initially, the two fluorophores are covalently bound to each other and move correlated before they are cleaved by a UV light pulse and their diffusive

separation gives access to low diffusion coefficients of down to 10^{-21} m^2 s^{-1} and beyond.

DF 25.7 Thu 17:15 ZEU 114

Intermittent Quakes on Surface of Soft Glassy Suspensions — •Tadashi Kajiya[1], Tetsuharu Narita[2], Velonique Schmitt[3], Francois Lequeux[2], and Laurence Talini[2] — [1]Max Plank Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — [2]PPMD-SIMM, UMR 7615 CNRS, UPMC, ESPCIParisTech, 10 rue Vauquelin, 75231 Paris Cedex 05, France — [3]CRPP, UPR 8641 CNRS, Universite Bordeaux 1, 115 Avenue Schweitzer, 33600 Pessac, France

We present measurements of the thermal fluctuations of the free surface of oil-in-water emulsions which exhibit a glassy behavior. The Surface Fluctuation Specular Reflection (SFSR) technique was applied to measure the free surface fluctuation. SFSR technique permits to probe the height of the fluctuations of liquid surface using the reflection of a laser beam projected on the target surface [1].

We found that when the volume fraction of the oil droplets is close to or larger than the disordered packing volume fraction, the free surface exhibits abnormal fluctuations, consisting of rare but large amplitude quakes. From a statistical analysis of the fluctuation signal, we also found that such large fluctuations become more prominent as the system ages. These quakes correspond to large changes in the local slope of the free surface over a few tenths of a second. We conjecture that such quakes reflect the dynamics peculiar to glassy systems driven by the relaxations of internal stress [2].

[1] A. Tay et al. Rev. Sci. Instrum. 79, 103107 (2008) [2] T. Kajiya et al. Soft Matter. 9, 11129 (2013).

DF 26: Metamorphic structures: Bringing together incompatible materials I (Joint Focus Session with HL and DS)

This session is devoted to the challenge to epitaxially combine materials, which differ strongly in their basic properties like lattice constant or symmetry and hence seem to be incompatible. It shall provide a discussion forum about understanding, how such material combinations can be grown with high yield, i.e. low defect densities in the final active region, in order to realize device structures of a given material system on a substrate of another system. Examples where such combinations are needed are materials, where adequate substrates are not available, like In-rich GaInN structures for green light emitting devices on GaN, or complex device structures like multi-junction solar cells requiring the combination of incompatible layers.

Organizers: Ferdinand Scholz, Universität Ulm, and Andreas Hangleiter, TU Braunschweig.

Time: Thursday 9:30–13:00 Location: POT 251

Topical Talk DF 26.1 Thu 9:30 POT 251

Metamorphic III-V-on-IV structures and its application to optoelectronic devices — Yoshiaki Nakano, •Masakazu Sugiyama, and Takuo Tanemura — Department of Electrical Engineering and Information Systems, University of Tokyo, Japan

There has been a considerable interest to combine merits of different III-V semiconductors with group IV-based materials and devices. One obvious example is the integration of InGaAs FETs with Si MOSFETS for enhancing CMOS performance. Another example is the "silicon photonics" where III-V materials are integrated on silicon substrates to have them perform light emission and control functions. Such integration is brought about by either heteroepitaxy or wafer bonding. The former is regarded better in terms of manufacturablity but in general more difficult than the latter, and therefore, its applicability has been limited. In this talk, our trial of integrating III-nitrides and III-phosphides/arsenides on silicon and germanium by metal-organic vapor phase epitaxy and wafer bonding is reviewed, together with its application to light emitting, controlling, and receiving devices, including micro lasers on Si and multi-junction solar cells.

