Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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Overview of Invited Talks and Sessions

(lecture rooms MÜL Elch, KÖN Farb, HSZ 101, HSZ 04, GER 38, ZEU 114; Poster P1)

Invited Talks

DF 1.1	Mon	10:15–10:55	MÜL Elch	**Design and Fabrication of Quantum-Enhanced Capacitors for CMOS-Applications** — •Jochen Mannhart, Thilo Kopp, Christoph Richter, Lu Li, Ashoori Ray
DF 3.1	Mon	14:45–15:25	MÜL Elch	**Advances of and by phase-field modelling in condensed matter physics** — •Heike Emmerich
DF 6.1	Tue	10:15–10:55	MÜL Elch	**Ultrafast X-ray Diffraction and all-optical Pump-Probe Spectroscopy on Oxide Multilayers** — •Matias Bargheer
DF 10.1	Wed	10:15–10:55	MÜL Elch	**Ferroelectric domains: Investigation, fabrication, and applications** — •Elisabeth Soergel

Invited talks of the joint symposium SKM-SYDT

See SKM-SYDT for the full program of the symposium.

SKM-SYDT 1.1	Thu	10:30–11:00	TRE Ma	**Domain boundaries as active elements in multiferroics and martensites: steps towards Domain Boundary Engineering** — •Ekhard K.H. Salje
SKM-SYDT 1.2	Thu	11:00–11:30	TRE Ma	**Intermediate Phases in Perovskite Solid Solutions** — •Ian Reaney, Clive Randall, David Woodward
SKM-SYDT 1.3	Thu	11:30–12:00	TRE Ma	**Adaptive martensite and giant strain effects in multiferroics** — •Ulrich K. Rössler
SKM-SYDT 1.4	Thu	12:00–12:30	TRE Ma	**Nature of magnetic coupling in Ni-Mn-based martensitic Heusler alloys** — •Mehmet Acet, Seda Aksoy, Eberhard F. Wassermann, Lluis Manosa, Antoni Planes
SKM-SYDT 1.5	Thu	12:30–13:00	TRE Ma	**Orthorhombic to tetragonal transition of $SrRuO_3$ layers in $Pr_{0.7}Ca_{0.3}MnO_3/SrRuO_3$ superlattices** — •Michael Ziese, Francis Bern, Ionela Vrejoiu, Eckhard Pippel, Elizaveta Nikulina

Sessions

DF 1.1–1.7	Mon	10:15–13:00	MÜL Elch	**Dielectric and ferroelectric thin films 1**
DF 2.1–2.5	Mon	11:00–12:40	KÖN Farb	**Nonlinear dielectrics, phase transitions, relaxors**
DF 3.1–3.7	Mon	14:45–17:30	MÜL Elch	**Dielectric and ferroelectric thin films 2**
DF 4.1–4.8	Mon	14:45–17:00	HSZ 04	**Multiferroics I (Joint Session of MA, DF, DS, KR, TT)**
DF 5.1–5.7	Mon	17:00–18:45	HSZ 04	**Multiferroics II (Joint Session of MA, DF, DS, KR, TT)**
DF 6.1–6.7	Tue	10:15–13:00	MÜL Elch	**Optical and nonlinear optical properties, photonic**
DF 7.1–7.1	Tue	10:15–10:45	HSZ 04	**Multiferroics III (Joint Session of MA, DF, DS, KR, TT)**
DF 8.1–8.6	Tue	10:45–12:15	HSZ 04	**Multiferroics IV (Joint Session of MA, DF, DS, KR, TT)**
DF 9.1–9.6	Tue	13:45–15:15	GER 38	**High-k and Low-k Dielectrics (Joint Session of DS, DF)**
DF 10.1–10.7	Wed	10:15–13:00	MÜL Elch	**Nano- and microstructured dielectrics**
DF 11.1–11.11	Wed	10:15–13:00	KÖN Farb	**Glasses I (Joint Session of DY, DF, CPP)**

DF 12.1–12.17	Wed	15:00–17:30	P1	**Poster**
DF 13.1–13.3	Thu	10:15–11:20	MÜL Elch	**Electrical and mechanical properties**
DF 14.1–14.2	Thu	11:20–12:00	MÜL Elch	**Dielectric composites and functionally graded materials; ceramics**
DF 15.1–15.7	Thu	10:45–13:00	ZEU 114	**Glasses and Glass Transition II (Joint Session of CPP, DY, DF)**
DF 16.1–16.5	Thu	14:15–16:00	MÜL Elch	**Dielectric surfaces and interfaces**
DF 17.1–17.6	Thu	14:00–16:45	HSZ 101	**Crystallography in Materials Science (Joint Session of KR, DF)**
DF 18.1–18.4	Thu	16:00–17:20	MÜL Elch	**Applications of dielectric solids**

Annual General Meeting of the Dielectric Solids Division

Mittwoch 17:45–19:00 MÜL Elch

- Bericht des Fachverbandleiters
- Tagungsnachlese
- Invited Talks 2012
- Tutorial, Focus Sessions, Plenary Talks and Symposia 2012
- Verschiedenes

DF 1: Dielectric and ferroelectric thin films 1

Time: Monday 10:15–13:00 Location: MÜL Elch

Invited Talk DF 1.1 Mon 10:15 MÜL Elch

Design and Fabrication of Quantum-Enhanced Capacitors for CMOS-Applications — •Jochen Mannhart[1], Thilo Kopp[1], Christoph Richter[1], Lu Li[2], and Ashoori Ray[2] — [1]Center for Electronic Correlations and Magnetism, Institute of Physics, Augsburg University, Augsburg, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

As the miniaturization of electronic circuits reaches the quantum scale, new possibilities emerge for the realization of novel, quantum electronic devices which exploit the quantum nature of solids. Here we show that by using quantum effects, the capacitance of electronic devices can be optimized to a great extent, which is a key to the further miniaturization of electronic components.

It is shown that by optimizing the material of the conducting electrodes, the capacitance of capacitors reaching the quantum regime can be substantially enhanced or reduced. Dielectric capacitors with negative total capacitances are suggested and their properties analyzed. Resulting perspectives to enhance the performance of electronic devices are discussed.

5 min. break

DF 1.2 Mon 11:00 MÜL Elch

Observation of ultrafast structural dynamics in perovskite ferroelectrics under optical excitation — •Michael Vattilana[1], Dan Daranciang[2], Nathaniel Brandt[4], Matthew Highland[3], Harold Hwang[4], Haidan Wen[2], Paul Fuoss[3], John Goodfellow[2], Jorgen Larsson[5], Keith Nelson[4], Andrew Rappe[6], David Reis[2], Brian Stephenson[3], Klaus Sokolowski-Tinten[1], and Aaron Lindenberg[2] — [1]Universität Duisburg-Essen — [2]SLAC/Stanford University — [3]Advanced Photon Source, Argonne National Lab — [4]Massachusetts Institute of Technology — [5]Lunds Universitet — [6]University of Pennsylvania

We used femtosecond time-resolved x-ray diffraction to investigate the dynamic structural evolution of thin $PbTiO_3$ films after optical excitation with intense fs laser pulses at 400 nm. The experiments were performed at the XPP pump-probe station of the Linac Coherent Light Source (SLAC) using ultrashort (60 fs) hard X-ray pulses at 9 keV. Our data reveal a complex structural response depending on the temperature (i.e. below and above the ferroelectric Curie-temperature) and the domain structure of the sample. We attribute this behavior to the strong coupling between the ferroelectric polarization, lattice strain and electronic degrees of freedom.

DF 1.3 Mon 11:20 MÜL Elch

Low voltage ferroelectric electron emission from $Pb(Zr_{0.4}Ti_{0.6})$ thin films — •Jana Becherer[1], Oliver Mieth[1], Vinay Shankar Vidyarthi[2], Gerald Gerlach[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden — [2]Institut für Festkörperelektronik, Technische Universität Dresden, D-01062 Dresden

We report on the electron emission from 600 nm thin ferroelectric $Pb(Zr_{0.4}Ti_{0.6})$ films. Based on a monolayer of polystyrene beads, structured top electrodes were prepared on the PZT films revealing nanometer-sized and regularly arranged apertures. The application of an ac voltage between top and bottom electrode initiates electron emission from the apertures. The emission current is measured under UHV conditions using a single electron detector for small signals and an amperemeter for larger currents.

The onset of the electron emission process could be accomplished at voltage values as low as 10 V. Emission current densities up to $3 * 10^{-8}\, Acm^{-2}$ for excitation voltages of 60 V were achieved. Using Piezoresponse Force Microscopy (PFM), the polarization state within the apertures was imaged for different voltages applied between top and bottom electrode. An increasing fraction of the free surface area was found to exhibit the reversed polarization orientation for rising voltage amplitudes. Thus, it is shown that the emission process in thin PZT films is strongly correlated to the switching of the ferroelectric polarization.

DF 1.4 Mon 11:40 MÜL Elch

Transient surface charging of insulators — •Björn Martin, Andrey Ostroskiy, and Herbert Kliem — Saarland University, Germany

The time dependent surface potential of insulators is investigated after charging of the surface with an electrical field. The surface potential is measured contactless using a scanning Kelvin probe or the Kelvin option of an atomic force microscope (AFM).

In a first experiment, a small point on the surface of an one side metallized insulator is charged with the cantilever of the AFM. The surface potential around this point is measured afterwards. On the position of the charged point a potential difference in relation to the uncharged regions is found. A transient decay and spread of the surface potential is observed in the long time range.

In another experiment, regions around evaporated top electrodes are charged by applying linear increasing voltages. Simultaneously the charging current is measured. Peaks are found in the measured current during the charging process. After application of a short circuit the surface potential at the electrode edge is measured. A potential peak near the electrode is found. The width and the temporal decay of this potential peak depend on the electrode material. The peaks during the charging process are correlated to the appearance of the potential peak. It is remarkable and not yet understood that positive surface charges are found near the electrode edge after application of a positive voltage.

DF 1.5 Mon 12:00 MÜL Elch

Comparative study of ferroelectric properties in Langmuir-Blodgett and spin-coated thin films of poly(vinylidene fluoride/trifluoroethylene) copolymers — •Manfang Mai, Bjoern Martin, and Herbert Kliem — Institute of Electrical Engineering Physics, Saarland University, Campus Building A5 1, D-66123, Saarbruecken, Germany

Poly(vinylidene fluoride/trifluoroethylene) copolymer thin films were prepared by Langmuir-Blodgett technique with thickness d ranging from 37 to 139nm and spin coating method (d=53-327nm). Their ferroelectric behavior has been investigated and compared by polarization switching measurements. Both kinds of films exhibit almost the same switching behaviour with varying thicknesses. As sample thickness reduces, the hysteresis loops tend to slant and the switching transients become broader. The coercive field increases with decreasing sample thickness, whereas the remanent polarization is nearly independent of sample thickness. The switching time decreases with increasing field and it is independent of thickness down to 69nm in LB films and 71nm in spun films. Slower switching is observed for a thickness below 60nm in both LB films and spun films. This could be due to the depolarization field induced by the surface oxidation layers of Al electrodes which becomes the more pronounced the thinner the sample is. The switching voltage suggests thin films in the range of 60-100nm are promising candidates for technical applications.

DF 1.6 Mon 12:20 MÜL Elch

Ferroelectric poly(vinylidene fluoride) films crystallized with ionic liquids: Structure-property relations — •Feipeng Wang[1], Alexander Lack[1], Zailai Xie[2], Peter Frübing[1], Werner Wirges[1], and Reimund Gerhard[1] — [1]Applied Condensed-Matter Physics, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam-Golm, Germany — [2]Institute of Chemistry, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam-Golm, Germany

Ferroelectric polymer films from poly(vinylidene fluoride) (PVDF) and its copolymers are often used in all-organic electronics. However, preparation of thin ferroelectric β-phase PVDF films is a challenging task due to the various crystalline phases of PVDF. In this work, ferroelectric PVDF films were obtained by spin coating from a solution containing a small portion of the ionic liquid 1-Ethyl-3-methylimidazolium nitrate ([EMIM][NO3]) and subsequent drying and annealing at elevated temperatures. The films show clear ferroelectric hysteresis behavior, with a remnant polarization of about 60 mC/m2 and a relatively high coercive field of about 200 MV/m. The quasi-static pyroelectric coefficient increases from 14 to 18 μC/(m2K) at temperatures between -20 and 40 °C. However, the measured pyroelectricity drops rapidly to 5 μC/(m2K) when the films are heated up to 70 °C. The

pyroelectric activity remains 60 % after the films were heated to 120 °C for 1 h and cooled back to 20 °C. X-ray diffraction measurements prove that addition of the ionic liquid enhances the films' crystallinity.

DF 1.7 Mon 12:40 MÜL Elch

Ferro- and pyroelectric characterization of thin poly(vinylidene fluoride) films — •Alexander Lack, Feipeng Wang, Peter Frübing, Werner Wirges, and Reimund Gerhard — Applied Condensed-Matter Physics, Department of Physics and Astronomy, Faculty of Science, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam-Golm, Germany

Ferroelectric poly(vinylidene fluoride) (PVDF) films with a thickness of about 430 nm were prepared by spin coating from DMF/acetone solution with addition of the ionic liquid 1-Ethyl-3-methylimidazolium nitrate ([EMIM][NO3]). After drying and annealing at elevated temperature, Fourier-transform infrared (FTIR) spectra and X-ray diffraction (XRD) measurements indicate dominance of the ferroelectric β phase. Ferroelectric hysteresis loops were obtained by integrating nonlinear current-voltage characteristics from a uni/bipolar electric-field sweep that allows separation of ferroelectric switching from capacitive charging and conduction. The nano-scale films show a relatively high coercive field of 200 MV/m. The remnant polarization is about 60 mC/m2, which agrees with the degree of crystallinity. The pyroelectric coefficient is determined by analyzing the short-circuit current response during low-frequency temperature oscillations at different temperatures. From XRD measurements, the crystallinity, and the size and the distribution of the crystallites are determined.

DF 2: Nonlinear dielectrics, phase transitions, relaxors

Time: Monday 11:00–12:40 Location: KÖN Farb

DF 2.1 Mon 11:00 KÖN Farb

Pressure induced Griffiths-like phase in $Sn_2P_2S_6$ ferroelectrics with three-well potential — •Konstantin Z. Rushchanskii[1], M. Kempa[2], P. Ondrejkovic[2], J. Hlinka[2], P. Saint-Grégoire[3], Ph. Bourges[4], and Yu. M. Vysochanskii[5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics AVCR, Prague, Czech Republic — [3]University de Nimes, Nimes, France — [4]Laboratoire Leon Brillouin, Saclay, France — [5]Uzhgorod National University, Uzhgorod, Ukraine

The origin of the second-order phase transition in uniaxial $Sn_2P_2S_6$ (SPS) monoclinic ferroelectrics is the relaxation of a lone-pair electron localized on Sn^{2+} cations, which results in nonlinear interaction of the soft polar and fully symmetrical optic modes and leads to a three-well potential in corresponding energy surface [1]. It is known [2] that systems with three-well potential, which are described by two order parameters (dipolar and quadrupolar), present a variety of stable, unstable and metastable phases at different temperatures. Combining *ab initio* derived effective Hamiltonian with Monte Carlo statistical simulations on large supercells, we first predict and then confirm experimentally by neutron diffuse scattering an existence of a pressure induced Griffiths-like phase in the PT-diagram near 0.6 GPa. KZR gratefully acknowledge the support from HGF Nachwuchsgruppe Programme VH-NG-409. [1] K.Z. Rushchanskii *et al*, Phys. Rev. Lett. **99**, 207601 (2007); [2] C. Ekiz *et al*, Physica A 293, 215 (2001).

DF 2.2 Mon 11:20 KÖN Farb

Effect of the substrate on the insulator-metal transition of vanadium dioxide films — •Gyoergy Kovacs, Danilo Buerger, Ilona Skorupa, Helfried Reuther, and Heidemarie Schmidt — HZDR, Dresden-Rossendorf

Vanadium dioxide is a potential candidate for on-chip memristive applications due to its hysteretic insulator-metal transition, which can be triggered by electronic pulses. Therefore it is interesting to investigate the details of the growth of VO2 on different substrates to see how the film structure and the electronic properties [1] depend on the underlying substrate. Here we show that single-phase vanadium dioxide films grown on (0001) sapphire and (001) silicon show a very different hysteretic insulator-metal electronic transition. The reason for this difference is that (tri-)epitaxy-stabilized columnar growth of VO2 takes place on the sapphire substrate, while on silicon the expected Zone II growth is identified [2]. The former ensures high crystalline quality so a narrow and high amplitude hysteresis loop, while in the latter case material transport between the substrate and the growing film alters the structure, resulting in a wider and lower amplitude hysteresis loop.

[1] V. A. Klimov, I. O. Timofeeva, S. D. Khanin, E. B. Shadrin, A. V. Ilinskii, and F. Silva-Andrade, Technical Physics 47, 1134 (2002). [2] György J. Kovács, D. Bürger, I. Skorupa, H. Schmidt, submitted

DF 2.3 Mon 11:40 KÖN Farb

Structural transformations in relaxor ferroelectrics on the mesoscopic scale — •Bernd J. Maier[1], Boriana Mihailova[1], Evgeniy A. Dul'kin[2], Tim Prüssmann[1], Carsten Paulmann[1], Marin Gospodinov[3], and Ulrich Bismayer[1] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg — [2]Faculty of Science, The Hebrew University of Jerusalem, Israel — [3]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

$Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST) is a canonical relaxor, undergoing on cooling a series of structural transformations without developing long-range ferroelectric order. Recently, it has been established that perovskite-type relaxors exhibit a characteristic temperature $T^\star$, at which initially formed polar clusters slow down and merge into larger polar nanoregions (PNRs). For PBST the temperature $T^\star$ is near 490 K as revealed by Raman scattering (RS) and acoustic emission (AE). RS data indicate that the transformation processes near $T^\star$ are realized via coupling of off-centred octahedral cations from adjacent polar clusters. AE experiments reveal that the coupling is highly anisotropic and is strongest along ⟨110⟩ cubic directions. AE measurements also demonstrate a temperature hysteresis of ∼15 K. Since PNRs generate strong x-ray diffuse scattering (XDS) along the ⟨110⟩* directions, the XDS intensity was used as an order parameter to determine the thermodynamical character of the phase transformation occurring at $T^\star$. The temperature evolution of XDS in PBST measured with synchrotron radiation reveals a near-tricritical behaviour in terms of the Landau theory.

DF 2.4 Mon 12:00 KÖN Farb

Origin of polar nano regions (PNR) in relaxor ferroelectrics: nonlinearity, polaron formation and charge transfer — •Annette Bussmann-Holder — Max-Planck-Institut für Festkörperforschung, Heisenbersgtr. 1, D-70569 Stuttgart, Germany

A central issue in the physics of relaxor ferroelectrics is the origin of the formation of PNRs below some characteristic temperature scale. While it is often attributed to chemical disorder, random bond * random field appearance, local symmetry lowering, it is shown here that the huge intrinsic nonlinearity of ferroelectrics gives rise to spatially limited solutions of discrete breather type, which interact strongly with the remaining lattice. This scenario corresponds to a two-component approach to relaxor physics with decisive signatures in the dielectric spectra and strong charge transfer.

DF 2.5 Mon 12:20 KÖN Farb

Complex polarization ordering in PbTiO3 nanowires: A first-principles computational study — Ghanshyam Pilania[1] and •Rampi Ramprasad[2] — [1]University of Connecticut, Storrs, USA — [2]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany

Based on parameter-free density-functional-theory calculations, we demonstrate the possibility of nonrectilinear curling vortex electric dipole configurations in PbTiO3 nanowires [1]. We predict that the critical size for the genesis of the vortex polarization instability with an axial toroidal moment is 16 Å. We also report previously unknown phase transitions between the nonrectilinear vortex and conventional rectilinear axial polarization configurations mediated by strain and surface terminations. The ability to switch reversibly between the vortex clockwise/counterclockwise and axial positive/negative polarization states may open up transformative technological possibilities.