Topical Talk DF 26.2 Thu 10:00 POT 251

Two types of buffer layer for the growth of GaN on highly lattice mismatched substrates and their impact on the development of sustainable systems — Tadashi Mitsunari[1], Koji Okuno[1], Yoshio Honda[1], Shigeyasu Tanaka[2], and •Hiroshi Amano[1,3] — [1]Department of Electrical Engineering and Computer Science, Nagoya University — [2]EcoTopia Science Institute, Nagoya University — [3]Akasaki Research Center, Nagoya University

There are two types of buffer layer for the growth of commercially available GaN-based blue LEDs on a sapphire substrate. One is the low-temperature deposited AlN or GaN buffer layer and the other is the sputter-deposited AlN buffer layer. In both cases, deposition condition, thickness and the annealing condition are critical for the fabrication of high performance blue LEDs. In this presentation, detailed study on the deposition and growth process of the low-temperature deposited AlN buffer layer and the following GaN growth will be discussed. We applied the sputter-deposited AlN buffer layer for the growth of GaN on Si. Details of the quality of GaN on a sputter-deposited AlN layer will be shown.

DF 26.3 Thu 10:30 POT 251

Influence of the substrate quality on the structural properties of short-period GaN/AlGaN superlattices grown by MBE — •Felix Schubert[1], Ulrich Merkel[2], Thomas Mikolajick[1,2], and Stefan Schmult[2] — [1]NaMLab gGmbH, Nöthnitzer Straße 64, D-01187 Dresden — [2]Institute of Semiconductor and Microsystems, TU Dresden, Nöthnitzer Straße 64, D-01187 Dresden

Short-period AlGaN/GaN superlattices have been established as versatile test structures to investigate the influence of the GaN substrate quality on the structural properties of AlGaN/GaN heterostructures. Of particular interest are surface roughness, layer accuracy and aluminum mole fraction in the MBE-grown superlattices. A variety of GaN substrates prepared by MBE, MOCVD, HVPE and ammothermal growth was investigated. For the best substrate quality theoretically expected properties like narrow high-order satellite peaks and interface fringes can be recovered from high resolution x-ray diffraction scans of the superlattices.

DF 26.4 Thu 10:45 POT 251

Strain engineering in a-plane GaN - Investigations on anisotropic strain behaviors — •Matthias Wieneke, Martin Feneberg, Michael Winkler, Peter Veit, Armin Dadgar, Jürgen Bläsing, Rüdiger Goldhahn, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, FNW/IEP, Universitätsplatz 2, 39106 Magdeburg

The use of low temperature AlN interlayers (LT AlN) is a successful technique to prevent crack formation in thick c-plane GaN films, but also to reduce the density of basal plane stacking faults in semipolar GaN. Here, we studied the impact of LT AlN on a-plane GaN films grown by metal-organic vapor-phase epitaxy on 2-inch r-plane sapphire substrates. The curvature increases during the growth of tensely-strained a-plane GaN buffer layers, while it decreases after inserting LT AlN. However, an increasing asphericity evaluated by a 3-spot-curvature measurement indicates an anisotropic strain relaxation. Consequently, after cooling-down various ex-situ X-ray diffraction (XRD) measurements reveal an increase in compressive strain along the in-plane GaN m-direction, while it marginally decreases along the in-plane GaN c-direction for layers with a LT AlN interlayer. The non-biaxial strain behavior mirrors in energy shifts of the characteristic photoluminescence features which is compared to the results of 4-band $\mathbf{k}\cdot\mathbf{p}$ theory. Furthermore, XRD and transmission electron microscopy measurements exhibit a degradation in the crystalline quality of GaN layers grown on LT AlN interlayer.

DF 26.5 Thu 11:00 POT 251

Growth and characterization of non- and semipolar AlInN and possibilities for relaxed buffer layer engineering — •Ernst Ronald Buss[1], Uwe Rossow[1], Heiko Bremers[1], Tobias Meisch[2], Ferdinand Scholz[2], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Germany — [2]Institute of Optoelectronics, Ulm University, Germany

The different a/c-ratios of group-III-nitrides open the possibility of strain engineering for relaxed buffer layers of AlInN in non- and semipolar GaN based structures. In this contribution, we present the very first results on low pressure MOVPE grown AlInN on semipolar $(11\bar{2}2)$ GaN templates, m-plane GaN templates, as well as m-plane pseudo-bulk GaN substrates. AlInN layers exhibit a macroscopic tilt due to the activation of basal plane slip for all non-c-plane orientations. For the m-plane case we will show that there is no shear of the unit cells of the different layers of the sample. Growth rates and indium incorporation efficiencies of m-plane and $(11\bar{2}2)$ oriented material could be estimated to be similar and the same as on c-plane GaN. While c- and m-plane AlInN shows extreme roughening with increasing layer thickness, $(11\bar{2}2)$ AlInN does not. Furthermore, we will present first experiments demonstrating a proof of concept of the specific relaxation of AlInN in different in-plane directions for $(11\bar{2}2)$ orientation. Depending on the indium content we are able to initiate relaxation only in $[1\bar{1}00]$ direction for 18% of indium, or $[11\bar{2}\bar{3}]$ direction for 28% of indium, respectively. All these results make AlInN quite promising for relaxed buffer layers and strain engineering for further growth.

Coffee break (15 min.)

Topical Talk DF 26.6 Thu 11:30 POT 251

Development of High Performance Semipolar GaN-based Blue and Green Lasers: Control of Stress Relaxation — •James Speck — UCSB Materials Department, Santa Barbara, CA USA

Nonpolar and semipolar GaN-based emitters have demonstrated low droop for LEDs and high performance for laser diodes. In this talk, we present two approaches to high performance blue and green laser diodes: the first using intentionally relaxed InGaN buffer layers for (11-22) oriented laser diodes and the second using selective area growth for (20-21) laser diodes.

For the relaxed (11-22) lasers we used strain compensated AlGaN/InGaN superlattice electron/hole blocking layers on intentionally relaxed InGaN buffer layers. Using this design, lasing at 447 nm was achieved with a threshold currentdensity of 7.2 kA/cm2, which is remarkably lower than previous results. Furthermore, wedemonstrate a 497 nm aquamarine-emitting semipolar (11-22)laser diode under pulsed operation.

For the coherent (20-21) lasers we used limited area epitaxy to minimize the misfit dislocation (MD) formation by preventing pre-existing TDs from entering a patterned mesa. Significant MD formation was suppressed by at least a factor of four for Al0.1Ga0.9N/GaN superlattices, enabling AlGaN-clad structures similar to those used in c-plane LDs. We then demonstrate AlGaN-clad blue (456 nm) LDs with threshold current density (Jth) of 4.5 kA/cm2 and GaN-clad true green (523 nm) LDs with Jth of 12 kA/cm2.

DF 26.7 Thu 12:00 POT 251

Improved X-ray diffraction simulations taking into account inhomogeneities exceeding the coherence length — •Christoph Berger, Dennis Schmidt, Jürgen Bläsing, Armin Dadgar, and Alois Krost — Otto-von-Guericke-Universität, Magdeburg, Deutschland

In many cases simulated diffraction patterns of semiconductor thin films or superlattices differ significantly from experimental data. The reason is that structural imperfections are often neglected in the simulation model. Indeed, many software packages can include the influence of compositional or thickness variations, but these variations occur on a shorter length scale than the coherence length of the diffractometer and have to be treated by dynamical theory. Including these influences often does not improve the simulation result. Due to the large area that is usually probed by the X-ray beam, one has to take into account structural variations larger than the coherence length as well, for instance lateral gradients across the wafer. These variations can be described by a sum of the diffracted intensity from the different parts of the specimen. In our method, a series of ideal simulations, each multiplied with a weighting factor, is summed up by a MATLAB routine that minimizes the deviation between the measurement and the sum of the weighted ideal simulations. The distribution of the weighting factors enables the estimation of the lateral variation width within the sample and the fit between simulated and experimental data is significantly improved.