[1] G. Pilania and R. Ramprasad, Phys. Rev. B 82, 155442 (2010).

DF 3: Dielectric and ferroelectric thin films 2

Time: Monday 14:45–17:30 Location: MÜL Elch

Invited Talk DF 3.1 Mon 14:45 MÜL Elch

Advances of and by phase-field modelling in condensed matter physics — •Heike Emmerich — Lehrstuhl Matrial- und Prozesssimulation Universität Bayreuth

Phase-field modelling as it is understood today is still a young discipline in condensed matter physics, which established itself for that class of systems in condensed matter physics, which can be characterised by domains of different phases separated by a distinct interface. Driven out of equilibrium their dynamics results into the evolution of those interfaces, during which those might develop into well defined structures with characteristic length-scales at the nano-, micro- or mesoscale. Since the material properties of such systems are to a large extend determined by those small scale structures, acquiring a precise understanding of the mechanisms that drive the interfacial dynamics is a great challenge for scientists in this field. Phase-field modelling is an approach that allows to tackle this challenge simulation-based. This contribution provides a critical overview over the conceptual background of the phase-field method, the most relevant fields of condensed matter physics, approached by phase-field modelling until now, as well as the respective model formulations and the insight gained via their simulation and analysis so far. Moreover, it discusses directions of further development and the quality of the scientific contributions to be expected from those, highlightening them via examples from advances in nucleation theory and austenite-martensite type transitions.

5 min. break

DF 3.2 Mon 15:30 MÜL Elch

Orbital ordering in head-to-head domain walls — •Kourosh Rahmanizadeh, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, oxide polar interfaces have attracted considerable attention due to the emerging novel behaviors. E.g. the $LaAlO_3$ / $SrTiO_3$ interface can induce new properties since the electric potential diverges due to the polar discontinuity at the interface. Electronic localization or defects can help to avoid the divergence of the electric potential and keep an insulating interface.

Also at a ferroelectric head-to-head domain wall there is an uncompensated charge, which could form a two-dimensional electron gas in the insulator. However, the uncompensated charges can be accommodated by partial occupation of the Ti 3*d* band. We carried out density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as implemented in the FLEUR code (www.flapw.de) to study the $PbTiO_3$ and $BaTiO_3$ head-to-head domain wall. The structures have been optimized with GGA and GGA+U. The optimized structure and electronic structure depend on the choice of the Coulomb U. For vanishing U a broad, conducting domain wall is obtained, while increasing U leads to an insulating and sharp domain wall. Also in GGA+U calculations an orbital ordering and a $GdFeO_3$-like rotation of the TiO_6 octahedra have been found at domain wall.

This work was partly supported by IFOX project of EU-FP7

DF 3.3 Mon 15:50 MÜL Elch

Tunneling through ferroelectrics: the role of the electronic structure of the barrier — •Daniel Wortmann and Stefan Blügel — Peter Grünberg Institut and Institute for Advanded Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich

Some of the proposed novel functionalities of future oxide-based electronics will drive their physical origin in the use of ferroelectric materials for tunneling barriers. With different directions of the ferroelectric polarization the tunneling conductance is modified, thereby allowing to utilize the polarization state for data storage. In direct analogy to the tunneling-magneto-resistance (TMR) a tunneling-electroresistance (TER) can be defined. One of the most basic microscopical sources of the TER is the change of the electronic transmission though the ferroelectric insulator because of the modified barrier potential.

We will discuss the basic theory of TER and we will demonstrate how a realistic description of the electronic structure as provided by density functional theory and the Green function formalism implemented in our FLEUR code [1,2] can be used to estimate the significance of the electronic structure of the barrier to the TER. We show that the change of the barrier potential in the simple prototype ferroelectric insulators $BaTiO_3$ and $PbTiO_3$ will lead to a very weak TER effect and thus the TER in junctions based on these materials will be dominated by interface effects.

[1] http://www.flapw.de

[2] D.Wortmann, H. Ishida and S. Blügel, PRB **66**,075113 (02)

DF 3.4 Mon 16:10 MÜL Elch

Electroresistance effects in ultrathin ferroelectric barriers — •Daniel Pantel, Silvana Goetze, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle (Saale)

Electron transport through ultrathin, fully depleted ferroelectric barriers sandwiched between two metal electrodes and its dependence on ferroelectric polarization direction are investigated by simulation and experiment.

In our calculations, we assume a polarization direction dependent ferroelectric barrier and include various transport mechanisms, namely direct tunneling, Fowler-Nordheim tunneling and thermionic injection. Electroresistance is found for all three transport mechanisms. Large electroresistance is favored in thicker films (on the expense of current density) or by switching between two transport mechanisms, e.g. direct tunneling and Fowler-Nordheim tunneling, by polarization switching.

Furthermore, we show some experimental results on $PbZr_{0.2}Ti_{0.8}O_3$ / $La_{0.7}Sr_{0.3}MnO_3$ heterostructures grown on $SrTiO_3$ substrates with nanoscale elemental metal top-electrodes. We find that the polarization direction influences the transport at room temperature.

DF 3.5 Mon 16:30 MÜL Elch

Growth of epitaxial multiferroic tunnelling heterostructures by pulsed laser deposition — •Silvana Goetze, Daniel Pantel, Marin Alexe, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

A multiferroic tunnelling heterostructure is a system of a thin ferroelectric film sandwiched between ferromagnetic electrodes, which could be applied in next generation of storage devices. Furthermore, they can be used to investigate electroresistance and magnetoelectric effects at interfaces. Here, we report on the growth of such structures by pulsed laser deposition. We have chosen $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) as the ferroelectric layer and $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) as the ferromagnetic bottom and top electrode grown on $SrTiO_3$ (100) (STO) substrate. For tunnelling junctions a low resistivity and a low surface roughness of the LSMO bottom electrode is crucial. Therefore, we optimized the growth conditions (temperature, oxygen pressure, laser energy, laser frequency) accordingly. Transmission electron microscopy images demonstrate the epitaxial growth of LSMO and PZT. Both are fully strained to the STO substrate as can be seen by x-ray diffraction. Hence, thicker PZT films show good ferroelectric hysteresis loops with high remnant polarization. Piezo-response force microscopy proves the ferroelectric behaviour for thinner PZT films.

DF 3.6 Mon 16:50 MÜL Elch

Electrical properties of ultrathin $CaTiO_3$ layers in MIM capacitor stacks — Andreas Krause[1], •Walter M. Weber[1], Uwe Schroeder[1], Johannes Heitmann[1,2], and Thomas Mikolajick[1,3] — [1]NaMLab gGmbH, Noethnitzer Strasse 64, D-01187 Dresden — [2]Institut fuer Angewandte Physik, TU Bergakademie Freiberg — [3]Institut fuer Halbleiter- und Mikroelektronik IHM, TU Dresden, Noethnitzer Strasse 64, D-01187 Dresden

$CaTiO_3$ is a promising material for high-k dielectric applications in metal-insulator-metal capacitors, combining a high dielectric constant (k) with low leakage current values. $CaTiO_3$ was deposited by rf-sputtering at different deposition temperatures. The dielectric constants and leakage current properties were optimized by improvement of the bottom electrode material and roughness. k-values between 51 and 180 were reached depending on the degree of crystallinity of the $CaTiO_3$ layer. The electrical results correlate well with the structural properties. The reduced leakage current values for the lower k samples are associated with the passivation of the grain boundaries in an amorphous matrix, while the leakage current for completely crystallized films is the result of conduction along the grain boundaries [1].

[1] A. Krause et al., Evaluation of the electrical and physical properties of thin calcium titanate high-k insulators for capacitor applications, JVST B accepted

DF 3.7 Mon 17:10 MÜL Elch

Piezoelectric properties of BNT-BT epitaxial thin films by electroacoustic measurement — •Mehrdad Baghaie Yazdi[1,2], Wook Jo[1], Philipp Komissinskiy[1], Pavel Klang[2], Joachim Hillenbrand[1], Jürgen Rödel[1], and Lambert Alff[1] — [1]Technische Universität Darmstadt — [2]Technische Universität Wien

The need for environmental friendly, non-hazardous materials have motivated the scientific community to increase their efforts in the development of lead free piezoceramics, as the electronic market faces an ever increasing need for such devices. Thin films of such a promising lead free piezoceramic, (1-x)$Bi_{0.5}Na_{0.5}TiO_3 \cdot x BaTiO_3$ for $x = 0.6$, have been deposited using pulsed laser deposition (PLD) on 5% niobium doped $SrTiO_3$(STO:Nb) substrates. The lattice constant of the films was determined using high resolution X-ray diffraction. Out of plane measurements, $c = 3.89$ Å, suggest the growth of a highly epitaxial cubic phase ($a = 3.90$ Å) on STO:Nb ($a = 3.905$ Å). The piezoelectric properties have been studied using an unconventional approach, namely electroacoustics, allowing the determination of d_{33} in the frequency range from 1 mHz to 1 MHz.

DF 4: Multiferroics I (Joint Session of MA, DF, DS, KR, TT)

Time: Monday 14:45–17:00 Location: HSZ 04

DF 4.1 Mon 14:45 HSZ 04

DFT calculation of $ACrO_3$ perovskites using hybrid functionals — •Martin Schlipf[1], Alessandro Stroppa[2], Silvia Picozzi[2], and Marjana Ležaić[1] — [1]Forschungszentrum Jülich, Peter Grünberg Institut and JARA, Germany — [2]CNR-SPIN, L'Aquila, Italy

Density-functional theory (DFT) is a very powerful tool for understanding the properties of several crystals and molecules. Novel hybrid exchange-correlation functionals, which include a fraction of Hartree-Fock exchange, improved the predictive power of DFT further. In this contribution, we have studied the $ACrO_3$ (A = Ca, Sr, Pb) perovskite compounds by DFT. These materials have recently gained a renewed interest, because they offer a rich phase-space of electronic, magnetic and structural transitions. The origins of several of these transitions are not understood, yet. In $SrCrO_3$ different authors report different electronic (metal/insulator) and magnetic (Pauli paramagnetic/Curie Weiss) configurations. It is not clear yet what is the ground state of this compound. In $PbCrO_3$ theoretical calculations predict a conducting state whereas experimentally a metal is found. We use a multi-code approach and clarify these issues from first-principles.

We gratefully acknowledge the support from HGF Nachwuchsgruppe Programme VH-NG-409.

DF 4.2 Mon 15:00 HSZ 04

Optical properties of $BiCrO_3$ — •Cameliu Himcinschi[1], Ionela Vrejoiu[2], Silvia Bahmann[1], Kannan Vijayanandhini[2], Adreas Talkenberger[1], Christian Röder[1], Dietrich R.T. Zahn[3], Alexei A. Belik[4], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, D-06120 Halle — [3]TU Chemnitz, Semiconductor Physics, D-09107 Chemnitz — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

Multiferroic materials that simultaneously show polarization and magnetization ordering are envisaged to play a significant role in developing devices with large magnetoelectric coupling. An interesting candidate for intrinsic multiferroism is $BiCrO_3$ (BCO). In this work, the optical properties of polycrystalline BCO ceramics and epitaxial BCO films deposited on $NdGaO_3$(110) substrates are investigated by Raman spectroscopy and spectroscopic ellipsometry. The spectral changes seen in temperature-dependent Raman measurements correlate well to a structural phase transition from a monoclinic structure (space group *C2/c*) to an orthorhombic structure (space group *Pnma*) at about 420 K. The room temperature dielectric function of a 55 nm thick BCO film deposited on $NdGaO_3$ substrate is determined by analyzing ellipsometry data and exploited to estimate the BCO band-gap. The imaginary part of the dielectric function calculated by means of density functional theory shows good agreement with the experimental one. *This work was supported by the German Research Foundation DFG HI 1534/1-1.*

DF 4.3 Mon 15:15 HSZ 04

Pressure induced phase transitions in $MnTiO_3$: Insights from First Principles calculations — •Carmen Quiroga and Rossitza Pentcheva — Section Crystallography, Dept. of Earth and Environmental Sciences, University of Munich

$MnTiO_3$ crystallizes in the ilmenite structure at ambient conditions and remains stable at least up to 26 GPa [1]. A denser $LiNbO_3$ phase can be quenched from high pressure and high temperature experiments to ambient conditions [2]. Our density functional theory calculations, including an on-site Coulomb repulsion term (LDA/GGA+U), show a transition from the $LiNbO_3$ to the perovskite phase at 2.5 GPa in agreement with experiments [3]. A transition from perovskite to the post-perovskite phase ($CaIrO_3$-type) is predicted at pressures above 50 GPa. Furthermore, the magnetic coupling of the Mn ions and the possibility of spin transitions in the different phases are explored.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] X. Wu et al. Geoscience Frontiers, in press (2010).
[2] J. Ko and C.T. Prewitt. Phys. Chem. Minerals **15**, 355 (1988).
[3] N. Ross et al. Phys Chem Minerals **16**, 621 (1989).

DF 4.4 Mon 15:30 HSZ 04

Resonant Soft X-ray Scattering (RSXS) Studies on Multiferroic YMn2O5 — •Sven Partzsch[1], Stuart Wilkins[2], John Hill[2], Enrico Schierle[3], Eugen Weschke[3], Dmitri Souptel[1], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW Dresden — [2]BNL Upton — [3]Helmholz-Zentrum Berlin

Multiferroic RMn_2O_5 (R = Y, rare earth, Bi) displays a complex magnetic behavior with transition into a ferroelctric phase as a function of temperature. The intensity of the magnetic superlattice reflection $(1/2, 0, 1/4)$ displays a strong resonance at the Mn L_{23}-edge, due to the strongly increased magnetic sensitivity close to the absorption edge.

Surprisingly, we also observe that this magnetic peak also displays a strong resonance at the oxygen K-edge. The measured integrated intensity of this reflection at the Mn L_3-edge in the commensurate and incommensurate magnetic phase is essentially unchanged. At the oxygen K-edge, however, a strong drop of the temperature dependent integrated intensity is observed at the corresponding phase transition, which resembles the temperature dependence of the ferroelectric polarization. Therefore RSXS at the different edges might provide more information about the origin of ferroelectricity in these frustrated magnets.

The experimental data together with LSDA+U calculations provide evidence that magnetically driven charge transfer between oxygen and manganese plays an important role for the ferroelectricity in these frustrated magnets.

DF 4.5 Mon 15:45 HSZ 04

Dilatometric studies of the multiferroic $FeTe_2O_5Br$ — •Christian Balz[1], Mariano de Souza[1], Matej Pregelj[2], Helmuth Berger[3], Denis Arčon[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany — [2]Institute "Jozef Stefan", Jamova 39, 1000 Ljubljana, Slovenia — [3]Institute of Physics of Complex Matter, EPFL, 1015 Lausanne, Switzerland

We report on high-resolution directional dependent thermal expansion measurements of the novel multiferroic system $FeTe_2O_5Br$ [1]. Our results reveal two distinct phase transition anomalies centered at $T_{N1} = 11.0$ K and $T_{N2} = 10.6$ K, which coincide with the transitions observed in other quantities [2]. A rounded minimum in α_c shows that short-range magnetic correlations within the crystal layers start to develop already above T_N. At T_{N1}, the system undergoes a magnetic phase transition into the high-T incommensurate (HT-ICM) phase. Interestingly, at T_{N2}, a second phase transition into the low-T incommensurately modulated (LT-ICM) phase is observed, which is accompanied by a spontaneous electric polarization. When mag-

netic field is applied, the transition temperatures shift depending on the field orientation. In the case of $B \| b > 4.5$ T, the HT-ICM phase merges into the LT-ICM phase. Despite the pronounced lattice effects observed at T_{N2} at 6 T, the electric polarization is destroyed. The rich low-T magnetic phase diagram of $FeTe_2O_5Br$ will be discussed in details [2].

[1] M. Pregelj *et al.*, Phys. Rev. Lett. **103**, 147202 (2009).
[2] M. Pregelj *et al.*, Phys. Rev. B **82**, 144438 (2010).

DF 4.6 Mon 16:00 HSZ 04

Investigation of multiferroic order in M_3TeO_6 (M=Co, Mn, Ni) by second harmonic generation — •Vera Carolus[1], Thomas Lottermoser[1], Sergey A. Ivanov[2], Matthias Weil[3], Roland Mathieu[4], Matthias Hudl[4], Per Nordblad[4], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Department of Inorganic Materials, Karpov' Institute of Physical Chemistry, Vorontsovo pole, 10 105064, Moscow K-64, Russia — [3]Institute of Chemical Technologies and Analytics, Vienna University of Technology, Austria — [4]Department of Engineering Sciences, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden

Orthotellurates with the formula M_3TeO_6 are structurally well characterized and can be divided into six different structure types. According to this, these materials show a wide range of magnetic phases. Recently it was suggested, that in some of the orthotellurates multiferroic order is possible.

Among this are: Co_3TeO_6 (space group C2/c) and Mn_3TeO_6 ($R\bar{3}$) with two magnetic phase transitions as well as Ni_3TeO_6 (R3) with one magnetic phase transition. However, a direct proof of ferroelectricity has not been reported so far.

Here, we investigate the multiferroic order by second harmonic generation (SHG) spectroscopy. For Co_3TeO_6 we measured a intense SHG contribution in the low temperature phase below 18 K, which is a strong evidence for multiferroic order. This interpretation is supported by the observation of complex domain patterns using SHG imaging techniques.

DF 4.7 Mon 16:15 HSZ 04

Optical Spectroscopy on the triangular antiferromagnet $CuCrO_2$ — •Michael Schmidt, Zhe Wang, Franz Mayr, Vladimir Tsurkan, Joachim Deisenhofer, and Alois Loidl — Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of physics, Augsburg University, Germany

$CuCrO_2$ belongs to the class of triangular lattice antiferromagnets and shows ferroelectricity below $T_{FE} \approx 24$ K [1] while the spins order in a proper screw [2]. Already a moderate magnetic field of 5.3 T can flop the plane of the spins and the polarization. A microscopic theory [3] explains this by the variation of the spin-orbit coupling with the metal-ligand (d-p) hybridization. Recently, electromagnons (magnetic excitations excited by electric field) have been detected in the related compound $Cu(Fe,Al)O_2$ [4] in the submillimeter range. We report on the optical excitation spectrum of $CuCrO_2$ including phonons, crystal-field excitations and magnon sidebands. The relation of magnon lifetime with the possible formation of Z_2 vortices in this system is discussed.

[1] K. Kimura et al., Phys. Rev. B 78, 140401 (2008)
[2] S. Seki et al., Phys. Rev. Lett. 101, 067204 (2008)
[3] T. Arima J. Phys. Soc. Jap. 76, 073702 (2007)
[4] S. Seki et al., Phys. Rev. Lett. 105, 097207 (2010)

DF 4.8 Mon 16:30 HSZ 04

New design for magnetoelectric switch from first principles — •Michael Fechner[1], Peter Zahn[2], Sergey Ostanin[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik Halle, Germany — [2]Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg

Saving information in a magnetic bit requires at least two stable magnetic states that can be distinguished. In conventional hard disks two opposite directions of the magnetization provide these two states. The magnetic state is changed by an external magnetic field thus writing information, whereas reading is performed by the usage of the GMR effect (giant magnetoresistance) [1]. Based on ab intio material design we propose a new hybrid magnetoelectric that allows this switching of the magnetic states by an applied electric field instead of the magnetic field. The switching in the proposed multilayer system is based on internal electronic couplings without any strain. Thus, it is a promising candidate for application in future magnetoresistive random access memory (MRAM).