DF 26.8 Thu 12:15 POT 251

Interactions between dislocations and overgrown v-shaped defects in GaN epitaxial layers — Phillip Weidlich[1], Michael Schnedler[1], Holger Eisele[2], Rafal E. Dunin-Borkowski[1], and •Philipp Ebert[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Due to the lack of large bulk substrates, most group III-nitride epitaxial layers have to be deposited on lattice-and thermal-mismatched substrates. The mismatch induces high dislocation concentrations. A variety of methods were invented to reduce the dislocation concentration in epitaxial GaN. Their common principle is the introduction of interfaces or inclined growth facets, which influence the line directions of threading dislocations. Inclined growth facets are also introduced by one of the most common extended defect in GaN layers, so called v-shaped defects. Therefore, we investigate the interactions between dislocations and v-shaped defects by mapping the spatial distribution and projected line directions of dislocations intersecting a cross-sectional (10-10) cleavage plane of GaN epitaxial layers using STM. The data is correlated with the spatial positions of v-shaped defects. The dislocations are found to be bent away from the inclined semipolar facets of v-shaped defects, due to a strain-induced repulsive interaction. The dislocation distribution is characterized by agglomerations and intersecting bundles of dislocations with parallel projected line directions, stabilized by many-body effects in the repulsive strain interactions.

DF 26.9 Thu 12:30 POT 251

Optical and structural investigations of the effect of barrier growth on GaInN quantum well structures — •Fedor Alexej Ketzer, Heiko Bremers, Torsten Langer, Uwe Rossow und Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

We study the influence of the growth of the barriers in GaInN multiple quantum wells (MQW) on structural and optical parameters of the wells. Therefore several MQWs were grown via low pressure MOVPE. Because the growth with H_2 as carrier gas is known to impede the incorporation of indium but is necessary during the growth of other layers, and therefore present in the reactor and structure, we investigate the effects of H_2 on the structure. We compare MQWs with different additional H_2 buffer gas flows during barrier growth with our reference samples with N_2 carrier gas. The growth parameters for the wells of all samples remain unchanged and lead to a nominal thickness of 2 nm with an indium content of 18 %. While the well thickness and indium content determined by photoluminescence do not differ for the reference samples without and the samples with H_2 buffer gas, the data of high resolution X-ray diffraction contradicts at a first glance. Here we see a drastically lower effective indium content of 7 %. This can only be explained by a strong inhomogeneity of the quantum wells and that only a small fraction of the quantum well area remains after growth. The influence of these inhomogeneities on the optical parameters and the internal quantum efficiency is discussed in detail.

DF 26.10 Thu 12:45 POT 251

Metamorphic growth of UV-B LEDs on $Al_{0.5}Ga_{0.5}N$ on AlN/Sapphire by MOVPE — •Johannes Enslin[1], Frank Mehnke[1], Martin Guttmann[1], Christoph Reich[1], Jens Rass[1,2], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Univerät Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

For AlGaN-based LEDs emitting in the UV-B spectral region between 280 nm and 320 nm relaxed buffer layers enable pseudomorphic growth of the multiple quantum well active region. In our contribution we present a study of the effects of various superlattice designs on pseudomorphic growth. The superlattice consists of 80 periods of AlN and GaN layers. We found that the thickness of the GaN layer and the relative AlN to GaN layer thicknesses (i.e. AlN/GaN ratio) are crucial for the relaxation process. 4.5 μm thick $Al_{0.5}Ga_{0.5}N$ with an AlN/GaN ratio of one exhibits high densities of pits and cracks. LEDs grown on this layer show no luminescence most likely due to these defects. UV-B LEDs grown on templates with AlN/GaN ratios $\leq$ 0.4 exhibit

fewer pits and no cracks, but show only poor luminescence. A smooth morphology was obtained for GaN thicknesses $\leq$ 2 nm and AlN/GaN ratios between 0.4 and 0.8. XRD scans show a distinct superlattice reflection. Reduced densities of pits and cracks indicate metamorphic growth. The optical emission power obtained from 305 nm LEDs grown on those layers reaches values up to 2.3 mW at 60 mA.

DF 27: Metamorphic structures: Bringing together incompatible materials II (Joint Focus Session with HL and DS)

Continuation of the morning session 'Metamorphic structures: Bringing together incompatible materials I'

Organizers: Ferdinand Scholz, Universität Ulm, and Andreas Hangleiter, TU Braunschweig.

Time: Thursday 15:00–16:30 Location: POT 251

Topical Talk DF 27.1 Thu 15:00 POT 251

Integration of cubic III/V semiconductors on silicon (001) — •Kerstin Volz — Philipps-Universität Marburg, Fachbereich Physik & Wissenschaftliches Zentrum für Materialwissenschaften

GaP layers on Si(001) can serve as pseudo-substrates for a variety of novel optoelectronic devices, like integrated lasers, solar cells and n-channel layers. The quality of the GaP nucleation layer is a crucial parameter for the performance of such a device. This presentation will summarize our current understanding of III/V heteroepitaxy on Si substrates and give several examples of successful integration of multinary III/V semiconductors on GaP/Si(001) virtual substrates.

DF 27.2 Thu 15:30 POT 251

Optical and structural characterization of an InGaN SQW embedded between quaternary InAlGaN barriers of varying In-concentration — •Christopher Karbaum[1], Frank Bertram[1], Marcus Müller[1], Peter Veit[1], Jürgen Christen[1], Jürgen Bläsing[1], Alois Krost[1], Martin Feneberg[1], Rüdiger Goldhahn[1], Jan Wagner[2], Michael Jetter[2], and Peter Michler[2] — [1]Institute of Experimental Physics, OvGUniversity Magdeburg, Germany — [2]IHFG, University Stuttgart, Germany

The change of the optical and structural properties of an InGaN SQW within InAlGaN barriers have been investigated using time resolved SEM-CL and STEM-CL spectroscopy at liquid helium temperature, PL, and HRXRD. The set of samples was grown on an optimized 1 μm thick GaN:Si buffer ontop of a c-oriented sapphire substrate. Subsequently, an InGaN SQW was embedded between InAlGaN barrier layers. The In gas flow during the pulsed MOVPE growth of these barriers was varied from 3 sccm up to 50 sccm. PL-spectra are dominated by the bound exciton emission of GaN (355 nm), a DAP at about 380 nm, the broad emission band from the InGaN SQW between 450 nm and 500 nm and the quaternary InAlGaN barrier emission. The fundamental idea behind the variation of the In-flux during growth is to achieve polarization matched conditions to decrease the QCSE of the InGaN SQW emission. For higher In-fluxes the InGaN emission undergoes a blueshift (150 meV) accompanied by a decrease of initial lifetime from 18 ns down to 5 ns. The temperature dependence of the luminescence and the recombination kinetics will be discussed.

DF 27.3 Thu 15:45 POT 251

Characterization of strained GaN on nanometer scale by IR near field microscopy — •Fabian Gaussmann[1], Stefanie Bensmann[1], Jochen Wüppen[1], and Thomas Taubner[1,2] — [1]Fraunhofer-Institut für Lasertechnik ILT, Aachen — [2]1. Physikalisches Institut 1A, RWTH Aachen Universität

Near-field microscopy combines the high spatial resolution of an atomic force microscopy with the depth of information that comes with spectroscopical analysis techniques. By using laser light in the mid IR range this technique is amongst others sensitive to the structure of polar materials like SiC or GaN. Regardless of the wavelength of the input laser light, the spatial resolution of these analyses is typical only a few tens of nanometer. This talk is focused on the characterization of strained gallium nitride systems. For near field analyses of GaN, laser light in the spectral range of 12 μm to 16 μm is required. This range, combined with a sufficient power density, is first covered by a novel developed tunable broadband laser system at the Fraunhofer ILT. While the two dimensional visualization of local stress fields using monochromatic laser systems is a common technique for near field analyses, we will present a method to transfer this capability to broadband laser systems. By recording single near field spectra, the optical properties and subsequent information for example about the strain, doping concentration or electron mobility can be achieved. Applied to cross-sections of layered systems, this technique gives a unique insight to the relaxation of crystal strain along the layer structure.