[1] Baibich et al., PRL 61, 2472-2475, (1988)

15 min. break

DF 5: Multiferroics II (Joint Session of MA, DF, DS, KR, TT)

Time: Monday 17:00–18:45 Location: HSZ 04

DF 5.1 Mon 17:00 HSZ 04

Tuning magnetism by epitaxial strain in biferroic $Fe_{70}Pd_{30}$ films — •Sandra Weiss[1], Markus Ernst Gruner[2], Jörg Buschbeck[1,3], Ludwig Schultz[1], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden — [2]University of Duisburg-Essen, Theoretical Physics, Lotharstraße 1, D-47048 Duisburg — [3]ECE Department, University of California, Santa Barbara

Due to combination of ferromagnetic and ferroelastic properties magnetic shape memory alloys can be considered as multiferrorics. For the magnetic shape memory alloy Fe-Pd we could demonstrate recently, that strained epitaxial film growth allows a variation of the tetragonal distortion by 27 % [J. Buschbeck et al., PRL 103, 2009, 216101]. Density functional calculations revealed a flat energy landscape along the Bain path, explaining this soft behaviour of $Fe_{70}Pd_{30}$. Here we show that tetragonal distortions up to 43 % are possible. This exceeds the Bain transformation path connecting bcc and fcc structure. $Fe_{70}Pd_{30}$ films are produced by coherent epitaxial growth on MgO substrates covered by different metallic buffer layers. By adjusting the tetragonal distortion intrinsic magnetic properties like Curie temperature, saturation magnetisation and magnetocrystalline anisotropy can be controlled. The relevance of two mechanisms for relaxation of epitaxial strain - misfit dislocations and adaptive martensite - is discussed.

DF 5.2 Mon 17:15 HSZ 04

Strain effect on the magnetic properties of $SrRuO_3$ thin films on ferroelectric PMN-PT substrates — •Andreas Herklotz, Mikko Kataja, Ludwig Schultz, and Kathrin Dörr — IFW Dresden, IMW, Helmholtzstrae 20, 01069 Dresden, Germany

We investigate a two-component multiferroic system consisting of a ferroelectric $0.72PbMg_{1/3}Nb_{2/3}O_3$-$0.28PbTiO_3$ (PMN-PT) substrate and ferromagnetic $SrRuO_3$ (SRO) thin films. The inverse piezoelectric effect of the substrate is used to reversibly vary the strain state of the epitaxial SRO films in order to clarify the strain dependence of the magnetic film properties. Buffer films of $Sr_{1-x}Ba_xTiO_3$ are introduced to vary the as-grown state of the SRO films and to cover a wider range from compressive to tensile strain.

High resolution X-ray diffraction is deployed to structurally characterize the films and to determine Poisson's ratio of SRO, which is not known so far. SQUID magnetometry reveals that the Curie temperature is increasing with tensile strain, but starts to decrease again under high strain. Angular-dependent measurements provide that the easy axis orientation shows a complex dependence on strain and temperature. SQUID measurements on conventional substrates like $SrTiO_3$ and $LaAlO_3$ and electric transport measurements complete the data.

DF 5.3 Mon 17:30 HSZ 04

Strain effect on ferroelectric switching dynamics of epitaxial $PbZr_{0.52}Ti_{0.48}O_3$ films — •Kathrin Dörr[1], Andreas Herklotz[1], Michael Biegalski[2], and Hans Christen[2] — [1]IFW Dresden, IMW, Helmholtzstr.20, Dresden — [2]CNMS, Oak Ridge National Laboratory, TN, USA

Elastic strain is known to change ferroic properties of thin films such as the remanent polarization. Less understood and little measured is the influence of the lattice strain induced by film-substrate mismatch on the switching dynamics. In this work, reversible biaxial strain has been applied to films on piezoelectric substrates for a study of their strain-dependent ferroelectric switching. $PbZr_{0.52}Ti_{0.48}O_3$

(PZT) films have been epitaxially grown by pulsed laser deposition on piezoelectric substrates of $0.72PbMg_{1/3}Nb_{2/3}O_3$-$0.28PbTiO_3$(001) (PMN-PT) buffered with a $SrRuO_3/SrTiO_3$ double layer. Four-circle x-ray diffraction has been employed to confirm the tetragonal symmetry and to measure the lattice parameters of the films. Measurements of the characteristic ferroelectric switching time at various temperatures and strains show an increase of several percent under compression, revealing a similarly strong strain sensitivity of the switching dynamics as that of the remanent polarization. We attempt to identify the strain dependence of the domain wall velocity.

DF 5.4 Mon 17:45 HSZ 04

Fabrication and multiferroic properties of $BiFeO_3/BiCrO_3$ perovskite heterostructures — •Vijayanandhini Kannan, Florian Johann, Alessio Morelli, Miryam Arredondo, Eckhard Pippel, and Ionela Vrejoiu — Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle.

Bi-based multiferroic materials have attracted strong research interests due to the presence of sterochemical active $6s^2$ lone pair electrons in Bi^{3+} ions and high ordering temperatures, e.g., $BiMeO_3$ (Me = Fe, Cr, Mn, etc). In the present work, epitaxial films of $BiCrO_3$ and $BiFeO_3$ of different thickness (5 nm to 250 nm) were grown on $SrTiO_3$ (100) using pulsed laser deposition technique. Reciprocal space mapping XRD measurements showed that both $BiFeO_3$ (40 nm) and $BiCrO_3$ films (130 nm) are fully strained, having out-of-plane lattice constants of 4.075 Å, and 3.88 Å, respectively. The transmission electron microscopy (TEM) analysis of $BiCrO_3$(130nm)/$SrRuO_3$(16nm)/$SrTiO_3$ films revealed the presence of 45^o and 90^o domains along with the coexistence of three structurally different phases, (i) monoclinic (Space Group: C2/c) and (ii) orthorhombic (Space Group: Pnma) and (iii) an unknown monoclinic-like structure. $BiCrO_3$ film (160 nm) grown on $NdGaO_3$ (110) showed a coherent interface without any misfit dislocations or structural variants. A systematic approach on understanding the thickness evolution of these defects or strain induced structural variants of $BiCrO_3/SrRuO_3/SrTiO_3$ films is done. Furthermore, the fabrication and multiferroic properties of $BiCrO_3/BiFeO_3$ bilayers and multilayer heterostructures are investigated.

DF 5.5 Mon 18:00 HSZ 04

Microscopic Investigations of the Strain-Mediated Coupling in Magnetoelectric Ni/$BaTiO_3$ — •Robert Streubel[1], Denny Köhler[1], Lukas Eng[1], Rudolf Schäfer[2], Claudia Patschureck[2], Anja Wolter[2], Sebastian Gass[2], Stephan Geprägs[3], and Rudolph Gross[3] — [1]Institute of Applied Physics, Technische Universität Dresden — [2]Leibniz Institute for Solid State and Materials Research Dresden — [3]Walther-Meißner-Institute for Low Temperature Research

Coupling the (anti-)ferromagnetic and ferroelectric phases within magnetoelectrics allows affecting the magnetic properties by electric fields. Magnetoelectric heterostructures thus may be considered as prospective candidates for future nanoscale memory devices. However, since only a few single-phase room temperature magnetoelectrics exist with rather poor permeability values, simple composite materials, e.g. amorphous nickel on barium titanate (Ni/$BaTiO_3$) may be used for this purpose. While the macroscopic characterization by monitoring magnetic hysteresis and other effects has been thoroughly carried out, microscopic investigations elucidating the mechanism of ferroelectric/ferromagnetic coupling are still missing.

We report here on the nanoscale inspection of the Ni/$BaTiO_3$ system by PFM, MFM and MOKE. In addition, the saturation magnetization and magnetic anisotropy were measured by SQUID. Both stress and anisotropy within the amorphous Ni film have been modeled showing an excellent agreement with experimental results.

DF 5.6 Mon 18:15 HSZ 04

Magnetoelectric properties of core-shell $CoFe_2O_4$-$BaTiO_3$ composites — •Vladimir Shvartsman[1], Firas Alawneh[2], Morad Etier[1], Shiwam Tiwari[1], and Doru Lupascu[1] — [1]Institut für Materilawissenschaft, Universität Duisburg-Essen — [2]The Hashemite University, Zarqa, Jordan

In recent years there has been growing interest in materials exhibiting the magnetoelectric (ME) effect. A large ME coupling has been achieved in composites, where a magnetostrictive phase is mechanically coupled to a piezoelectric phase. The magnitude of the ME effect in such systems depends on the properties of the phases and the type of connectivity. In particular, in core/shell-type structures, where the magnetostrictive core is surrounded by the piezoelectric shell, a large well-defined interface area should enhance the ME coupling.

We report on results of synthesis and ME characterization of $CoFe_2O_4$ - $BaTiO_3$ composites with the core-shell structure. The ceramic samples were prepared by covering cobalt ferrite nanoparticles by a shell of $BaTiO_3$ using a sol-gel technique. Scanning probe microscopy studies confirm formation of the core-shell structure with a magnetic core and piezoelectric shell. The ME effect was measured using a modified SQUID susceptometer. Though the relatively high conductivity of the samples prevents an efficient poling of the ferroelectric component, the obtained ME coefficients are comparable to those reported for similar systems. Effects of the microstructure and ratio between piezoelectric and magnetostrictive phases on ME performance are analysed.

DF 5.7 Mon 18:30 HSZ 04

Highly ordered multiferroic nanocomposite arrays: Fabrication and Properties — •Xiaoli Lu, Yunseok Kim, Silvana Goetze, Peter Werner, Marin Alexe, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

With the resurgence of interest in multiferroics, searching for materials with high coupling coefficient becomes more and more important from both fundamental and practical point of views. We report a new type of artificial nanocomposite, $BaTiO_3/CoFe_2O_4$ (BTO/CFO) heterostructured nanodot arrays. Using a stencil of ultra thin anodic aluminum oxide (AAO) membrane and pulsed laser deposition (PLD), BTO and CFO nanodots were epitaxially grown on top of each other. The size of the nanodots can be easily tuned from 60 to 400 nm. Piezoresponse force microscopy (PFM) and superconducting quantum interference device (SQUID) were used to study the nanocomposite. The local characterization of the piezoresponse and domain structure within single nanodots may shed new light on the strain-mediated magnetoelectric (ME) coupling. The epitaxial interface and reduced clamping from the substrate in this nanocomposite promise a better elastic coupling, which makes it a good prototype for nonvolatile ultrahigh-density memory unit with multi-state data storage capability.

DF 6: Optical and nonlinear optical properties, photonic

Time: Tuesday 10:15–13:00 Location: MÜL Elch

Invited Talk DF 6.1 Tue 10:15 MÜL Elch

Ultrafast X-ray Diffraction and all-optical Pump-Probe Spectroscopy on Oxide Multilayers — •Matias Bargheer — Institut für Physik und Astronomie, Universität Potsdam — Helmholtz-Zentrum Berlin

We present experimental results of ultrafast x-ray diffraction and ultrafast optical experiments that simultaneously measure optical reflection and transmission changes on various multilayer systems. The investigated multilayer samples include expitaxially grown oxides (STO, SRO, LSMO, PZT, BTO) with dielectric, metallic, ferromagnetic and ferroelectric character as well as polyelectrolyte multilayers with embedded gold nano-particles.

From the ultrafast x-ray techniques we assess the exact structural properties and structural changes. On the one hand we are able to measure transient relative changes of the lattice constant of STO as small as 10^{-7}. On the other extreme, we can induce changes of the x-ray diffraction efficiency of 2500% on particular superlattice Bragg-reflections by launching strain-waves with an amplitude of 1.8%.

Broadband visible and infrared pump-probe experiments are used to measure the changes in the dielectric function. We show how the information determined from ultrafast structural measurements can help with the interpretation of all-optical spectroscopies.

5 min. break

DF 6.2 Tue 11:00 MÜL Elch

Temperature dependent absorption and Urbach tail scaling in LuAG single crystals. — •Martin Letz[1], Alexander Gottwald[2], Matthias Richter[2], Vlad Liberman[3], and Lutz Parthier[1] — [1]Schott AG, Hattenbergstr. 10, 55128 Mainz — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin — [3]Lincoln Laboratory. MIT, 244 Wood St., Lexington, Massachusetts 02420-9108, USA

In the deep ultraviolet (DUV) spectral range the transmission of high purity $Lu_3Al_5O_{12}$, LuAG was measured using monochromatized synchrotron radiation. In the vicinity of the band gap below 7.8 eV, a scaling behavior of the absorption as a function of photon energy was observed. Temperature dependent measurements [1] allow us to distinguish different absorption mechanisms which differ by their ability to couple to phonon excitations. Interpreting the Urbach tails measured at different temperatures, we show that the temperature independent tail is due to defects in the lattice, whereas the temperature dependent part originates from the short term localization of exciton modes coupling to lattice distortions. These results allow us to extrapolate the maximum transmittance which can be obtained with LuAG crystals at the lithographic wavelength of 193.39 nm. Accurate determination of the maximum transmission limit is critical in deciding whether the material can meet industry's specification for 193-nm-based high index lithography.

[1] M.Letz, A.Gottwald, M.Richter, V.Liberman, L.Parthier, Phys. Rev. B, 81, 155109 (2010)

DF 6.3 Tue 11:20 MÜL Elch

A microscopic model for diffusive hopping charge transport in wide-bandgap oxide semiconductors — •Christoph Merschjann[1], Mirco Imlau[2], and Hauke Brüning[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Universität Osnabrück, Fachbereich Physik, Osnabrück, Germany

Relaxation and recombination processes of optically excited charge carriers in wide-bandgap oxide semiconductor crystals (e.g. niobates, phosphates, borates) often exhibit non-exponential decay shapes. In recent years, such relaxations have been phenomenologically described by stretched exponential functions after Kohlrausch, Williams and Watts (KWW). Although they describe the shapes fairly good, it is not possible to directly retrieve informations about the nature of the relaxation, i.e. the charge-transport process, from the KWW formalism.

We present a novel microscopic model for the diffusive hopping charge transport via strongly localized states (e.g. small polarons). This random-walk-based model directly incorporates microscopic quantities, such as lifetimes of single hopping events, electron and hole densities, and dimensionality of the system under study. We compare our numerical, analytical and experimental results. In the common case of equal electron and hole densities, as found in $KNbO_3$, our model yields the above named quantities with high accuracy.

Generalizations of our model, as well as relations to the KWW formalism, are discussed in the presentation.

DF 6.4 Tue 11:40 MÜL Elch

Tunability of the photofunctional properties in photochromic polypyridine ruthenium sulfoxide complexes — •Kristin Springfeld, Volker Dieckmann, Sebastian Eicke, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Ruthenium polypyridine sulfoxide compounds feature photo-triggered linkage isomerization into two metastable structural isomers. This isomerization is accompanied by a pronounced photochromism in the UV/VIS spectral range. The absorption changes are combined with a tremendous photosensitivity and a high thermal stability of the structural isomers. In this contribution, we discuss the modification of photochromic properties in the frame of ligand substitution and the replacement of the dielectric environment of the compounds. The complex $[Ru(bpy)_2(ROSO)]\cdot PF_6$ [1] (with OSO: 2-methylsulfinylbenzoate) is modified with the groups R = H, Bn, BnCl and BnMe [2] and studied in different solvents. The studies are performed by UV/VIS laserspectroscopy as a function of temperature and exposure. Our results reveal a selective tunability of the thermal stability in the compounds, while the photosensitivity and the characteristic absorption spectra remain unchanged. We discuss the impact of our findings in view of application of sulfoxide compounds in molecular photonic devices.

Financial support by the DFG (GRK 695) is gratefully acknowledged.

[1] Dieckmann et al., Opt. Express, 17, 15052 (2009)
[2] Dieckmann et al., Opt. Express, 18, 23495 (2010)

DF 6.5 Tue 12:00 MÜL Elch

Polarization controlled switching of optical nonlinearity in nanocomposite glass — •Sabitha Mohan and Gerhard Seifert — Physics Institute, Martin-Luther-Universität Halle-Wittenberg, von-Danckelmann-Platz 3, 06120 Halle (Saale)

Nonlinear optical properties of uniformly oriented anisotropic metal nanoparticles in a glass matrix are studied using the Femtosecond Z-Scan technique. The glass samples (thickness 200μm) contain spheroidal nanoparticles only in a thin surface layer of 1-2 micrometer thickness. The macroscopic structural anisotropy of the composite system allows to tailor the optical nonlinearities of longitudinal and transverse Plasmon band separately. Ultrafast excitation of the longitudinal plasmon band (peak at 550 nm) in the near-resonant regime with 1030nm excitation wavelength (280fs pulse duration, 1 kHz repetition rate) results in a saturable absorption along with a negative nonlinear refraction. Contrastingly in the non-resonant regime the excitation results in a positive nonlinear refraction with negligible nonlinear absorption, which stems from the pure glass substrate. The contribution from the transverse plasmon band is observed by tuning the excitation wavelength to 800nm (pulse duration τ=80fs, 1 kHz repetition rate) which is in two-photon absorption resonant with the transverse plasmon band (peak at 390 nm). Studying samples with different aspect ratio, we obtained the dispersion of third-order nonlinearity in the near resonant regime, showing a boosting of the nonlinear processes due to the dielectric field enhancement.

DF 6.6 Tue 12:20 MÜL Elch

Bestimmung der effektiven Ladungsträgerkonzentration in nominell undotierten Lithiumniobat-Kristallen mittels holographischer Methoden — •Fabian Lüdtke[1], Daniel Haertle[1], Boris Sturman[2] und Karsten Buse[1] — [1]Physikalisches Institut, Universität Bonn, Deutschland — [2]Institute of Automation and Electrometry, Novosibirsk, Russia

Lithiumniobat-Kristalle sind auf Grund ihrer nichtlinearen und elektrooptischen Eigenschaften von großer Bedeutung in den Bereichen Photonik und integrierte Optik. Doch selbst nominell hochreine Kristalle weisen Verunreinigungen, beispielsweise durch Eisen oder Chrom, von wenigen ppm oder geringer auf. Diese führen bei hohen Lichtintensitäten zu Erwärmung durch Absorption und zu optischem Schaden durch photorefraktive Fremdatome. Beide Effekte schränken die Anwendbarkeit der Kristalle stark ein. Um den Einfluss der Verunreinigungen quantitativ abzuschätzen und Verfahren zu deren Beseitigung zu optimieren, ist eine genaue Kenntnis der Konzentration notwendig. Standardmethoden wie Absorptionsspektroskopie versagen hier auf Grund unzureichender Empfindlichkeit. Allerdings ist es unter Ausnutzung von Raumladungsbegrenzung möglich, die effektive Ladungsträgerkonzentration mit holographischen Methoden zu messen. Typische Konzentrationen liegen im Bereich um 10^{20} m^{-3}. Die Empfindlichkeit des Verfahrens ist im Vergleich zur optischen Absorptionsspektroskopie etwa 100-mal höher.

DF 6.7 Tue 12:40 MÜL Elch

Photoakustische Absorptionsmessungen in Lithiumniobat-Kristallen — •Stephan Fieberg[1], Niklas Waasem[1], Daniel Haertle[1], Frank Kühnemann[2] und Karsten Buse[1] — [1]Physikalisches Institut, Universität Bonn, Deutschland — [2]Physics Department, German University in Cairo, Egypt

Lithiumniobat ist ein hochtransparenter, elektrooptischer Kristall, der in vielen Bereichen der Photonik verwendet wird. Bei sehr hohen Lichtintensitäten können jedoch schon kleine Absorptionskoeffizienten zu unerwünschten Effekten führen, z.B. thermischen Schäden oder Photorefraktion. Aus diesem Grund ist eine genaue Kenntnis der Absorptionsspektren erforderlich. Zudem können Absorptionsspektren Auskunft über die Bandstruktur, Art und Dichte von Fremdatomen und die Stöchiometrie geben. Sie sind daher nicht nur technisch, sondern auch wissenschaftlich von großem Interesse. Derzeit gängige Messmethoden erreichen entweder nicht die nötige Auflösung von $< 10^{-4}$ cm^{-1} oder sind zu aufwändig und langsam. Eine sowohl schnelle, als auch hochauflösende Alternative bieten Photoakustische Verfahren, die eine durch Absorption des Lichts hervorgerufene Schallwelle zum Nachweis der Absorption nutzen. Der vorliegende Beitrag beschäftigt sich mit der Anwendung dieser Verfahren auf Lithiumniobat.