DF 27.4 Thu 16:00 POT 251

Measurement of strain in the InGaN/GaN heterogeneous nanostructures — •Tomaš Stankevič[1], Simas Mickevičius[1], Mikkel Schou Nielsen[1], Robert Feidenhans'l[1], Olga Kryliouk[2], Rafal Ciechonski[2], Giuliano Vescovi[2], Zhaoxia Bi[3], and Anders Mikkelsen[3] — [1]University of Copenhagen, Niels Bohr Institute, Copenhagen, Denmark — [2]GLO AB, Lund, Sweden — [3]Lund University, Nanometer Structure Consortium, Lund, Sweden

Growth and electrical properties of the core-shell nanostructures are often infulenced by the lattice mismatch induced strain. In contrast to planar films nanostructures contain multiple facets that act as independent substrates for the shell growth. In this study we present experimental results obtained by X-ray diffraction showing that the InGaN shells grown on the GaN cores are strained along each of the facets independently. Reciprocal space maps (RSMs) reveal multiple Bragg peaks corresponding to different parts of the shell strained along individual facet planes. Strained lattice constants were found from the peak positions. Vegard's law and Hooke's law for an anisotropic medium were applied in order to find the composition and strain in the InGaN shell. Simple atomistic kinematic simulations of the RSMs showed good agreement with the experimental data. We conclude that 8 nm the InGaN shells of up to 27% indium composition were nearly fully strained bixially along each of the $10\bar{1}0$ facets of the nanowires and the $10\bar{1}1$ facets of the nanopyramids.

DF 27.5 Thu 16:15 POT 251

Direct correlation of optical and structural properties of InGaN/GaN core-shell microrods by STEM-Cathodoluminescence — •Benjamin Max[1], Marcus Müller[1], Gordon Schmidt[1], Anja Dempewolf[1], Thomas Hempel[1], Peter Veit[1], Frank Bertram[1], Jürgen Christen[1], Martin Mandl[2], Tilman Schimpke[2], and Martin Strassburg[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]OSRAM Opto Semiconductors GmbH, Regensburg, Germany

We present a direct nano-scale correlation of the optical properties with the crystalline real structure of InGaN/GaN core-shell microrods using highly spatially resolved cathodoluminescence spectroscopy (CL). The characterized three microrod samples were grown by MOVPE on c-plane GaN/sapphire template via selective area growth using a SiO_2 mask: a GaN microrod reference structure without shell, a sample with InGaN single quantum well (SQW), and finally a complete core-shell LED structure were investigated. In all samples the GaN NBE emission originates exclusively from the compressively strained GaN template with an emission line at 356 nm. Spatially resolved CL mappings of the undoped sample and the LED structure exhibit luminescence from the InGaN SQW on the non-polar facet at about 400 nm. In contrast, on the semi-polar facet at the tip of the microrod the InGaN SQW luminescence is shifted to longer wavelengths. Additionally, the final core-shell LED structure shows DAP recombination at 380 nm, superimposing the InGaN SQW emission at the non-polar facets.

DF 28: Slow Dynamics in Glasses and Granular Matter II (Joint Focus Session with DY and CPP)

The transition into an amorphous solid state is typically accompanied by the observation of slow dynamics. The understanding of such transitions from first principles has seen progress in many of its aspects recently, including nonlinear response, residual stresses, and non-affine deformations. The Focus Session provides an overview of common phenomena and of general concepts in the physical picture of disordered materials. (Organizers M. Sperl and A. Zippelius)

Time: Friday 9:30–12:15 Location: HÜL 186

Invited Talk DF 28.1 Fri 9:30 HÜL 186

Critical Rheology of Weakly Vibrated Granular Media — •Martin Van Hecke — Huygens-Kamerlingh Onnes Lab, Leiden University

We experimentally probe the rheology of weakly vibrated granular media, and show that much of it is controlled by a nontrivial 2nd order-like critical point that occurs at finite stress and vibration strength. Close to this critical points, fluctuations become strong, correlation times diverge, and the flow curves exhibit scaling. For smaller vibrations, a 1st order transition emerges which separates a glassy phase from a rapidly flowing phase.