DF 7: Multiferroics III (Joint Session of MA, DF, DS, KR, TT)

Time: Tuesday 10:15–10:45 Location: HSZ 04

Invited Talk DF 7.1 Tue 10:15 HSZ 04

Search for a permanent electric dipole moment of an electron: Multiferroics bring us a step closer — •Marjana Ležaić — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

Although it is conjectured that the Big Bang created equal amounts of matter and antimatter, the Universe that we know consists only of matter. It is not yet clear why the Nature treats matter and antimatter in a different way. One possibility that is being intensively explored lies in the existence of a permanent electric dipole moment (EDM) of an electron. Electron's EDM would violate time-reversal symmetry leading to charge-parity symmetry violation and as a consequence, would act as a source of the matter-antimatter asymmetry. The talk will present a multidisciplinary study [1] including theoretical solid state design, consequent synthesis and characterization of a multiferroic material, (Eu,Ba)TiO_3, with characteristics optimized for a search for electron's EDM.

[1] K. Z. Rushchanskii, S. Kamba, V. Goian, P. Vaněk, M. Savinov, J. Prokleška, D. Nuzhnyy, K. Knížek, F. Laufek, S. Eckel, S. K. Lamoreaux, A. O. Sushkov, M. Ležaić and N. A. Spaldin, Nature Mater. **9** 649 (2010).

DF 8: Multiferroics IV (Joint Session of MA, DF, DS, KR, TT)

Time: Tuesday 10:45–12:15 Location: HSZ 04

DF 8.1 Tue 10:45 HSZ 04

Polarization and magnetization dynamics of a field-driven multiferroic structure — •Alexander Sukhov[1], Chenglong Jia[1], Paul P. Horley[2], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06120 Halle/Saale, Germany — [2]Centro de Investigation en Materiales Avanzados, S.C. (CIMAV), 31109 Chihuahua, Mexico

A multiferroic chain with a linear magnetoelectric coupling induced by electrostatic screening at the ferroelectric/ferromagnet interface [1] is considered. We study theoretically the dynamic ferroelectric and magnetic response to external magnetic and electric fields by utilizing an approach based on coupled Landau-Khalatnikov and finite-temperature Landau-Lifshitz-Gilbert equations. Additionally, we make comparisons with Monte Carlo calculations. It is demonstrated [2] that for material parameters corresponding to $BaTiO_3$/Fe the polarization and the magnetization are controllable by oscillating external magnetic and electric fields, respectively.

[1] T. Cai, S. Ju, J. Lee, N. Sai, A.A. Demkow, Q. Niu, Z. Li, J. Shi and E. Wang, Phys. Rev. B **80**, 140415(R) (2009). [2] A. Sukhov, C.L. Jia, P.P. Horley and J. Berakdar, J. Phys.: Condens. Matter **22**, 352201 (2010).

DF 8.2 Tue 11:00 HSZ 04

Rare-earth induced magnetoelectric effect in multiferroic $TbMn_2O_5$ — •Naëmi Leo[1], Dennis Meier[2], Roman V. Pisarev[3], Sang-Wook Cheong[4], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]UC Berkeley, USA — [3]Ioffe Institute, St. Petersburg — [4]Rutgers University, USA

The presence of magnetic frustration and multi-dimensional magnetic order parameters leads to remarkable effects like magnetically induced ferroelectricity. Such a particularly interesting compound is $TbMn_2O_5$ due to the associated magnetic-field controllable electric polarization. The gigantic magnetoelectric coupling originates in the presence of three independent ferroelectric contributions, which can be separatedly accessed by optical second harmonic generation (SHG). Two of these contributions are related to the manganese Mn^{3+} and Mn^{4+} magnetism. The third one is attributed to the spin arrangement of the Tb^{3+} sublattice which also mediates the intricate field-dependent cross-coupling. We confirm this model by measurements taken on isostructural YMn_2O_5 with non-magnetic Y^{3+} ions.

Also we perform spatially resolved domain topography to show that the magnetic-field induced polarization reversal in $TbMn_2O_5$ does not include domain wall motion but is indeed due to a reversal of only one ferroelectric contribution.

This work was supported by the DFG through SFB 608.

DF 8.3 Tue 11:15 HSZ 04

Three-dimensional distribution of protected ferroelectric vortices in multiferroic hexagonal $YMnO_3$ — Tobias Jungk[1], •Martin Lilienblum[2], Ákos Hoffmann[1], Manfred Fiebig[2], and Elisabeth Soergel[1] — [1]PI, Universität Bonn, Wegelerstraße 8, 53115 Bonn, Germany — [2]HISKP, Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany

Multiferrroics are a rich source for "unusual" forms of ferroelectric order. The spontaneous polarizations is induced by magnetism, charge order, geometric effects, etc., and may lead to novel domain states and functionalities. Here we show by piezoresponse force microscopy that ferroelectric domains in hexagonal multiferroic $YMnO_3$ form vortex-like structures around the direction of polarization. Although one would intuitively associate the sixfold character of the domain vortices to the uniaxial hexagonal structure, sixfold vortices are also present perpendicular to the direction of the spontaneous polarization. We will explain the intriguing topology on the basis of a simple geometric model. In addition, we will show how individual domain vortices are affected by application of an electric field applied along the polarization axis.

DF 8.4 Tue 11:30 HSZ 04

Poling of ferrotoroidic domains in $LiCoPO_4$ with toroidal fields — •Anne S. Zimmermann[1], Jean-Pierre Rivera[2], Hans Schmid[2], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Department of Inorganic, Analytical and Applied Chemistry, University of Geneva, Switzerland

Ferrotoroidicity denotes a fourth, space- and time-asymmetric form of ferroic order with a spontaneous uniform alignment of magnetic vortices. Space and time asymmetry also relates ferrotoroidic materials to multiferroics and magnetoelectrics. After ferrotoroidic domains have been observed in $LiCoPO_4$ by second harmonic generation (SHG) experiments [1] controlled manipulation of these ferrotoroidic domains is the next step in demonstrating the ferroic nature of the toroidal state. This can be achieved by a toroidal field, i.e., a field behaving asymmetric under space inversion and time reversal, which can be realized by crossed electric and magnetic fields.

Here we report on the behaviour of ferrotoroidic domains in applied toroidal fields. The ferrotoroidic domain structure in various field experiments was investigated by phase-sensitive SHG. We demonstrate that it is possible to orient and switch the ferrotoroidic domains with an appropriate toroidal field. Furthermore the critical field strengths required to orient the ferrotoroidic domains and the relation of ferrotoroidic poling with magnetoelectric annealing are discussed. - Work supported by the SFB 608.

[1] B. B. Van Aken et. al., Nature 449, 702 (2007)

DF 8.5 Tue 11:45 HSZ 04

Time resolved measurements of the multiferroic switching in MnWO4 — •Max Baum[1], Thomas Finger[1], Jeannis Leist[2], Karin Schmalzl[3], Louis-Pierre Regnault[4], Petra Becker[5], Ladislav Bohatý[5], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Georg-August-Universität Göttingen — [3]Jülich Centre for Neutron Science (JCNS) at ILL, Grenoble — [4]Institut Nanosciences et Cryogénie, CEA-Grenoble — [5]Institut für Kristallographie, Universität zu Köln

Multiferroic materials or compounds with a strong magnetoelectric effect posses a large application potential in data storage techniques. Quite recently, systems with a peculiar spiral magnetic order were shown to directly induce a spontaneous electric polarisation and to exhibit giant magnetoelectric and magnetocapacitance effects, among

them MnWO4. Neutron scattering with spherical polarisation analysis gives direct access to the chiral component of the magnetic structure which is directly linked to the electric polarisation and thus may be tunable by an electric field. In MnWO4 it is possible to drive multiferroic hysteresis loops at constant temperature as a function of the electric field. We broadened our investigations in this topic and present time resolved measurements of magnetoelectric switching. We applied stroboscopic techniques in order to investigate how fast the chiral component of the magnetic structure adapts to an instantaneously switched electric field. The time scale of the response is remarkable slow, in the range of 3 - 20 ms.

DF 8.6 Tue 12:00 HSZ 04

Time resolved reversal of spin-spiral domains by an electric field in multiferroic $MnWO_4$ — •Philip Thielen[1], Tim Hoffmann[1], Petra Becker[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]University Bonn, HISKP, Germany — [2]Institut für Kristallographie, Universität zu Köln

The interaction of magnetic and ferroelectric order is intrinsically strong in spin-spiral multiferroics. Here the complex magnetic long range order breaks inversion symmetry and induces a spontaneous electric polarization. The interaction allows for switching of the magnetization by means of an applied electric field and is thus of great interest for possible applications. So far there exists little information on the time scale and dynamics of the actual switching process. Here we report time resolved measurements of the reversal of spin-spiral domains in multiferroic $MnWO_4$ by optical second harmonic generation. Magnetic single-domain states are created by the application of an electric field. By reversing its polarity, a reversal of the magnetic domain state occurs. The time scale of the dynamic switching process is found to be in the ms region. Images of the domain-reversal process are obtained. The dynamic domain pattern differs substantially from that of quasi-statically switched multi domain structures.

DF 9: High-k and Low-k Dielectrics (Joint Session of DS, DF)

Time: Tuesday 13:45–15:15 Location: GER 38

DF 9.1 Tue 13:45 GER 38

Nondestructive Hard X-ray Photoelectron Spetroscopy Study of Resistive Switching TiN/Ti/HfO_2/TiN RRAM Cells — •Małgorzata Sowińska[1], Sebastian Thiess[2], Christian Walczyk[1], Damian Walczyk[1], Christian Wenger[1], Mindaugas Lukosius[1], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]P09 beamline at Petra III (DESY), Notkestrasse 85, 22607 Hamburg, Germany

Resistive switching metal-insulator-metal (MIM) diodes present a promising approach for back-end-of-line (BEOL) integration of embedded nonvolatile memory (NVM) cells in Si integrated circuits. Research in our group focused on TiN/Ti/HfO_2/TiN devices and one-resistor (1R) as well as one-transistor, one-resistor (1T1R) architectures were successfully processed under Si CMOS BEOL conditions. Switching characteristics in sweep as well as pulse mode were electrically investigated to study NVM characteristics (retention, endurance etc.). To unveil the microscopic origin of the switching mechanism, the Ti/HfO_2 interface was studied by nondestructive Hard X-ray Photoelectron Spectroscopy (HAXPES) studies at the recently constructed P09 beamline at Petra III (Hamburg). Results on RRAM cells in as-deposited, ON and OFF, as well as hard breakdown state will be presented.

DF 9.2 Tue 14:00 GER 38

Improvement of dielectric properties of $Sr_xZr_{(1-x)}O_y$ grown by Molecular Beam Deposition and Sputtering — •Matthias Grube[1], Dominik Martin[1], Walter M. Weber[1], Thomas Mikolajick[1,2], Lutz Geelhaar[3], and Henning Riechert[3] — [1]Namlab gGmbH, 01187 Dresden — [2]Lehrstuhl für Nanoelektronische Materialien, TU Dresden, 01062 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

Following the demand of replacing conventional dielectrics in the semiconductor industry, a material screening for new high-k dielectrics with nanometer-scale thicknesses is required. Among the many investigated potential materials are ZrO_2 as well as laminates and mixtures of ZrO_2 with HfO_2, Ta_2O_5 and Al_2O_3. We concentrated our efforts to the growth and characterisation of ZrO_2 with the admixture of SrO to form $Sr_xZr_{(1-x)}O_y$. We employed the molecular beam deposition technique (MBD) in a co-deposition regime for this purpose. The capability of MBD for high-k material screening was verified by comparison to deposition via sputtering a stoichiometric $SrZrO_3$ target. The investigated test structures were metal-insulator-metal capacitors (MIM) with a TiN bottom electrode on n^{++}-Si substrates. I-V and C-V measurements revealed a k-value of 19 for amorphous $Sr_xZr_{(1-x)}O_y$ grown by either MBD or sputtering. After surpassing a crystallisation temperature of approximately 650°C the k-value increases to 30 while the dielectric changes into a polycrystalline film with a cubic phase. A comparison of MBD and sputtering of ZrO_2 and $Sr_xZr_{(1-x)}O_y$ will be presented in detail.

DF 9.3 Tue 14:15 GER 38

Phase equilibria at Si-HfO_2 and Pt-HfO_2 interfaces from first principles thermodynamics — •Rampi Ramprasad[1] and Hong Zhu[2] — [1]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of Connecticut, Storrs, USA

In this work, two types of interfaces found in the emerging technologically important high-k MOSFETs have been studied. The phase diagrams of Si-HfO_2 and Pt-HfO_2 interfaces as a function of temperature and oxygen pressure have been determined using first principles thermodynamics (FPT), i.e., by combining conventional density functional theory results with thermodynamics [1]. The vibrational and configurational entropic contributions to the free energies of the condensed phases are explicitly included in this treatment. We demonstrate that the predictions of the FPT approach are in quantitative agreement with experiments for the classes of interfaces considered here. In particular, under UHV conditions, we show that FPT methods predict the correct Si-HfO_2 silica-like interface configurations. Likewise, we also show that an interfacial oxygen coverage of 0.5-1.0 monolayer is favored under UHV conditions at the Pt-HfO_2 interface before rapid oxidation of Pt may be expected (for higher oxygen pressures). These results have important implications both for the applicability of FPT methods for the considered classes of interfaces as well as for high-k dielectrics-based electronic devices in which such interfaces are expected.

[1] H. Zhu, C. Tang and R. Ramprasad, Phys. Rev. B, in print (2010).

DF 9.4 Tue 14:30 GER 38

Bottom-up Modeling of the Elastic Properties of Organosilicate Glasses and their Relation to Composition and Network Defects — •Jan M. Knaup[1,2], Han Li[3], Joost J. Vlassak[3], and Efthimios Kaxiras[1,2,3] — [1]Department of Physics, Harvard University, Cambridge MA, USA — [2]EPFL, Lausanne, Suisse — [3]School of Engineering and Applied Sciences, Harvard University, Cambriudge MA, USA

Organosilicate glasses (OSG), also known as SiCOH or carbon-doped oxide are used as low-k inter-metal dielectrics for integrated circuits. The material must fulfill two conflicting requirements: It has to have low density to reduce the dielectric constant and be mechanically stable enough to withstand mechanical stress during subsequent production steps. Experimental advances in improving their mechanical and electrical properties have not yet been theoretically examined at the ab initio level, due to the relatively large model sizes necessary for amorphous materials. We employ the density-functional based tight-binding (DFTB) method to achieve an accurate description of OSG properties at different compositions. We analyze the influence of composition and topological defects on the density and bulk modulus of non-porous OSG. We find that the dependence of density and stiffness on chemical composition is of different nature. This difference is traced to a transition between different mechanisms of elastic deformation in silica glass and in silicon hydrocarbide, which is also the reason for different sensitivity to topological defects in the two materials.

DF 9.5 Tue 14:45 GER 38

Local I-V characteristics of high-k ultra-thin ZrO_2- and

$ZrO_2/Al_2O_3/ZrO_2$-films. — •Dominik Martin[1], Matthias Grube[1], Elke Erben[1], Johannes Müller[2], Wenke Weinreich[2], Uwe Schroeder[1], Lutz Geelhaar[3], Walter Weber[1], Thomas Mikolajick[1,4], and Henning Riechert[3] — [1]namlab Gmbh, D-01187 Dresden — [2]Fraunhofer-CNT, D-01099 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin — [4]Chair of Nanoelectronic Materials, 01062 Dresden, Germany

In order to produce ultra thin ZrO_2-films, with a dielectric constant high enough to satisfy industry demands, it is necessary to reach the tetragonal crystalline phase. This can be achieved either by high temperature deposition or by a post deposition annealing step. Both however induce high leakage currents. Small amounts of Al_2O_3 can be incorporated in ZrO_2 to reduce leakage current. To get more insight into the charge carrier transport mechanisms involved, a thickness series of ultra thin ZrO_2- and $ZrO_2/Al_2O_3/ZrO_2$-films were deposited by ALD and subjected to different rapid thermal annealing processes. These layers were examined by GI-XRD, TEM, I-V-, C-V-Spectroscopy and conductive atomic force microscopy. Thus, leakage currents are reduced to $3.2 \cdot 10^{-8} \frac{A}{cm^2}$ at 1 V while maintaining the high k value (CET=1 nm at 1V for a 10 nm film) . CAFM studies demonstrate how the crystallization effects the charge transport mechanisms on the mesoscopic scale. Local I-V curves acquired on amorphous films and at grain boundaries in nanocrystalline films in yield lower breakdown voltages and higher leakage currents at crystallite grain boundaries.

DF 9.6 Tue 15:00 GER 38

Post-etch cleaning mechanisms at ultra low k surfaces — •Roman Leitsmann[1], Oliver Böhm[1,2], Philipp Plänitz[1], Christian Radehaus[1], Michael Schreiber[2], and Matthias Schaller[3] — [1]GWT-TUD GmbH, Material Calculations, Chemnitz, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [3]Globalfoundries Dresden Module Two GmbH & Co. KG, Germany

The usage of materials with an ultra low dielectric constant is necessary due to the decreasing feature size of integrated circuits, which results in smaller distances between the conduction layers, and hence to an increasing resistance capacitance delay. However, the application of such ultra low k (ULK) materials is connected to several problems. For example a fluorocarbon film at the ULK-surfaces at the sidewalls of trenches or vias is formed during the etch process. To remove this film a post-etch cleaning procedure have to be applied. In this study we investigate the cleaning efficiency of diluted HF using state of the art density functional theory. In particular different desorption mechanisms of CF-polymer fragments will be discussed in detail.

DF 10: Nano- and microstructured dielectrics

Time: Wednesday 10:15–13:00 Location: MÜL Elch

Invited Talk DF 10.1 Wed 10:15 MÜL Elch

Ferroelectric domains: Investigation, fabrication, and applications — •Elisabeth Soergel — Physikalisches Institut, Universität Bonn

Ferroelectric materials posses a permanent spontaneous polarization that can be reversed by the application of an electric field. In this way, ferroelectric domain patterns are fabricated which can be used for various applications ranging from efficient frequency conversion to high-density data storage. Although known since more than half a century, there are still open questions regarding ferroelectrics: For example the physical properties of the domain walls are still under discussion.

I will introduce ferroelectric materials and their applications, the fabrication of domain patterns and their investigation by piezoresponse force microscopy will constitute the principal part in my talk. Finally, as an example for a new application of ferroelectric domains, I will outline how they can be used to fabricate *m-sized single crystal structures suitable for photonic micro-components.

5 min. break

DF 10.2 Wed 11:00 MÜL Elch

Lithiumniobat-Nanokristall-Hybridsysteme für optisch-nichtlineare Prozesse — •Bastian Knabe, David Dung, Matthias Ackermann, Daniel Schütze und Karsten Buse — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Wir untersuchen die optischen Eigenschaften ferroelektrischer Lithiumniobat-Nanokristalle, insbesondere ihre optische Nichtlinearität, mittels kohärenter Frequenzkonversion. Diese Nanokristalle ermöglichen es optische Nichtlinearität in isotrope und amorphe Trägermaterialen einzubringen, wie z. B. Polymere oder Flüssigkeiten. Dabei sind sie, durch ihre Kristallinität, stabiler als organische Chromophore. Die nichtlineare Antwort einzelner Lithiumniobat-Partikel mit 50 nm Durchmesser wird polarisationsabhängig studiert. Es deutet sich an, dass die nichtlinearen Koeffizienten so groß wie die des Volumenkristalls sind.

*Wir danken der Deutschen Forschungsgemeinschaft (BU 913/21) und der Deutschen Telekom AG für finanzielle Unterstützung.

DF 10.3 Wed 11:20 MÜL Elch

Lithiumniobat-Nanopartikel für optische Anwendungen* — •Matthias Ackermann, Bastian Knabe, Daniel Schütze und Karsten Buse — Physikalisches Institut, Universität Bonn, Wegelerstraße 8, 53115 Bonn

Die Kombination von Lithiumniobat-Nanopartikeln mit Trägermaterialien wie z. B. Flüssigkeiten verspricht, Hybridmaterialien mit variablen ferroelektrischen und optischen Eigenschaften zu erzeugen. Dafür ist es notwendig, die Partikel ausrichten zu können und den Ausrichtungsmechanismus zu verstehen. Wir betrachten die Partikelorientierung in elektrischen Feldern, die durch induzierte und permanente Dipolmomente bestimmt wird. Bei einer Feldstärke von 3 kV/mm richten sich 80 Prozent der Partikel in einem Kegel mit einem Öffnungswinkel von 70° aus. Durch Ausnutzung des pyroelektrischen Effekts, also mittels Temperaturänderungen, wird die Größe der permanenten Dipolmomente beeinflusst und damit das Ausrichtungsverhalten der Partikel manipuliert.

*Wir danken der Deutschen Forschungsgemeinschaft (BU 913/21) und der Deutschen Telekom AG für finanzielle Unterstützung.

DF 10.4 Wed 11:40 MÜL Elch

Nonlinear Optics on Inversion-Domain Nanostructures in $Fe_2O_3(ZnO)_m$ — •Thomas Lottermoser[1], Simon Eichhorn[2], Werner Mader[2], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Institute of Inorganic Chemistry, University of Bonn, Germany

We prepared surfaces of ZnO single crystals with thin layers of Fe_2O_3 on top. Diffusion of Fe^{3+} ions generates a layer with the composition $Fe_2O_3(ZnO)_m$ with small $m \approx 15$ at the surface of the ZnO single crystal. Investigation with transmission electron microscopy reveals that in this layers regular patterns of triangular shaped ZnO inversion domains on a nanometer scale are formed by self organization. Additional measurements with electron energy loss spectroscopy show that the Fe^{3+} ions form monolayers at the domain boundaries while the domains itself consist of pure ZnO. The size of the inversion domains can be tuned by controlling the concentration of the Fe^{3+} ions.

These type of nano-structured materials has the potential to exhibit new magneto-optical properties that are tunable in various ways, e.g., by the Fe^{3+} concentration, the structure size and orientation of the iron-'doped' layers. The periodic and spatial inversion symmetry breaking nature of this compounds makes nonlinear optics an obvious characterization tool. Here, we report on our first experiments using optical second-harmonic generation (SHG). We observed an enhancement of the SHG intensity by about one order of magnitude compared to bulk ZnO. Polarization analysis indicates that this enhancement can be attributed to the meta-structure of the doped layers.

DF 10.5 Wed 12:00 MÜL Elch

Computation of dielectric permittivities: comparison of different crystal structures, amorphous systems and nanocomposites — •Andreas Leschhorn and Herbert Kliem — Universität des Saarlandes , Lehrstuhl für Grundgebiete der Elektrotechnik , Campus A5 1 , 66041 Saarbrücken

We investigate the influence of the microscopic structure on the dielectric properties of a dielectric material. To that, effective dielectric

permittivities of a system of induced dipoles are simulated numerically on a microscopic scale by calculating the local electric fields. In contrast to macroscopic calculations the method of local fields considers all dipolar fields within the sample taking account of the electrodes by the method of images. In this way all depolarizing fields in inhomogeneous samples are regarded.

Results for amorphous dielectrics and materials with different crystal structures are compared. For example, we found that a fcc structure leads to a higher relative permittivity than a sc lattice at the same parameters. Here the product $n\alpha$ of particle density n and polarizability α has been kept constant. Another example is the calculation of the permittivity of a bcc structure which also exhibits a higher value than a comparable sc structure. Also the permittivity of dielectrics consisting of atoms with different polarizabilities is computed. Furthermore, nanocomposites are investigated, with regions of different structures and species of atoms.

DF 10.6 Wed 12:20 MÜL Elch

Advancement of $Ba_{0.6}Sr_{0.4}TiO_3$ varactors by MgO micro dots — •Stefan Hirsch[1], Yuliang Zheng[2], Shunyi Li[1], Philipp Komissinskiy[1], Andreas Klein[1], Rolf Jakoby[2], and Lambert Alff[1] — [1]TU Darmstadt, Institut für Materialwissenschaft, Darmstadt, Germany — [2]TU Darmstadt, Institut für Elektrotechnik, Darmstadt, Germany

We report on the improvement of high frequency losses of Pt / $Ba_{0.6}Sr_{0.4}TiO_3$ / Pt thin film parallel plate varactors with MgO micro dots produced by pulsed laser deposition. Varactors are measured at frequencies from 1 MHz to 10 GHz. At 1 MHz losses are reduced by 30 % by using MgO micro dots in the BSTO layer. The figure of merit of the varactor is increased by 25 %. The influence of size and geometry of the micro dots on the varactor properties is investigated. The authors thank DFG GK 1035.

DF 10.7 Wed 12:40 MÜL Elch

On the Interpretation of Small Angle Diffraction Experiments on Opaline Photonic Crystals — •Frank Marlow, Mulda Muldarisnur, and Parvin Sharifi — MPI für Kohlenforschung, Kaiser-Wilhelm-Platz 1

Artificial opals are the most important approach to self-assembled photonic crystals. They have been characterized optically and by electron microscopy, but detailed structural information is still missing. Classical methods fail because of the small scattering angles. Recently, interesting structure investigations with neutron reactor sources and synchrotrons have been published. Theses studies reveal a surprisingly high degree of order in the scattering pattern but also some unexpected scattering features.

In this contribution we will add two points to the current interpretation of the diffraction data. First, the exclusion of the allowed (002) diffraction peaks by a small atomic form factor is not fully justified and, second, surfaces scattering has to be included as a possible source for the diffraction peaks. Our neutron diffraction data indicate that surface scattering is the main reason for the lowest detected order in the diffraction patterns.

DF 11: Glasses I (Joint Session of DY, DF, CPP)

Time: Wednesday 10:15–13:00 Location: KÖN Farb

DF 11.1 Wed 10:15 KÖN Farb

Boson-peak in glasses and random-matrix statistics — •Walter Schirmacher — Institut für Physik, Univ. Mainz — Physik-Department E13, TU München

The enhancement of the vibrational density of states (DOS) with respect to the Debye expectation ("boson peak"), which is universally observed in glasses, is considered by means of of symmetry arguments. Low-frequency wave-like excitations in a disordered solids probe a homogeneous and isotropic material. Due to these symmetries the vibrational wave-like states are highly degenerate (Debye regime). This degeneracy is lifted at higher frequencies. In this regime the discretized equation of motions are governed by a sparse random matrix. The eigenvalues of this matrix are non-degenerate and show the distance statistics of the Gaussian orthogonal ensemble ("level repulsion"). It is conjectured that the integrated density of levels in this regime increases linearly. The cross-over from the Debye regime to the random-matrix regime leads in three dimensions to an enhancement of the DOS. In two dimensions this is not the case. Model calculations using a field-theoretical approach [1] and inspection of simulation data [2] confirm this reasoning.

[1] W. Schirmacher, Europhys. Lett. Europhysics Letters, 73, 892 (2006); [2] see e.g. S. K. Sarkar, G. S. Matharoo, A. Pandey, Phys. Rev. Lett. 92,215503 (2004)

DF 11.2 Wed 10:30 KÖN Farb

Identification of facilitation effects in supercooled liquids — •Andreas Heuer and Christian Rehwald — Institute of Physical Chemistry, University of Muenster

In a first step we analyze the information content of the finite-size effects of a glass-forming system. Interestingly, the diffusion constant shows a very weak and the structural relaxation time a very strong finite-size effect [1]. This result reflects the dynamic coupling of different regions in real space via a facilitation mechanism. We can formulate a minimum model of the glass transition which can reproduce in detail the observed features of these finite-size effets. It can be regarded as a generalization of the kinetically constrained models [2].

In a second step we search for a direct evidence of this facilitation mechanism in computer simulations. Using the setup of a highly non-equilibrium configuration these causal relations between successive relaxation events can indeed be found and characterized.

[1] C. Rehwald, O. Rubner, A. Heuer, Phys. Rev. Lett. 105, 117801 (2010).

[2] Y. J. Jung, J. P. Garrahan, and D. Chandler, Phys. Rev. E 69, 061205 (2004).

DF 11.3 Wed 10:45 KÖN Farb

Dynamics of shear transformation zones during mechanical cycling of glassy CuTi - a molecular dynamics study — •Lennart Fricke und S. G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

Plastic deformation of bulk metallic glasses at low temperatures occurs in highly localized regions, called shear-transformation-zones (STZ) [1] - as corroborated recently in detailed experimental and simulational studies. After activation, these STZs should possess a memory of their configuration prior to transformation due to confinement by the surrounding elastic matrix, i.e. the Eshelby back-stress. While this picture surely is intuitive, it is particularly interesting whether it applies in a strict or only statistical sense and up to what strain levels. With this background we study shear behavior during mechanical cycling of CuTi with a maximum of 1% to 10% shear strains in large–scale MD simulations using realistic embedded atom method (EAM) potentials. Evaluating suitable quantities, including non-affine displacements and atomic-level Basinski–Duesbery–Taylor (BDT) stresses, we address the reversibility of STZs and the underlying physics on the atomic scale.

[1] A. S. Argon, Acta Metall. 27, 47 1979

This project is funded by the German DFG - PAK 63

DF 11.4 Wed 11:00 KÖN Farb

Describing experimentally obtained stress overshoots in sheared colloidal dispersions with schematic MCT — •Christian Peter Amann[1], Matthias Fuchs[1], Miriam Siebenbürger[2], and Matthias Ballauff[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Helmholtz Zentrum für Materialien und Energie, 14109 Berlin, Germany

Sheared viscoelastic media show a stress overshoot between elastic and plastic deformation regime, i.e. a maximum in the shear stress vs. strain plot after switching on a constant shear rate. We found a way to model such overshoots with the $F_{12}^{(\dot{\gamma})}$ model, a schematic model of a microscopic mode-coupling theory (MCT) approach to describe glass forming liquids. The enhancement of the schematic model is tested by fitting experimental strain-stress curves from sheared colloidal dispersions of thermosensitive core-shell particles. Flow curves and linear

stress response moduli of the same experimental setup could be fitted well with the $F_{12}^{(\dot{\gamma})}$ model [1]. Furthermore this model has been able to describe nonlinear stress response to oscillatory shear rates [2]. The implementation of stress overshoots in this schematic model was motivated and guided by the recently identified mechanism within microscopic MCT framework causing such overshoots to occur [3]. This mechanism is also identified to be highly connected to a super-diffusive motion regime of the colloids [3].

[1] M. Siebenbürger et al., *J. Rheol.* **53**, 707–726 (2009)
[2] J.M. Brader et al., arXiv:1010.2587v1 (2010)
[3] J. Zausch et al., *J. Phys.: Condens. Matter* **20**, 404210 (2008)

DF 11.5 Wed 11:15 KÖN Farb

Evaluation of MD force fields for ion transport in glassy materials — •Christian Trott[1], Martin Körner[1], Michael Schuch[2], and Philipp Maass[2] — [1]Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [2]Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany

Ion conducting glasses are an interesting class of materials with a wide range of possible applications, including batteries, supercapacitors, and smart windows. Considerable efforts have been undertaken to understand their properties with the help of experimental and theoretical investigations such as molecular dynamics (MD) simulations. Most of the previous MD studies of ion conducting glasses have been limited to structural analysis and the existing investigations of ion transport were almost all performed at comparatively high temperatures just below the "computer glass transition" temperature. Recent advances in hardware and MD software, namely the development of the GPU-MD code $\text{LAMMPS}_{\text{CUDA}}$, allow for a much more comprehensive investigation of long term dynamics. We assess the power of a number of interaction models for investigating long range ion transport in glasses. Specifically we determine diffusion constants and selected activation energies in several ion conducting glass systems for which force fields have been suggested in the literature.

DF 11.6 Wed 11:30 KÖN Farb

Lorentz-like power-law decay of velocity anti-correlations in a supercooled liquid — •Felix Höfling[1] and Peter Colberg[2,3] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [2]Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Canada — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln

Harnessing the compute power of recent graphics processors, we have measured the velocity-autocorrelation function (VACF) in the supercooled Kob-Andersen mixture for large systems of 50,000 particles, providing data with an excellent signal-to-noise ratio. The emergence of glassy dynamics upon supercooling is systematically accompanied by a power-law decay of the VACF at intermediate times with exponent 5/2 and negative prefactor, similarly as observed recently for the hard sphere liquid (Williams *et al.*, PRL 2006). Such anti-correlations are reminiscent of the well-known, universal long-time tail in the Lorentz model with the same exponent and sign. The role of dynamic heterogeneities for the power-law decay is addressed by considering correlation functions that are restricted to the most mobile or immobile particles. We find that the Lorentz-like decay is absent in the VACF of the most mobile particles and conclude that the power law is *not* a manifestation of dynamic heterogeneities. For the most immobile particles, however, the power-law decay is well pronounced and we propose that the relevant mechanism is given by repeated encounters with the quasi-arrested, microscopic particle cages.

DF 11.7 Wed 11:45 KÖN Farb

Universal jamming phase diagram in the hard-sphere limit and comparison of the dynamics of soft and hard spheres — •Michael Schmiedeberg[1], Thomas K. Haxton[2], Sidney R. Nagel[3], and Andrea J. Liu[4] — [1]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [2]Theory of Nanostructured Materials, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [3]The James Franck Institute, The University of Chicago, Chicago, IL 60637, USA — [4]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA

We present a new formulation of the jamming phase diagram for a class of glass-forming fuids consisting of spheres interacting via finite-ranged repulsions. Our phase diagram is universal at low pressure, i.e. observables such as the relaxation time are insensitive to details of the interaction potential and collapse onto the values for hard spheres.

Furthermore, we show that the dynamics of soft spheres can be described in terms of the dynamics of hard spheres. By introducing an effective hard sphere diameter that is determined from the soft-sphere pair potential via the Andersen-Weeks-Chandler approximation, the relaxation times of soft spheres can be mapped onto the curve known for hard-sphere liquids. These results indicate that the dynamics of soft spheres depend on an effective free volume in a universal way.

DF 11.8 Wed 12:00 KÖN Farb

Investigation of the dephasing of tunneling systems in glasses using two-pulse polarisation echo experiments — •Masoomeh Bazrafshan, Paul Fassl, Martin Schwarze, Angela Halfar, Annina Luck, Andreas Fleischmann, and Christian Enss — Kirchhoff Institut für Physik, Universität Heidelberg

Low temperature properties of glasses are governed by atomic tunneling systems. Many aspects are well described within the phenomenological standard tunneling model. Tunneling systems couple to their local strain fields which gives rise to a strain-mediated coupling among them. These interactions cause time-dependent variations in the energy splittings of tunneling systems when their neighbors undergo thermal transitions. This is the basis of the spectral diffusion model, which describes the dephasing of tunneling systems at very low temperatures. Experimentally, this dephasing of tunneling systems can be studied by two-pulse polarisation echo experiments. We have performed such echo decay measurements with an improved setup allowing us to observe echoes at very long delay times where the echo has decayed five orders of magnitude from its original amplitude. We have analysed the time and temperature dependent results in the framework of spectral diffusion model, finding very good qualitative agreement for the echo decay, but clear shortcoming in terms of the temperature dependence.

DF 11.9 Wed 12:15 KÖN Farb

Structural investigations on Eu-doped fluorobromozirconate glass ceramics. — •Marie-Christin Wiegand[1], Bernd Ahrens[2], Bastian Henke[2,3], and Stefan Schweizer[2,3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33100 Paderborn, Germany — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany — [3]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale), Germany

Modified Eu-doped fluorozirconate glasses are regarded as promising materials for photovoltaic and medical applications. In these glasses, a substantial fraction of the fluorine ions was replaced by bromine ions resulting in the formation of $BaBr_2$ nanocrystals upon subsequent thermal treatment of the as-made glass. Interestingly, the metastable hexagonal phase of $BaBr_2$ is always formed first before further annealing leads to the formation of orthorhombic phase $BaBr_2$, i.e., a phase transition from hexagonal to orthorhombic phase $BaBr_2$ occurs upon annealing. During the annealing a part of the doped Eu^{2+} is incorporated into the $BaBr_2$ nanocrystals enabling fluorescent transitions of Eu^{2+} in hexagonal and orthorhombic $BaBr_2$, respectively, upon ultraviolet excitation. The nanocrystal size and the structural phase depend on the addition of InF_3 and YF_3 and on the Br/(F+Br)-ratio, which was investigated by differential scanning calorimetry and x-ray diffraction. In addition, photoluminescence experiments were performed to monitor the phase transition by optical means.

DF 11.10 Wed 12:30 KÖN Farb

Optical and structural properties of fluorozirconate-based glass ceramics doped with divalent and trivalent europium. — •Christian Passlick[1], Bastian Henke[1,2], Jacqueline Anne Johnson[3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA

Eu-doped fluorozirconate-based glass ceramics can be used for x-ray detection in medical diagnostics as well as for down-converting top layers in photovoltaics. A modified ZBLAN composition consisting of a mixture of Zr, Ba, La, Al, and Na fluorides was additionally doped with chlorine ions to initiate the formation of $BaCl_2$ nanocrystals upon thermal treatment of the as-poured glasses. During annealing some of the Eu^{2+} ions are incorporated into the nanocrystals enabling a strong

blue fluorescence upon ultraviolet excitation or x-ray irradiation. In this work, focus is put on the amount of divalent and trivalent Eu fluoride and chloride additives since it is known that the expensive Eu^{2+} can be produced by melting the cheaper Eu^{3+} raw material. Influences of the different Eu oxidation states on the $BaCl_2$ crystallization and the optical response of the glass ceramics are presented.

DF 11.11 Wed 12:45 KÖN Farb

Multi-phonon relaxation in Eu-doped fluorozirconate-based glasses and glass ceramics — •Charlotte Pfau[1], Christian Bohley[1], Manuela Miclea[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[2,1] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle — [3]Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle

Eu-doped fluorozirconate(FZ)-based glasses are of interest for various fluorescence applications such as photon down-conversion layers for high efficiency solar cells or ionizing radiation imaging plates. Multi-phonon relaxation (MPR) is one of the major quenching processes of the rare-earth (RE)-related fluorescence therein. The MPR is significantly reduced in hosts providing low phonon frequencies such as FZ-based glasses and glass ceramics; the latter contain barium halide nanocrystals with even lower phonon frequencies. However, the MPR rate depends not only on the phonon frequency, but also on the electron-phonon coupling between the rare-earth ion and the host lattice. The local vibrational environment of the RE ion is investigated by phonon sideband spectroscopy. To analyze the vibrational spectra and their influence on the fluorescence properties, a series of Eu-doped FZ-based glasses and glass ceramics has been studied by Raman, phonon sideband, and fluorescence spectroscopy. The MPR rate is determined for the levels involved in the fluorescence process.

DF 12: Poster

Time: Wednesday 15:00–17:30 Location: P1

DF 12.1 Wed 15:00 P1

Strontium titanate/barium titanate heterostructures grown by pulsed-laser deposition — •Jan Zippel, Tammo Böntgen, Michael Lorenz, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentalphysik II, Linnéstraße 5, 04103 Leipzig

Recently, ferroelectric thin films such as $BaTiO_3$ (BTO) and $SrTiO_3$ (STO) have been attracted considerable attention due to their properties like ferroelectricity and piezoelectricity being suitable for applications in memories and sensors [1]. Differences in the electronic structure in combination with nearly no optical interface between STO and BTO and the probability to tune the optical properties for superlattices formed by STO and BTO is of interest for optical applications.