DF 28.2 Fri 10:00 HÜL 186

THz scattering from granular media — •Philip Born[1], Heinz-Wilhelm Hübers[2], Nick Rothbart[2], and Matthias Sperl[1] — [1]DLR Institute of Materials Physics in Space, Cologne, Germany — [2]DLR Institute of Planetary Research, Berlin, Germany

The structure and dynamics of driven dissipative granular media seems to be captured well by simulations. However, the results still evade experimental verification. The dynamics in colloidal suspension in contrast can be investigated comprehensively using light scattering techniques. The particle sizes in common experimental realisations of dense driven granular media, usually with particle sizes above 0.1mm, prevent application of imaging methods and established light scattering methods. Here we present approaches to the structure and dynamics of granular media using Thz radiation based light scattering. The matched wavelength ensures high sensitivity to geometric features of granular particle packings and paves the way for in-situ investigations of driven granular media.

DF 28.3 Fri 10:15 HÜL 186

Correlations and response in sheared hard sphere glasses — •Suvendu Mandal[1], Dierk Raabe[1], and Fathollah Varnik[2] — [1]Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Universitätsstr. 150, 44801 Bochum, Germany

Via event-driven molecular dynamics simulations, we study the packing-fraction and shear-rate dependence of single-particle fluctuations and dynamic correlations in hard-sphere glasses under shear [1]. At packing fractions above the glass transition, correlations increase as shear rate decreases: the exponential tail in the distribution of single-particle jumps broadens and dynamic four-point correlations increase. Interestingly, however, upon decreasing the packing fraction, a broadening of the exponential tail is also observed, while dynamic heterogeneity is shown to decrease. An explanation for this behavior is proposed in terms of a competition between shear and thermal fluctuations. We further address the issue of anisotropy of the dynamic correlations [2,3].

[1] Suvendu Mandal, Markus Gross, Dierk Raabe, and Fathollah Varnik, PRL. 108, 098301 (2012). [2] Suvendu Mandal, Vijaykumar Chikkadi, Bernard Nienhuis, Dierk Raabe, Peter Schall, and Fathollah Varnik, PRE. 88, 022129 (2013). [3] Vijaykumar Chikkadi, Suvendu Mandal, Bernard Nienhuis, Dierk Raabe, Peter Schall, and Fathollah Varnik, EPL. 100, 56001 (2012).

DF 28.4 Fri 10:30 HÜL 186

Granular matter composed of shape-anisotropic grains under shear — Ralf Stannarius[1], Sandra Wegner[1], Tamás Börzsönyi[2], and •Balázs Szabó[2] — [1]Inst. of Experimental Physics, University of Magdeburg, Germany, — [2]Institute for Solid State Physics and Optics, HAS, Budapest, Hungary

This contribution establishes a link between two different soft matter systems that can develop orientational order, liquid crystals and granular matter. We present shear experiments with prolate (ellipsoids, cylinders) and oblate (lentils) particles and discuss the observed order and alignment. Positions and orientations of the individual grains in the bulk are resolved by X-ray tomography. Shear experiments show that many observations are qualitatively and even quantitatively comparable to the behavior of the well-understood molecular liquid crystal mesophases, even though the types of interactions are completely different. We establish a quantitative relation between shear alignment and aspect ratio and investigate the interrelations to shear dilatancy and macroscopic friction properties. Long-range effects like particle rearrangements by creeping motion far from the shear band are detected.