Here, we present the optimized growth of BTO and STO on STO (100) substrates using pulsed-laser deposition (PLD) with an in-situ reflection high energy electron diffraction (RHEED) system. The oxygen partial pressure ($p(O_2)$), the substrate temperature (T_{sub}) as well as the repetition rate of the laser and the energy density were varied in order to optimize both, the surface quality, controlled by atomic force microscopy (AFM) and the crystalline properties, checked by X-ray diffraction (XRD). The optical properties measured by spectral ellipsometry hardly depend on the crystalline structure. We were able to tune the index of refraction to a point, where optically nearly no difference between STO and BTO is observable at certain wavelength. [1] James F. Scott, Carlos A. Paz de Araujo, Science (1989), **246**, 1400-1405.

DF 12.2 Wed 15:00 P1

Polarisation switching dynamics by Inhomogeneous Field Mechanism in ferroelectric polymers — •Jörg Schütrumpf, Sergej Zhukov, Yuri Genenko, and Heinz von Seggern — Technische Universität Darmstadt, Darmstadt, Deutschland

The temporal behaviour of polarisation reversal in ferroelectric polymers like Polyvinylidene Fluoride (PVDF) cannot be satisfactory explained by simple models such as the classical Kolmogorov-Avrami-Ishibashi model for ferroelectric ceramics or by models considering stretched exponential laws. In the present contribution the Inhomogeneous Field Mechanism model recently proposed for PZT ceramics has been applied to polymer ferroelectrics for the first time. The model is based on the assumption that the switching volume is divided into many regions with independent dynamics, only determined by the local electric field. The local field values are randomly distributed over the ensemble of regions due to intrinsic inhomogeneities of the material. Therefore an inhomogeneous switching behaviour is induced by the varying local fields of each region. The electric field distribution can be directly extracted from the experimental data. The model satisfactory describes virgin and fatigued samples over a broad time-field domain covering nine orders of magnitude of the poling time and electric field values from 50-200 kV/mm. In the same way we can conclude that the IFM model is adaptive to ferroelectric ceramics and semi-crystalline polymers at once.

DF 12.3 Wed 15:00 P1

Surface modeling of $SrO(SrTiO_3)_n$ Ruddlesden-Popper phases — •M. Zschornak[1,2,3], S. Gemming[1], E. Gutmann[2], T. Weissbach[2,4], H. Stöcker[2,3], T. Leisegang[1,2], T. Riedl[5,6], M. Tränkner[5,6], T. Gemming[5], and D.C. Meyer[3] — [1]Ionenstrahlphysik u. Materialforschung, HZ Dresden-Rossendorf — [2]Strukturphysik, TU Dresden — [3]Experimentelle Physik, TU Bergakademie Freiberg — [4]Theoretische Physik, TU Bergakademie Freiberg — [5]IFW Dresden — [6]Werkstoffwissenschaft, TU Dresden

Strontium titanate (STO) is a preferred substrate material for functional oxide growth, whose surface properties can be adjusted through the presence of Ruddlesden-Popper (RP) phases. In this work[1], density functional theory (DFT) is used to model the (100) and (001) surfaces of $SrO(SrTiO_3)_n$ RP phases. Relaxed surface structures, electronic properties and stability relations have been determined. In contrast to pure STO, the near-surface SrO-OSr stacking fault can be employed to control surface roughness by adjusting SrO and TiO_2 surface rumpling, to stabilize SrO termination in an SrO-rich surrounding or to increase the band gap in the case of TiO2 termination. RP thin films have been epitaxially grown on (001) STO substrates by chemical solution deposition. In agreement with DFT results, the fraction of particular RP phases $n = 1 - 3$ changes with varying heating rate and molar ratio Sr:Ti. This is discussed in terms of bulk formation energy. [1] M. Zschornak, S. Gemming, E. Gutmann, T. Weißbach, H. Stöcker, T. Leisegang, T. Riedl, M. Tränkner, T. Gemming, D.C. Meyer: Acta Materialia 58 4650 (2010).

DF 12.4 Wed 15:00 P1

Preparation of nano-crystalline $BaTiO_3$ powder in a sol-precipitaion process — •Yanling Gao, Vladimir Shvartsman, and Doru C. Lupascu — Institut für Materialwissenschaft, Universität Duisburg-Essen, Essen, Germany

We are trying to synthesize uniform-sized nanoparticles having a high dielectric permittivity to be used in conjunction with conducting polymer in order to alter the electric properties of the latter. For this purpose, the synthesis of hydrophobic nano-crystalline $BaTiO_3$ is investigated. Cubic and hydrophobic $BaTiO_3$ nanopowders with a size below 20 nm were directly synthesized by sol-precipitaion under alkaline conditions at 100°C using the water - insoluble titanium (IV) isopropoxide oleate ($Ti(OR)_{4-x}(RCOO)_x$) precursor. The latter prepared by reacting titanium (IV) isopropoxide with oleic acid. The crystallinity and phase purity of the nanopowders were studied with X-ray diffraction spectrometry (XRD). The size and the microstructure of the $BaTiO_3$ nanopowder were analysed by Scanning Electron Microscopy (SEM). The XRD pattern of as-precipitated nanopowders showed weak and broad reflections characteristic of crystalline $BaTiO_3$ with evidence of the presence of $BaCO_3$. The as-prepared nanopowders were calcined at 500°C/6hrs in air to obtain perovskite of $BaTiO_3$ phase. The obtained $BaTiO_3$ were further pressed into pellets and sintered at 950°C/4hrs in air to get dense ceramics. Dielectric properties of these ceramics are measured as a function of temperature.

DF 12.5 Wed 15:00 P1

Ultrafast X-ray Diffraction with Synchrotron Pulses —

•Yevgen Goldshteyn[1], Roman Shayduk[1], Hengameh Navirian[1], Marc Herzog[2], Peter Gaal[2], Wolfram Leitenberger[2], and Matias Bargheer[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahm-Meitner-Platz 1, 14109 Berlin — [2]Institute of Physics and Astronomy, University Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam

The technique of time resolved X-ray diffraction with synchrotron pulses allows probing structural dynamics of matter with time resolution of approximately 100 ps. First time-resolved X-ray diffraction experiments at the EDR beamline at BESSY II have been performed on epitaxial $La_{0.8}Sr_{0.2}MnO_3$ (LSMO) and $SrTiO_3$ (STO) superlattices (SL) grown on single crystalline STO substrate. The heat transport in both the SL and the substrate has been studied on timescales of 50 ps to 4 μs. A Ti:Sa laser with 350 fs pulse duration is used to rapidly heat up the sample. Monochromatized X-ray pulses are used to measure SL diffraction peak profiles as a function of pump-probe delay. The peak shift is proportional to the strain in the SL caused by thermal expansion. The transient strain is detected with an accuracy of 10^{-7} and compared to simulations.

In addition, this poster presents the conceptual upgrade of the EDR beamline, which aims at shortening the X-ray pulses down to 1 ps pulse duration. First tests of controlled shortening have been successfully performed at ESRF and SLS.

DF 12.6 Wed 15:00 P1

Photoacoustic absorption spectroscopy in lithium niobate crystals — •Niklas Waasem[1], Stephan Fieberg[1], Daniel Haertle[1], Frank Kühnemann[2], and Karsten Buse[1] — [1]Physikalisches Institut, Bonn, Germany — [2]Physics Departmentof the German University, Cairo, Egypt

Lithium niobate is a highly transparent material that exhibits large non-linear optical coefficients, but for high-power applications even very small absorption coefficients can be a critical problem. Thus, determining the absorption spectra is a task of practical and scientific relevance. Existing methods of absorption spectroscopy fail either because they do not provide the necessary sensitivity of $\alpha < 10^{-4}$ cm^{-1} (grating absorption spectroscopy) or because of insufficient measuring speed needed for a wavelength scan (laser calorimetry). Therefore, we use a photo-acoustic approach. A sample is locally illuminated with nanosecond laser pulses, which heat and expand the exposed region. The resulting acoustic pressure waves are detected by fast and extremely sensitive piezo transducers. The amplitude of the measured signal is proportional to the product of pulse energy and absorption coefficient.

DF 12.7 Wed 15:00 P1

Impulsive Stimulierte Ramanstreuung: Prinzip und Anwendungen — •Peter Gaal, Yevgeni Goldsteyn, Daniel Schick und Matias Bargheer — Universität Potsdam Institut für Physik und Astronomie, Potsdam, Deutschland

Wir verwenden Impulsive Stimulierte Ramanstreuung (ISRS) zur Impuls-selektiven Anregung von Phonon-Polariton Moden in in oxidischen Materialien wie z.B. Lithium-Niobat oder Stronthium-Titanat und weisen diese durch Vierwellen-Mischprozesse nach. Durch die Überlagerung mehrerer Replika des gleichen Pumppulses wird in der Probe ein transientes Polarisationsgitter erzeugt, das mit einem Abtastimpuls ausgelesen wird. Wir diskutieren verschiedene Bereiche der Dispersionsrelation mit unterschiedlich starker Kopplung von Phononen- und Lichtcharakter. In Vorbereitung ultraschneller Röntgendiffraktionsexperimente bestimmen wir die k-Vektor-Selektivität der Anregung und geben eine Abschätzung für die erreichbare Phononenamplitude an.

DF 12.8 Wed 15:00 P1

Photofunctional ruthenium sulfoxide compounds for molecular photonics — •Volker Dieckmann, Sebastian Eicke, Kristin Springfeld, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Ruthenium polypyridine sulfoxide compounds are promising photofunctional molecules, which comply with the key requirements of (ultra-)fast all-optical devices, e.g. in information and telecommunication industry. These small molecular compounds provide a fast phototriggered linkage isomerization located at the SO ligand into two structural metastable states. The isomerization is accompanied by a pronounced photochromism with a tremendous photosensitivity. An advantage of these compounds is their adaptability on the optical requirements (e.g. spectral sensitivity) by two possibilities: Substitution of ligands or modification of the (dielectric) environment of the complex. We highlight the optical properties of these sulfoxides in the view of material design for the field of nonlinear molecular photonics: This includes the possibility of tailoring the optical properties studied by linear and nonlinear optical spectroscopy. Dynamical control of light by optical recording of 2D-photonic structures is verified by a spatially modulated phototriggered linkage isomerism using a single-pulse two-beam interferometer. Our findings are discussed in the frame of pronounced photochromism and presence of refractive index changes accompanying the phototriggered isomerism. The latter is explained satisfactorily both by Kramers-Kronig-relation as well as Lorentz-Lorenz relation. Financial support by the DFG (GRK 695).

DF 12.9 Wed 15:00 P1

Study of transient photocurrents in nominally pure $LiNbO_3$ depending on the reduction — •Andreas Buescher, Hauke Bruening, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

In thermally reduced, nominally pure $LiNbO_3$ the steady-state absorption is characterized by a broad absorption band at $\lambda = 500$ nm due to the presence of stable $(Nb_{Li}^{4+}{:}Nb_{Nb}^{4+})$-bipolarons. Upon illumination with intense pulse laser light in the blue green spectral range ($\tau = 8$ ns, $\lambda = 532$ nm) these bipolarons can be dissociated into metastable small free (Nb_{Nb}^{4+})-polarons and small bound (Nb_{Li}^{4+})-polarons. This mechanism is responsible for the strong photochromic properties of this material. Furthermore, but less often studied, these polarons contribute to the conductivity comparable to the features of extrinsic Fe-doping. We present first results of measurements to detect the transient photocurrents associated to bound polarons using a fast operational amplifier. Our study highlights the impact of the number density of optically generated small polarons, which can be controlled by the reduction pre-treatment. We discuss the results in the framework of optical and electrical properties of small polarons in $LiNbO_3$.

*Financial support by the DFG (project IM37/5-1) and DAAD (50445542) is gratefully acknowledged.

DF 12.10 Wed 15:00 P1

Photostable imaging by second-harmonic-generating nanoparticles — •Thomas Kämpfe, Philipp Reichenbach, Stefan Grafström, and Lukas M. Eng — Institute for Applied Photophysics, University of Technology Dresden, 01062 Dresden

Fluorescence microscopy is a widespread and elaborate method in imaging. However, in practice several disadvantages, most notably bleaching and blinking, can be observed. Second-harmonic generation (SHG) in noncentrosymmetric nanocrystals with diameters up to 100 nm seem to be a promising alternative. These particles circumvent the mentioned constraints as no real transition is invoked and thereby no phototoxic or dark state can be excited.

Long-time stability as well as sufficient signal strength for standard microscopy techniques was obtained for barium titanate nanoparticles with tetragonal crystal structure. The SHG signal increases quadratically with the excitation intensity (typ. 10^9 W/cm^2); these nanoparticles outshine all fluorescent markers at dye saturation. Moreover, the emitted second-harmonic radiation is spectrally sharp (~ 6 nm) so that the signal-to-noise ratio can be augmented by means of narrow bandpass filters. We present the experimental results on the nonlinear optical properties of single $BaTiO_3$ nanoparticles including the dependence on intensity, excitation wavelength and in-plane polarization as well as obtain the according crystal axis theoretically.

DF 12.11 Wed 15:00 P1

Temperature dependence of x-ray diffuse scattering near $T^\star$ for $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ relaxor. — •Tim Prüssmann[1], Bernd J. Maier[1], Boriana Mihailova[1], Carsten Paulmann[1], Marin Gospodinov[2], and Ulrich Bismayer[1] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg, Germany — [2]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Synchroton single-crystal x-ray diffraction was applied to the canonical relaxor $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST) to study the development of polar nanoregions. The temperature evolution of x-ray diffuse scattering (XDS) along $\langle 110\rangle^\star$ was followed by the ratio of the intensity of the XDS I_{diff} to the intensity of the corresponding Bragg peak I_{Bragg}. By using $I_{\mathrm{diff}}/I_{\mathrm{Bragg}}$ the thermodynamical character of the phase transformation near the intermediate temperature $T^\star$ associated with coupling of polar nanoregions was analysed. It is shown

that the transformation process near $T^\star$ is not of second-order and is most likely of tricritical character.

DF 12.12 Wed 15:00 P1

Supercritical and Subcritical Period Doubling Bifurcations - Influence of Near-Resonant and Resonant Perturbations — •Sebastian Lemm, Kay Barz, and Martin Diestelhorst — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, von-Danckelmann-Platz 3, D-06120 Halle, Deutschland

Using different ferroelectrics as nonlinear capacitors in a series resonance circuit gives rise to different kinds of bifurcations. Both supercritical and subcritical period doubling bifurcations could be observed depending on the choice of the ferroelectric. Whereas triglycine sulphate (TGS) in the circuit caused supercritical period doubling bifurcations, we observed subcritical period doubling bifurcations when we used a relaxor ferroelectric lead magnesium niobate-lead titanate (PMN-PT). In both systems we investigated the influence of both near resonant and resonant perturbations on the bifurcations experimentally. We observed the shift of the bifurcation points under the influence of perturbation compared to the unperturbed bifurcation. The phenomena are discussed in the framework of the corresponding center manifold. It was predicted earlier that tuning the resonance circuit towards a period doubling bifurcation under the action of a near resonant or resonant perturbation, may yield an amplification of the perturbation in the vicinity of the bifurcation. This effect of small signal amplification was investigated with respect to its applicability as a detector for signals, which may be coupled into the circuit via the special properties of the ferroelectric materials.

DF 12.13 Wed 15:00 P1

Thermal polarization noise of silver sodium nitrite — •Jumna Mehlis, Ulrich Straube, Martin Diestelhorst, Jörn Petersson, and Horst Beige — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

The thermal polarization fluctuations of ferroelectric crystals in the vicinity of the phase transition are discussed in detail in thermodynamic theories. These could be observed experimentally in a ferroelectric liquid crystal [1]. However, there is no publication about the experimental proof of the polarization noise in solid ferroelectric crystals. For this reason it was our aim to prove the spontaneous fluctuations of the polarization field in a ferroelectric AgNa(NO2)2-crystal. This was achieved by measurements of the thermal current noise in short * circuit of the single crystal. The noise current was made measurable with the help of a current - voltage amplifier. The thermal polarization and current noise power spectra of the silver sodium nitrite crystal could be described by the generalized Nyquist theorem. The possibility to determine the phase transition by noise measurements is discussed.

[1] I. Musevic, A. Kityk, M. Skarabot, and R. Blinc, Phys. Rev. 79, 1062-1065 (1997).

DF 12.14 Wed 15:00 P1

Theoretical investigation of the ferroelectric transition in $BaTiO_3$ and $LiNbO_3$ — •Simone Sanna and Wolf Gero Schmidt — Lehrstul für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

Barium titanate ($BaTiO_3$, BT) and lithium niobate ($LiNbO_3$, LN) are the most important ferroelectric materials. The first is the prototypical ferroelectric oxide, as many features and properties caused by or related to ferroelectricity have been found for the first time in BT [1]. The second is one of the most important optic materials, being the equivalent in the field of optics, non-linear optics and optoelectronics to silicon in electronics [2]. Despite the extensive interest in BT and LN, the knowledge of the mechanisms underlying the ferroelectric phase transitions is rather poor. The nature of the phase transition itself (displacive or order-disorder) is still argument of debate [3]. In this contribution we report on our first-principles theoretical studies of the ferroelectric transition in the two systems. Total energy calculations, molecular dynamics and frozen-phonon calculations are used to understand the mechanisms driving the transition at microscopic level. The Curie temperatures are estimated by *ab initio* thermodynamics. Similarities and differences between the two systems are discussed. *[1] R. Waser, Nanoelectronics and Information Technology: Advanced Electronic Materials and Novel Devices (Wiley- VCH, Weinheim, 2003). [2] A. Räuber, Chemistry and Physics of Lithium Niobate (North-Holland Publ. Company, Current Topics in Mat. Sci., 1978). [3] I. Inbar and R. E. Cohen, Phys. Rev. B* ***53****, 1193 (1996).*

DF 12.15 Wed 15:00 P1

Eigenschaften des Hyperfeinfeldes für ^{111}In in Al_2O_3 bei tiefen Temperaturen — •Michael Steffens und Reiner Vianden — HISKP, Universität Bonn, Nußallee 14-16, 53115 Bonn

In früheren Arbeiten [1,2] wurde der Elektronentransport in einem Isolator (Al_2O_3) bei hohen Temperaturen mit der Methode der gestörten γ - γ-Winkelkorrelation (PAC) untersucht. Dabei zeigte sich, dass der Einfluss des im Kristall vorliegenden Feldgradienten auf den PAC-Sondernkern ^{111}In durch einen aus dem Zerfall des In zu Cd resultierenden "after effect"(AE) überlagert wurde. Der Rückgang des AE bei hohen Temperaturen konnte mit einer erhöhten Eletronenbeweglichkeit begründet werden.

In dieser Arbeit wurden die Messreihen um Messungen bei tiefen Temperaturen erweitert. Auch bei Probentemperaturen < 50 K kann ein Rückgang des AE-Einflusses beobachtet werden.

[1] J. Penner, R. Vianden, Hyperfine Interactions 158(1), 389 (2004)
[2] M. Steffens et al., Hyperfine Interactions (2010), in print

DF 12.16 Wed 15:00 P1

Lattice dynamics of HgI_2 — •Lydia Nemec[1,2], Dieter Strauch[1], Bruno Dorner[3], Dieter Schwarzenbach[4], Peter Fischer[5], and Martin Böhm[3] — [1]Universität Regensburg, Regensburg, Deutschland — [2]*current address:* Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Deutschland — [3]Institut Laue-Langevin, Grenoble, France — [4]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [5]Paul Scherrer Institute, Villingen, Switzerland

We present a first principle study of the vibrational properties of tetragonal red mercury(II)iodide (α-HgI_2), an important material for X- and γ-ray detection at room temperature. Linear response theory within density-functional theory is used to calculate phonon frequencies and eigenvectors with special emphasis on vibrations in the [110]-plane. The full phonon band structure is investigated and compared with experimental data. We study the LO-TO splitting by calculating the dielectric constant and Born effective charges. The theoretical scattering intensities show fair agreement with experiment. Predictions are made for the scattering intensities in the [110]-direction, and data are provided for future neutron scattering experiments.

DF 12.17 Wed 15:00 P1

Zum Mechanismus der elektrostatischen Aufladung von Polymeren — •Frank Simon[1], Victoria Albrecht[1], Andreas Janke[1], Edith Reinsch[2] und Urs Peuker[2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, D-01069 Dresden — [2]Technische Universität Bergakademie Freiberg, Institut für Mechanische Verfahrenstechnik und Aufbereitungstechnik, D-09596 Freiberg

Die triboelektrische Aufladung von nichtleitenden Polymeren ist ein gut bekanntes und häufig beobachtetes Phänomen. Überraschend ist, daß die Mechanismen für die triboelektrische Aufladung weitgehend unbekannt sind. Gehen wir von der Annahme aus, daß beim Kontakt von zwei Stoßpartnern ein Elektronentransfer stattfindet, kann die Tendenz der funktionellen Gruppen eines Polymers zum Abgeben oder Aufnehmen von Elektronenpaaren genutzt werden, das Aufladeverhalten qualitativ zu beschreiben. Die Kontaktzone zweier sich berührender Polymeroberflächen beinhaltet jedoch eine Vielzahl solcher Gruppen. Diesen kooperativen Effekt konnten wir mittels rasterkraftmikroskopischer Untersuchungen visualisieren. Weiterhin ist bekannt, daß die Aufladung von Polymeren von der Umgebung abhängig ist. Wassermoleküle vermögen fixierte Ladungen zu mobilisieren und tragen zur Entladung bei. Dieses Abklingverhalten haben wir in Abhängigkeit der relativen Luftfeuchte und der Zeit untersucht. Die Kinetik des Entladeprozesses ist nicht nur abhängig von der molekularen Struktur des Polymers, sondern auch von Überstrukturen im polymeren Volumen.

DF 13: Electrical and mechanical properties

Time: Thursday 10:15–11:20 Location: MÜL Elch

DF 13.1 Thu 10:15 MÜL Elch

High-pressure crystal structure and Raman spectra of $Bi_{12}TiO_{20}$ sillenite — •Leonore Wiehl, Alexandra Friedrich, Eiken Haussuehl, Wolfgang Morgenroth, and Bjoern Winkler — Institut für Geowissenschaften, Goethe-Universität Frankfurt/Main, Germany

Sillenites, $Bi_{12}MO_{20}$ (M = Si, Ge, Ti), show outstanding electric and optical properties used in many applications, especially the photorefractive effect and a high photoconductivity, which are assumed to be correlated with the stereochemical activity of the $6s^2$ lone electron pair of Bi^{3+}. At ambient conditions the Bi^{3+} lone pair is oriented towards an unoccupied corner in the distorted $BiO_5\square$ octahedron. Thus the stereochemical activity is expected to decrease under high external pressure. The crystal structure of $Bi_{12}TiO_{20}$ (BTO) was determined from a single crystal at 9.2(2) GPa in a diamond anvil cell by X-ray diffraction with synchrotron radiation at HASYLAB (D3), Hamburg. Powder diffraction experiments were performed with synchrotron radiation at ESRF (ID09A), Grenoble up to a pressure of 37 GPa. On pressure release of the same sample, Raman spectra were measured in the pressure range from 37 GPa to ambient conditions. The bulk modulus is $B_0 = 50(1)$ GPa. The Bi^{3+} lone pair remains stereochemically active up to the highest pressure reached in this study.

Financial support from the DFG (HA 5137/3-1) and from HASYLAB is gratefully acknowledged. We thank HASYLAB and ESRF for synchrotron beamtime, Martin Tolkiehn for assistance at D3 and Michael Hanfland for assistance at ID09A.

DF 13.2 Thu 10:35 MÜL Elch

PVD grown high-k $SrTiO_3$ for capacitor applications: reliability and leakage current behavior — •Steve Kupke[1], Uwe Schröder[1], Steve Knebel[1], Sebastian Schmelzer[2], Ulrich Böttger[2], and Thomas Mikolajick[1] — [1]NaMLab gGmbH, Nöthnitzer Straße 64, D-01187 Dresden, Germany — [2]Institut für Werkstoffe der Elektrotechnik 2, RWTH Aachen University, Sommerfeldstraße 24, D-52074 Aachen, Germany

Low rate rf-sputtering was used to grow a 12 nm $SrRuO_3/SrTiO_3/SrRuO_3$ thin film capacitor with high dielectric constant and low leakage current behavior [1]. Leakage current analysis and time dependent dielectric breakdown (TDDB) measurements as a function of temperature were performed. Poole-Frenkel emission and trap assisted tunneling were found to explain the leakage current behavior at different electric field ranges. Shallow trap levels between 0.75 - 0.85 eV below the conduction band were found whereas at higher temperatures conduction is governed by deeper traps at 1.2 eV. Constant voltage stress (CVS) measurements indicate that electron trapping is predominant and stress induced leakage current occurs before hard breakdown. Based on the Weibull model a projected lifetime of several years was obtained at product conditions. The high lifetime in combination with a high effective permittivity of approximately 200 making it a promising candidate for future DRAM applications.

[1] S. Schmelzer et al., Appl. Phys. Lett. 97, 132907 (2010)

DF 13.3 Thu 10:55 MÜL Elch

Spectroscopic investigation of electro-coloration in Fe:$SrTiO_3$ — •Christian Lenser[1], Regina Dittmann[1], Kristof Szot[1], Aleksandr Kalinko[2], Alexei Kuzmin[2], Juris Purans[2], and Rainer Waser[1,3] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich, Jülich, Germany — [2]Institute of Solid State Physics, University of Latvia, Riga, Latvia — [3]Institut für Werkstoffe der Elektrotechnik, RWTH Aachen, Aachen, Germany

Electro-coloration of single crystals can be used as a model for the electroforming process of valence-change non-volative memory materials such as $SrTiO_3$ and TiO_2, which is necessary to access the switching properties of the material. Fe-doped $SrTiO_3$ single crystals are electro-colored by applying a DC-voltage between two evaporated Au-electrodes and stepwise increasing the current until metallic conductivity is reached.

The regions near the anode and cathode of the single crystal are investigated by X-ray absorption fine structure (XAFS), electron paramagnetic resonance (EPR) and Raman spectroscopy. EPR data show the presence of Fe^{3+}-oxygen vacancy complexes in the cathodic region, as well as their absence in the anodic region. The concentration gradient of oxygen vacancies created by the electro-coloration process is correlated to the local environment of Fe-centers as investigated by XAFS, and the effect of complexation and oxidation state on the pre-edge intensity and Fe-O bond length is discussed.

5 min. break

DF 14: Dielectric composites and functionally graded materials; ceramics

Time: Thursday 11:20–12:00 Location: MÜL Elch

DF 14.1 Thu 11:20 MÜL Elch

Dielectric properties of $BaTiO_3$ composites below the percolation threshold due to finite size effects — •Hans Lustfeld[1] and Martin Reissel[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D52425 Jülich — [2]Fachhochschule Aachen, Abteilung Jülich, D52428, Jülich

The high dielectric permittivity of $BaTiO_3$ can be enhanced further by adding metallic nanoparticles, e.g. Ni[1,2] or Ag[3]. This enhancement becomes high near the concentration c_p of the percolation threshold[4]. Therefore computing dielectric properties close to c_p is of great interest. However, near this limit finite size effects become important for modern **M**ulti **L**ayer **C**eramic **C**apacitors (MLCC's) having a layer thickness of a few μ only. Here we discuss these effects for the dielectric permittivity, energy storage and conductivity using the brick layer model[5] and a modified brick-layer model.

[1] C. Pithan et.al., Int. J. Mater. Res. **97**, 5 (2006)
[2]Y-C. Huang et.al., J. Am. Ceram. Soc., **90**, 1438 (2007)
[3]Y.Cheng et.al., Appl. Phys. Lett. **91**, 252903 (2007)
[4]W.T. Doyle, J. Appl. Phys. **85**, 2323 (1999)
[5]N.J. Kidner et.al., J. Am. Ceram. Soc. **91**, 1733 (2008)

DF 14.2 Thu 11:40 MÜL Elch

Piezoelectric characterisation of single ceramic fibres — •Sabine Kern, Ralf Steinhausen, Christoph Pientschke, and Horst Beige — Martin-Luther-University Halle-Wittenberg, Physics Department, PFM, 06099 Halle, Germany

Ceramic-polymer composites containing embedded piezoelectric ceramic fibres in a polymer matrix are favourable for application as ultrasonic transducers due to their low acoustic impedance, the high electromechanical coupling coefficient, as well as the high aspect ratio of the ceramic part. To optimise the composite's properties, knowledge of the electromechanical properties of the fibre itself is advantageous. A method to measure the piezoelectric strain loops for single ceramic fibres was developed. Using a capacitive displacement sensor, the present measurement method also allows the determination of the low-voltage piezoelectric coefficient d_{33} due to its high sensitivity. Reference measurements had shown that the electromechanical properties were measured with good accuracy. PZT fibres with diameters of 250-750 μm were characterised regarding the high-field bipolar and unipolar strain-field dependence and also the low-field piezoelectric coefficient. Moreover, the dependence of the polarisation regime was studied and discussed.

DF 15: Glasses and Glass Transition II (Joint Session of CPP, DY, DF)

Time: Thursday 10:45–13:00 Location: ZEU 114

Topical Talk DF 15.1 Thu 10:45 ZEU 114

Local Anisotropy of Fluids, Glasses and Jammed Bead Packs — •Gerd Schroeder-Turk — Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr 7B, 91058 Erlangen

The local structure of particle ensembles is important for physical properties of normal or super-cooled fluids, jammed bead packs or structural glass phases. It is often characterized by order parameters such as q_4 or q_6, defined by spherical harmonics of particle neighborhoods. Here we show that a Minkowski tensor analysis of the particles' Voronoi cells provides shape indices that give a clear signature of various structural transitions in particle systems. In particular, all of the above mentioned systems consist of locally anisotropic environments. We show that the degree of cell anisotropy shows a clear signature of the jamming transition in bead packs, the transition to partially ordered states at the random close packing limit, and of the transitions from fluid to ordered phases in simple liquids. For jammed bead packs, these findings suggest an inherent geometrical reason why anisotropic shapes can fill space more efficiently than spheres.

[1] Schröder-Turk *et al*, Europhys. Lett., **90**(3), 34001 (2010)
[2] Kapfer *et al*, J. Stat. Mech. (2010) P11010

DF 15.2 Thu 11:15 ZEU 114

In-situ characterization of vapor-deposited glasses of toluene by differential AC chip nanocalorimetry — •Mathias Ahrenberg[2], Heiko Huth[2], Katie Whitaker[1], Mark D. Ediger[1], and Christoph Schick[2] — [1]University of Wisconsin - Madison — [2]University of Rostock

We use ac nanocalorimetry to investigate extraordinarily stable glasses of toluene prepared by vapor deposition. For that purpose we have built a vapor deposition chamber that allows in-situ characterization of vapor-deposited organic glasses down to liquid nitrogen temperature. With highly sensitive nanocalorimeters in a differential setup, we are able to measure ng-samples over a frequency range from 0.1 Hz up to 8 kHz. The device was used to investigate the transformation of as-deposited stable toluene glasses into ordinary glasses. For films about 100 nm thick, the transformation was studied as a function of time at constant temperature above the common glass transition and as function of temperature at constant heating rate. The stability of the thin films was investigated as a function of substrate temperature and deposition rate.

DF 15.3 Thu 11:30 ZEU 114

Structural relaxation times in high-density amorphous ice (HDA) — •Philip H. Handle[1], Markus Seidl[1], Erwin Mayer[2], and Thomas Loerting[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of General, Inorganic & Theoretical Chemistry, University of Innsbruck, Austria

Solid water (H2O) exists in a variety of different forms. Besides common hexagonal Ice (Ih) today 15 different crystalline and three different amorphous forms are known. It is under discussion whether the amorphous forms are glassy (related to liquid water [1]) or nano-crystalline (related to ice). In case of high-density amorphous ice (HDA) this question has been addressed in some studies [2-4], yet remains controversial. In our work we measured structural relaxation times of HDA at elevated pressures (0.1 and 0.2 GPa) and different temperatures (125-135 K) on the basis of differential scanning calorimetry (DSC) at 1 bar. Our data suggest that at 135 K the structural relaxation time is only slightly higher than 100s, i.e., HDA is on the borderline to the glass transition.

[1] Poole, P. H.; et al.; Nature 360, 324-328 (1992). [2] Tse, J. S.; et al.; Nature 400, 647-649 (1999). [3] Mishima, O.; J. Chem. Phys. 115, 4199-4202 (2001). [4] Andersson, O.; Phys. Rev. Lett. 95, 205503-205507 (2005).

DF 15.4 Thu 11:45 ZEU 114

Dynamics of glass forming liquids in soft confinement — •Emmanuel Gouirand[1], Thomas Blochowicz[1], Andreas Blank[1], Bernd Stühn[1], and Bernhard Frick[2] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut Laue-Langevin, Grenoble, France

In search of a characteristic length scale associated with cooperative dynamics at the glass transition, intensive effort has been devoted to investigating the influence of confinement on the dynamics of glass forming liquids. Nevertheless, no generally accepted picture exists so far because of the complex interplay of surface, pressure and finite size effects affecting the dynamics. We investigate the dynamics in confinements of different nature in order to be able to disentangle these various effects. Therefore, we apply photon correlation spectroscopy and quasi elastic neutron scattering on glass formers confined within microemulsion droplets, the structure of which proved to remain stable over the whole temperature range by means of small angle scattering. First, we report on the dynamics of glycerol confined in AOT micelles where the glass transition temperature (T_g) of the matrix is chosen to be smaller than T_g of the glycerol core (fast soft confinement). We find glycerol to relax faster than in bulk with an Arrhenius temperature dependence [1]. Then we compare the dynamics of toluene in Cremophor ELP micelles. Contrary to the former situation, here the matrix relaxes slower than the core and slows down the latter due to interfacial effects. Finally, below T_g of the matrix actual hard confinement of toluene within the droplets is realized.

[1] Blochowicz et al., CPL 475, 171-174 (2009)

DF 15.5 Thu 12:00 ZEU 114

Crystallization and induced glass transition of n-alcohols in silicon-nanochannels — •Rolf Pelster, Rene Berwanger, Carsten Biehl, and Christoph Schuhmacher — FR 7.2 Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have investigated the molecular dynamics of n-alcohols (C_4H_9OH - $C_{11}H_{23}OH$) confined in mesoporous silicon and silicon oxide with pore radii ranging from 3.5 to 7 nm. Using dielectric and infrared spectroscopy we show that the temperature of the liquid-solid phase transition and the structure of the solid phase depend on both the chain length and the radius of the pores:

Long-chain alcohols exhibit a crystalline structure at low temperatures. The confinement induces a lowering of the freezing temperature. The shorter the chain length or the smaller the pore radius, the lower the freezing temperature. Below the phase transition only the dynamics of amorphous wall layers are observable [1].

Short-chain alcohols behave differently. While bulk alcohols still freeze upon slow cooling, we observe a glass transition for the confined phase. The glass transition temperature is close to that reported for quenched bulk alcohols. We thus conclude that nano-confinement suppresses the crystallization process and induces a glass transition.

[1] R. Berwanger, Ch. Schumacher, P. Huber, and R. Pelster, Eur. Phys. J. Special Topics 189, 239-249 (2010)

DF 15.6 Thu 12:15 ZEU 114

Glass Transition in Confined Geometry — •Simon Lang[1,2], Viatlie Botan[1], Martin Oettel[1], David Hajnal[1], Thomas Franosch[2], and Rolf Schilling[1] — [1]Johannes Gutenberg-Universität Mainz, Germany — [2]Universität Erlangen/Nürnberg, Germany

Confinement of a simple liquid is accompanied by introducing a further length scale in addition to the average distance of the particles. The interplay between them strongly influences the glass transition according to numerous significant experiments and simulations.

To achieve a theoretical description, we extend the microscopic mode-coupling theory to a liquid confined between two parallel flat hard walls [1]. The theory contains the standard mode-coupling equations in bulk and in two dimensions as limiting cases and requires as input solely the equilibrium density profile and the static structure factors of the fluid in confinement. We evaluate the phase diagram for a hard-sphere liquid as a function of the distance of the plates and obtain an oscillatory behavior of the glass transition line as a result of the structural changes related to layering. We detect a facilitation of the glass transition at half-integer values of the distance with respect to the hard-sphere diameter. In contrast, at commensurate packing particles can more easily slide along the walls and therefore the liquid phase remains favored for higher packing fractions.

[1] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, Phys. Rev. Lett. 105 125701 (2010)

Topical Talk DF 15.7 Thu 12:30 ZEU 114

Concentration fluctuations and intrinsic confinement effects in binary glass forming liquids: Insights from neutron scattering and X-ray photon correlation spectroscopy — •Thomas Blochowicz[1], Sebastian Schramm[1], Emmanuel Gouirand[1], Philipp Gutfreund[2], Bernd Stühn[1], Bernhard Frick[2], and Yuriy Chushkin[3] — [1]TU-Darmstadt, Darmstadt, Germany — [2]ILL, Grenoble, France — [3]ESRF, Grenoble, France

We investigate the dynamics in a series of binary glass forming liquids using dielectric spectroscopy (DS) in combination with quasielastic neutron scattering, dynamic light scattering and X-ray photon correlation spectroscopy (XPCS). It turns out that, although macroscopically the systems are fully miscible in the whole temperature range, two glass transitions can be clearly distinguished due to the high T_g contrast of the components. By means of DS the corresponding relaxation processes are identified, and it turns out that contrary to expectation the small molecules take part in both glass transitions, which suggests that two dynamical species can be distinguished among the small molecules. Moreover, the relaxation connected with the lower glass transition shows properties typical of dynamics in confinement like an Arrhenius-type temperature dependence and a broad distribution of relaxation times. On the other hand it is revealed by XPCS that the concentration fluctuations exhibit a significantly weaker temperature dependence than the α-relaxation and show a crossover from a diffusive to a so-called ballistic wave vector dependence and from stretched to compressed relaxation functions around the upper T_g.