15 min. break

Invited Talk DF 28.5 Fri 11:00 HÜL 186

A Granular Ratchet: Spontaneous Symmetry Breaking and Fluctuation Theorems in a Granular Gas — •Devaraj van der Meer[1], Sylvain Joubaud[2], Peter Eshuis[1], Ko van der Weele[3], and Detlef Lohse[1] — [1]University of Twente, The Netherlands — [2]ENS and University of Lyon, France — [3]University of Patras, Greece

We construct a ratchet of the Smoluchowski-Feynman type, consisting of four vanes that are allowed to rotate freely in a vibrofluidized granular gas. The necessary out-of-equilibrium environment is provided by the inelastically colliding grains, and the equally crucial symmetry breaking by applying a soft coating to one side of each vane. The onset of the ratchet effect occurs at a critical shaking strength via a smooth, continuous phase transition. For very strong shaking the vanes interact actively with the gas and a convection roll develops, sustaining the rotation of the vanes. From the experimental results we show that a steady state fluctuation relation holds for the work injected to the system, and that its entropy production satisfies a detailed fluctuation theorem. Surprisingly, we find that the above relations are satisfied to some extent even when a convection roll has developed and there exists a strong coupling between the motion of the vanes and the granular gas.

DF 28.6 Fri 11:30 HÜL 186

Granular Microrheology in the Large Force Regime — •Ting Wang[1], Matthias Grob[2], Annette Zippelius[2], and Matthias Sperl[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — [2]Georg-August-Universität Göttingen, Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

When pulling a particle in a driven granular system with constant force F, the probe particle may approach a steady velocity v. In the large force regime, it was found in our recent simulation that the effective friction coefficient F/v increases with increasing F, being proportional to the square-root of F, while some earlier Brownian dynamics simulations and theories predicted constant friction coefficient. Here, we study the behavior in granular microrheology by a schematic model of mode-coupling theory (MCT) and a simple kinetic theory. Our schematic model qualitatively reproduces the increase of friction tendency but fails to exhibit the square-root law. In the low density limit, the square-root law can be derived from the kinetic theory, based on which, we clarify the discrepancy of the large force behaviors in driven granular systems and Brownian ones.

DF 28.7 Fri 11:45 HÜL 186

Integration Through Transients Approach to the Rheology of a Sheared Granular Fluid — •Till Kranz[1], Fabian Frahsa[2], Matthias Fuchs[2], Matthias Sperl[3], and Annette Zippelius[1] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Fachbereich Physik, Universität Konstanz — [3]Institut für Materialphysik im Weltraum, DLR Köln

We generalize the Integration through Transients (ITT) formalism to

the non-equilibrium stationary state of randomly driven inelastic hard spheres. ITT was first developed for Brownian suspensions [1] and recently extended to thermostated Newtonian systems [2]. As a result we get generalized Green-Kubo-relations and an equation of motion for the transient density correlator.

Since the seminal work of Bagnold [3] it has been recognized that dissipative hard spheres (i.e. granular particles) have an unusual rheology. In particular, the shear stress σ varies with the square of the shear rate $\dot{\gamma}$, i.e., Bagnold scaling, $\sigma = \eta\dot{\gamma}^2$, holds. We will discuss the response to shear and the dependence on the degree of inelasticity and packing fraction. This includes the transient density correlator and the prefactor, η, of the Bagnold scaling relation. We will comment on the relation to the elastic [1,2] and the unsheared case [4], clarifying how Bagnold scaling emerges.

[1] M. Fuchs, M. E. Cates, J. Rheol. 53, 957 (2009)
[2] K. Suzuki, H. Hayakawa, Phys. Rev. E 87, 012304 (2013)
[3] R. A. Bagnold, Proc. R. Soc. Lond. A 225, 49 (1954)
[4] W. T. Kranz, *et al.*, Phys. Rev. E 87, 022207 (2013)

DF 28.8 Fri 12:00 HÜL 186

Nonlinear rheology of colloidal systems with attractive interactions: A mode-coupling theory analysis — •Madhu Priya and Thomas Voigtmann — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany

Hard spheres with a short-ranged attraction are a model system for colloid-polymer mixtures. These systems display two separate glasses, attractive and repulsive, connected with glass-glass transitions and higher-order glass-transition singularities. We study the nonlinear rheology of the square-well system in the vicinity of the glass-glass transition, using mode-coupling theory (MCT) in an isotropic-shear approximation. The yield strength and yield strains are studied, depending on packing fraction, attraction range, and strength. The findings of the model are compared with the observations made by recent experiments and computer simulation studies for colloid-polymer systems.