DF 16: Dielectric surfaces and interfaces

Time: Thursday 14:15–16:00 Location: MÜL Elch

DF 16.1 Thu 14:15 MÜL Elch

Ferroelectric properties of TiO_2 rutile investigated by ab inito calculations — •Anna Grünebohm[1,2], Heike C. Herper[1,2], and Peter Entel[1,2] — [1]Fachbereich Physik, Universität Duisburg-Essen, Deutschland — [2]Cenide

TiO_2 rutile is an incipient ferroelectric material [1] and theoretical studies have shown that a ferroelectric transition can be triggered by a lattice expansion or a strained lattice [2]. The experimental realization of ferroelectric TiO_2 would be of great technical impact as TiO_2 is a cheap material with well optimized processing and a variety of applications like optical coating, solar cells or catalysis. Most of this applications are based on properties of the rutile (110)-surface. Therefore, the knowledge of the ferroelectric properties at this surface is the key point, which has not been addressed in literature so far.
In order to get an insight into these properties, we have performed calculations within the projector augmented wave method using VASP [3]. We present a systematic study of the ferroelectric trends in rutile for the bulk systems as well as for the rutile (110) surface and TiO_2 nanoparticles. Although, the surface reduces the ferroelectric trends we find a ferroelectric phase for strained TiO_2(110). [1] C. Lee, P. Ghosez and X. Gonze, Phys. Rev. B **50**, 13379 (1994) [2] B. Montanari and N. M. Harrison, J. Phys. Condens. Matter **16**, 273 (2004) [3] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996)

DF 16.2 Thu 14:35 MÜL Elch

Polarisationsabhängige H_2O-Adsorption auf $LiNbO_3$ (0001) — •Rebecca Hölscher, Simone Sanna und Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn

Die Polarisation von ferroelektrischen Oxidoberflächen kann kontrolliert werden, um die Oberflächenreaktivität für gewisse Anwendungen gezielt anzupassen. Dieses „domain engineering“ ermöglicht die Realisierung von molekularen Detektoren und anderen Bauteilen auf Nanoebene. Hier werden ab initio Rechnungen vorgestellt, die den Effekt der Polarisation auf die Adsorption von H_2O-Molekülen auf der (0001) Oberfläche von $LiNbO_3$ (LN) untersuchen. Die Adsorption wird mittels Dichtefunktionalrechnungen innerhalb der generalisierten Gradienten Approximation (GGA) modelliert, da dies realistische Strukturen und Energien für das LN Volumensmaterial und dessen Oberflächen ergibt[1]. Die Adsorptionsenergie und -geometrie sowie die Oberflächenbedeckung auf der positiven und negativen (0001) Oberfläche werden bestimmt. Analog zu den Ergebnissen von TPD (temperature programmed desorption) Messungen[2], wird hier eine polarisationsabhängige Adsorption gezeigt (ebenso bei 2-Propanol auf LN[3]). Zudem zeigt sich, dass keine Adsorptionsbarriere vorliegt, im Sinne einer Physisoption und keine Dissoziation des Moleküls bei niedriger Bedeckung stattfindet.

*[1] W. G. Schmidt, M. Albrecht et al., Phys. Rev. B **77** (2008), 035106. [2] J.Garra, J.M. Vohs, D.A. Bonnel, Surf. Sci. **603** (2009) 1106. [3] Y. Yun, L. Kampschulte et al., J. Phys. Chem. C **111** (2007) 13951.*

DF 16.3 Thu 14:55 MÜL Elch

UV-induced domain wall conductivity at room temperature in Mg-doped lithium niobate single crystals — •Mathias Schröder, Alexander Haussmann, and Lukas M. Eng — Institute of Applied Photophysics, Technische Universität Dresden, D-01062 Dresden, Germany

Ferroelectric 180° domain walls (DWs) may play an important role in future electronic devices. The size and position of domains and DWs can be easily controlled. In addition, DWs in lithium niobate (LiNbO3: LNO) can be functionalized through depositing metallic and/or molecular nanowires by means of ferroelectric lithography [1,2]. Moreover, the same DWs become conductive under super-bandgap illumination, hence manifesting switchable, tunable, and nanoscale conductive channels that extend across the whole insulating bulk material. However, a detailed understanding of the underlying processes that lead to DW conductivity is still missing to date. Here, we report on conductive-AFM (c-AFM) measurements on 5 mol% Mg-doped congruent LNO single crystals. We compare the c-AFM results with the domain distribution recorded by piezoresponse force microscopy (PFM). Surprisingly, we find an enhanced current flow inside the 180° DWs under super-bandgap UV-illumination even at ambient conditions. The DW conductivity was studied as a function of wavelength, light intensity and doping concentration. Our results suggest a hopping transport being relevant for the reported DW conductivity.

[1] S.V. Kalinin, et al., Nano Lett. 2, 589 (2002).
[2] A. Haussmann et al., Nano Lett. 9, 763 (2009).

DF 16.4 Thu 15:15 MÜL Elch

Investigating electronic defects in strontium titanate by surface photovoltage analysis — •Elke Beyreuther, Jana Becherer, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

The energy distribution of electronic defect states within the bandgap of oxygen-reduced n-type strontium titanate has been analyzed by means of wavelength-dependent surface photovoltage (SPV) measurements using a Kelvin probe set-up. As a further result, the parameters of several surface states, i.e. the trap state density and the thermal and optical cross sections, were extracted from SPV transients.

Finally, the appropriateness of the method as a general tool for electrical characterization of complex oxide surfaces is illustrated by applying the SPV technique to comparable oxide crystals such as undoped $SrTiO_3$, Nb-doped $SrTiO_3$, or $BaTiO_3$.

DF 16.5 Thu 15:35 MÜL Elch

Defektanalyse in SiO_2-Schichten mit Hilfe der Positronen-Lebensdauer-Impuls-Korrelation — •Benjamin Löwe[1], Werner Egger[1], Andreas Bergmaier[1], Gottfried Kögel[1], Luca Ravelli[1], Peter Sperr[1], Christoph Hugenschmidt[2,3] und Günther Dollinger[1] — [1]LRT2, Universität der Bundeswehr, Neubiberg, Deutschland — [2]ZWE FRM II, TU München, Deutschland — [3]Physik-Department E21, TU München, Deutschland

Aus Positronenlebensdauermessungen in Festkörpern kann auf Art und Konzentration von leerstellenartigen Defekten geschlossen werden. Messungen der Energie der Annihilationsquanten, die bei der Vernichtung von Positronen mit Elektronen im Festkörper entstehen, lassen Rückschlüsse auf die chemische Umgebung der Defekte zu.

Korrelierte Messungen der Positronenlebensdauer und der Energie der Annihilationsquanten, die vom selben Annihilationsereignis stammen (AMOC = Age Momentum Correlation) liefern ein detailreicheres Bild der Defektsituation als die unkorrelierte Messung von Lebensdau-

er und Energie.

Mit Hilfe des gepulsten Positronenstrahlsystem PLEPS am FRM II wurden AMOC-Messungen an SiO_2-Schichten durchgeführt. Die Positronen wurden bei einer Energie von 2 keV in 100 nm dicke, unterschiedlich hergestellte SiO_2-Schichten implantiert. Aus den gemessenen AMOC-Spektren können verschiedene Schnitte extrahiert werden. Anhand des S(t)-Plots, der die Breite der Annihilationslinie als Funktion der Lebensdauer darstellt, lässt sich z.B. die Positroniumsbildung in unterschiedlich aufgetragenen SiO_2-Schichten vergleichen.

5 min. break

DF 17: Crystallography in Materials Science (Joint Session of KR, DF)

Time: Thursday 14:00–16:45 Location: HSZ 101

Invited Talk DF 17.1 Thu 14:00 HSZ 101

Crystallography of Nanowires — •Julian Stangl[1], Dominik Kriegner[1], Christian Panse[2], Bernhard Mandl[1,3], Kimberley A Dick[3], Mario Keplinger[1], Johan M Persson[4], Philippe Caroff[3,5], Daniele Ercolani[6], Lucia Sorba[6], Friedhelm Bechstedt[2], and Günther Bauer[1] — [1]Johannes Kepler University Linz, Austria — [2]Friedrich-Schiller-Universität Jena, Germany — [3]Lund University, Sweden — [4]Technical University of Denmark — [5]IEMN, UMR CNRS, France — [6]Scuola Normale Superiore Pisa, Italy

Semiconductor nanowires are interesting not only from physical and technological viewpoints, but also in a crystallographic sense. While most III-V semiconductors, except nitrides, crystallize exclusively in the cubic zinc-blende lattice in bulk or epitaxial layers, in nanowires very often hexagonal modifications such as wurtzite, but also the more complex 4H structure are observed. The wires grow mainly along the cubic <111> directions, where those lattice structures on first sight differ only by the stacking sequence of bilayers, changing from fcc to hcp. Detailed x-ray diffraction investigations for InAs and InSb nanowires reveal, however, that beside the stacking sequence also the atomic distances change, so that the unit cells deform compared what would be expected from a simple change of stacking. Comparisons to density functional theory calculations are in excellent agreement with the experimental data, and the combination of x-ray diffraction and theoretical calculations allow explaining the reason for the observed changes in atomic distances.

DF 17.2 Thu 14:45 HSZ 101

The Crystal structure of InAs nanorods grown onto Si[111] substrate — •Anton Davydok[1], Andreas Biermanns[1], Steffen Breuer[2], Manos Dimakis[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Festkörperphysik, Universität Siegen, Walter-Flex-Str. 3,57072, Siegen, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7,10117 Berlin, Germany

Nanowires are of particular interest due to the ability to synthesize heterostructures in the nanometer range. It was found that nearly any AIIIBV semiconductor material can be grown as NWs onto another AIIIBV or group IV [111] substrate independent from lattice mismatch. We presented an X-ray characterization of InAs NRs on Si [111] grown by assist free MBE method. Lattice mismatch of this materials is 11%. For study of strain realizing we concentrated our research on initial stages of growth process investigating samples set with different growth time. Using synchrotron radiation we have performed experiments in symmetrical and asymmetrical out-of plane scattering geometry and grazing-incidence diffraction. Combining the results we were able to characterize the transition between silicon silicon substrate and InAs NWs. We find in-plane lattice mismatch of -0.18% close to the interface compared to InAs bulk material. With help of microfocus setup we are able measure structural paramters of single NWs to determine the strain accomodation as function of NW size. In particular using asymmetric wurzite-sensitive reflections under coherent beam illumination we could quantify the number of stacking faults. In the talk we present details of the analysis and first simulation results.

DF 17.3 Thu 15:00 HSZ 101

X-ray characterization of Au-free grown GaAs nanowires on Si — •Andreas Biermanns[1], Steffen Breuer[2], Anton Davydok[1], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Semiconductor nanowires (NW) are of particular interest due to the ability to synthesize single-crystalline 1D epitaxial structures and heterostructures in the nanometer range. However, many details of the growth mechanism are not well understood. In this contribution we present a x-ray diffraction study of the early stage of Au-free GaAs nanowire growth on Si(111)-substrates with native oxide using the nano-focus setup available at the ID1 beamline of ESRF. The GaAs NWs were grown by molecular beam epitaxy (MBE), and their formation was induced by Ga droplets. Using a nanometer-sized x-ray beam, size and lattice parameters of individual wires were measured separately. Using asymmetric x-ray diffraction on particular zinc-blende (ZB) and wurtzite (W) sensitive reflections, we show that under the used conditions the NW growth starts with predominantly WZ phases and continues mainly in ZB phase. In addition we can show that the WZ segments of the NWs exhibit a different vertical lattice parameter compared to the zinc-blende segments. A combination of x-ray diffraction from single wires and grazing incidence diffraction shows that the base of the NW is compressively strained along the inplane direction. This strain is released within 20nm from the substrate-interface.

15 min. break

Invited Talk DF 17.4 Thu 15:30 HSZ 101

New Grounds in Materials Science: Complex Metallic Alloys — •Michael Feuerbacher — Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany.

Complex metallic alloys (CMAs) represent a class of materials increasingly receiving scientific attention. These materials possess characteristic structural features substantially deviating from those of simple metals. They have large lattice constants and, correspondingly, a high number of atoms per unit cell, ranging from some ten to some thousands. Their local order is dominated by icosahedral-symmetric atom coordination in the form of concentric cluster shells. These characteristic structural features are at the origin of novel physical properties.

Due to the crucial structure-property relations, transmission electron microscopy is an inevitable tool for the understanding of the physical properties of CMAs. We will present structural characterizations of various CMA materials by state-of-the-art techniques, such as aberration-corrected transmission electron microscopy and high-angle annular dark field scanning transmission electron microscopy. We will review recent experimental investigations of the physical properties of CMAs, and discuss these in the light of the particular cluster substructure. Basic scientific phenomena will be addressed, such as novel structural defects and deformation mechanisms, as well as application related issues, for example the use of CMAs as catalysts, as thermoelectric materials, and for digital data storage.

DF 17.5 Thu 16:15 HSZ 101

Local electronic structure of Ruddlesden-Popper films - a combined DFT and ELNES study — Thomas Riedl[1,2], Thomas Gemming[2], Torsten Weissbach[3,4], Gotthard Seifert[4], Emanuel Gutmann[5], Matthias Zschornak[6,7], Dirk C. Meyer[5,6], and •Sibylle Gemming[7] — [1]Werkstoffwissenschaft, TU Dresden, D-01062 Dresden — [2]IFW Dresden, PF 270116, D-01171 Dresden — [3]Theo. Physik, TU-BA Freiberg, D-09596 Freiberg — [4]Phys. Chemie, TU Dresden, D-01062 Dresden — [5]Strukturphysik, TU Dresden, D-01062 Dresden — [6]Exp. Physik, TU BA Freiberg, D-09596 Freiberg — [7]HZ Dresden-Rossendorf, PF 510119, D-01314 Dresden

Ternary oxides with the composition $AO(ABO_3)_n$, the Ruddlesden-Popper (RP) phases, and derived quaternary phases are versatile materials with complex structure-property relationships; due to their unusual conductivity properties such RP phases have attracted recent interest as materials for solid-oxide fuel cells or as thermoelectric. The present study focuses on the parent phases with A = Sr and B = Ti. Electron energy-loss near-edge fine structures of the $SrO(SrTiO_3)_{n=1}$ Ruddlesden-Popper system and of the reference compounds $SrTiO_3$ and SrO are analyzed by comparison with calculations. The fine struc-

tures of sol-gel-grown RP films have been experimentally recorded. All-electron density-functional calculations indicate that the appearance and shape of the experimental O-K and Ti-$L_{2,3}$ fine structure features result from the crystallography-dependent electronic structure of the investigated oxides, which - already without further modification - display technologically interesting dielectric and lattice properties.

DF 17.6 Thu 16:30 HSZ 101

Modeling the environment-controlled morphology changes of adsorbed two-component nanoparticles — •Sibylle Gemming[1], Gintautas Abrasonis[1], and Matthias Krause[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, PF 510119, D-01314 Dresden, Germany. — [2]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany.

The morphology and the local composition of binary nano-particles from two immiscible components are driven by the local interactions at the different interfaces within the material system. Especially in small nano-particles, atoms at interfaces cover a large part of the total amount of atoms. Therefore, the interface energetics crucially influences the relative stabilities of different possible atom arrangements both at the surface of the particles and at the interface with the support. Such a complex system can be mapped to a two-component phase-field model with a set of complex boundary conditions at the interfaces of the particle with the support and with the surrounding atmosphere. Numerical simulations have been performed to describe the morphology evolution of such particles in dependence on the external physical conditions. The results rationalize recent observations on the structural changes of oxide-supported bimetallic nano-particles cycled in oxidizing and reducing atmospheres. Funding via the ECEMP project D1 (EU-EFRE) is gratefully acknowledged.

DF 18: Applications of dielectric solids

Time: Thursday 16:00–17:20 Location: MÜL Elch

DF 18.1 Thu 16:00 MÜL Elch

Nanometer thin tantalum oxide capacitors: Characterization of temperature stability and built in electric fields. — •Katrin Bruder[1], Kevin Stella[2], and Detlef Diesing[2] — [1]Heraeus Clevios GmbH, Chempark Leverkusen — [2]Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Tantalum oxide based capacitors are widely used in electronic applications. A big amount of works exists for thicker oxide films $d > 10\,\mathrm{nm}$. However, for the production of high capacitance values per area thinner oxide films $d < 10\,\mathrm{nm}$ are of significant interest since the capacitance scales with d^{-1}. We present current-voltage experiments with 2 to 5 nm thick tantalum oxide capacitors. The temperature of the devices was varied from 40 K to 500 K. To avoid degradation of the devices the experiments were carried out under ultra high vacuum conditions. Tantalum oxide capacitors were found to be stable in the mentioned temperature range. By monitoring the temperature and voltage dependence of the device current one can determine the built in electric field $E_{\mathrm{built-in}} = 0.15\mathrm{V/nm}$. Deviations from the bulk dielectric behaviour were found for the dielectric permittivity ϵ_{rel}. Thin films only show values from 8 to 12 in contrast the bulk value of 28. This finding is attributed to asymmetric dipole layers at the oxide interfaces and smeared out band edges inside the vitreous oxide film. The asymmetry of the dipole layers may also evoke the built-in electric field.

DF 18.2 Thu 16:20 MÜL Elch

Colossal Dielectric Constants in Transition-Metal Oxides — •Stephan Krohns[1,2], Peter Lunkenheimer[1], and Alois Loidl[1,2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute for Materials Resource Management, University of Augsburg, Germany

Systems showing so-called colossal effects have an enormous potential as building blocks for future correlated electronics, including capacitors for energy storage and integrated circuits. For example, in the past decade the generation and investigation of very-high ("colossal") dielectric constants (CDC) has been an active field of basic and applied research. The measurement of the dielectric response to ac electric fields is one of the most powerful techniques to provide detailed insight into the underlying physics responsible for CDCs, which may comprise very different phenomena, e.g., charge order, molecular or polaronic relaxations, hopping charge transport, ferroelectricity or density-wave formation. Most of the materials exhibiting these effects, among them numerous transition-metal oxides [1], have complex ground states emerging from strong electronic correlations. For example, charge-ordered $La_{2-x}Sr_xNiO_4$ exhibits CDCs up to gigahertz frequencies at room temperature [2]. Here, we thoroughly discuss the mechanisms that can lead to colossal values of the dielectric constant in transition-metal oxides, especially emphasising effects generated by external and internal interfaces, including electronic phase separation.

[1] P. Lunkenheimer *et al.*, Eur. Phys. J. Special Topics **180**, 61 (2010). [2] S. Krohns *et al.*, Appl. Phys. Lett. **94**, 122903 (2009).

DF 18.3 Thu 16:40 MÜL Elch

CVD Diamond for sub-mm and THz applications — •Theo Scherer, Dirk Strauss, and Andreas Meier — Karlsruhe Institute of Technology KIT ; IMF-1 Hermann-von-Helmholtz-Platz 1 D-76344 Eggenstein-Leopoldshafen, Germany

Diamond is an outstanding material with a extremely high thermal conductivity and a very low loss tangent of < 10-5 for GHz frequencies and shows therefore a very small microwave absorption. To understand the loss mechanisms at the surface and in the bulk material of diamond the determination of loss tangent in dependence of the frequency in the range of several GHz up to THz is essential. The main absorption mechanisms for ultra-low loss materials will be described and prospects will be given for advancing these materials in the THz region. A reduction of the losses at the surface can be realized by special chemical treatment and surface finishing of the CVD diamond disk material. Resonator measurements and experimental setups for the GHz- and the THz-range will be discussed.

DF 18.4 Thu 17:00 MÜL Elch

Glass-ceramics with paraelectric phases for mobile applications in the GHz-range — •Hubertus Braun[1,2], Martin Letz[1], and Gerhard Jakob[2] — [1]Schott AG, Hattenbergstraße 10 Mainz — [2]Johannes Gutenberg-Universität Mainz

In the last years, handheld devices such as global positioning systems (GPS), satellite phones and radios have required antennas that communicate directly with the satellite. The most attractive technology for this purpose is based on dielectrically loaded antennas (DLA) which utilise microwave ceramics. The advantage of the dielectric antenna technology lies mainly in the miniaturisation by $\frac{1}{\sqrt{\varepsilon_r}}$ and in the resistance to detuning ("Body Loading") by nearby objects, as for example human tissue. Selective parameters for the needed ceramics are high quality factor Qf $>$ 5000 GHz, near zero temperature coefficient of resonance frequency $|\tau_f| \leq 20$ ppm/K and permittivity $\varepsilon_r > 20$. A possible alternative to usual ceramic fabrication techniques is the use of glass-ceramic technology in which the antenna cores can be cast to net shape followed by crystallisation to achieve intrinsic pore free materials with the desired microwave properties. In the current work, promising low melting temperature dielectric glass-ceramics in the La-Ti-Si System are analysed concerning suitability for DLA applications and lower cost fabrication techniques.