DIELECTRIC MATERIALS

DIELEKTRISCHE FESTKÖRPER (DF)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture rooms MÜL Elch, KÖN Farb, P1, HSZ 04)

Invited Talks

DF 1.1	Mon	09:30	(MÜL Elch)	**Barium Strontium Titanate Thin Film for RF Applications**, Ulrich Böttger
DF 2.1	Mon	14:30	(MÜL Elch)	**Size effects in ferroelectric nanostructures**, Andreas Rüdiger
DF 4.1	Tue	09:30	(KÖN Farb)	**Piezoelectric composite materials for smart structures applications** , Andreas Schönecker
DF 5.1	Tue	09:30	(MÜL Elch)	**Towards a Statistical Mechanics for Network Glasses**, Reimer Kühn, Jort M. van Mourik, Martin Weigt, Annette Zippelius
DF 8.1	Wed	14:30	(MÜL Elch)	**Phonons in multiferroics: BiFeO3 and related systems**, Jens Kreisel, Raphaël Haumont, Pierre Bouvier, Françoise Hippert
DF 9.1	Thu	09:30	(MÜL Elch)	**Driving a macroscopic state switching into materials with a laser pulse and probing atoms moving in real time with a X-ray pulse**, CAILLEAU Herve, COLLET Eric, BURON Marylise, LEMEE-CAILLEAU Marie-Helene, KOSHIHARA Shin-ya
DF 9.2	Thu	10:10	(MÜL Elch)	**Structural instabilities in Ferroelectric Aurivillius compounds**, J. Manuel PEREZ-MATO
DF 10.1	Thu	14:30	(MÜL Elch)	**Broadband Dielectric Spectroscopy in Functional Transition-Metal Compounds**, Joachim Hemberger, Peter Lunkenheimer, Robert Fichtl, Stefan Weber, Torsten Rudolf, Franz Mayer, Andrei Pimenov, Vladimir Tsurkan, Alois Loidl
DF 11.1	Fri	10:50	(MÜL Elch)	**Universal domain wall dynamics in ferroics and relaxors**, Wolfgang Kleemann

Sessions

DF 1	**Internal Symposium "Integrated Electroceramic Functional Structures"**	Mon 09:30–13:10	MÜL Elch	DF 1.1–1.10
DF 2	**Dielectric and Ferroelectric Thin Films and Nanostructures I**	Mon 14:30–17:30	MÜL Elch	DF 2.1–2.8
DF 3	**Poster Session**	Mon 09:30–17:00	P1	DF 3.1–3.29
DF 4	**Internal Symposium "Ferroelectric Materials for Smart Structures"**	Tue 09:30–12:50	KÖN Farb	DF 4.1–4.9
DF 5	**Glass I (together with division 'Dynamics and Statistical Physics' [DY])**	Tue 09:30–12:10	MÜL Elch	DF 5.1–5.7
DF 6	**Glass II (together with division 'Dynamics and Statistical Physics' [DY])**	Tue 14:30–16:10	MÜL Elch	DF 6.1–6.5

DF 7	**Dielectric and Ferroelectric Thin Films and Nanostructures II**	Wed	14:30–16:50	KÖN Farb	DF 7.1–7.7
DF 8	**Spectroscopy, Scanning and Diffraction Methods**	Wed	14:30–16:50	MÜL Elch	DF 8.1–8.6
DF 9	**Phase Transitions**	Thu	09:30–12:30	MÜL Elch	DF 9.1–9.7
DF 10	**Electric, Electromechanical and Optical Properties I**	Thu	14:30–18:10	MÜL Elch	DF 10.1–10.10
DF 11	**Electric, Electromechanical and Optical Properties II**	Fri	10:50–13:10	MÜL Elch	DF 11.1–11.6
SYMM	**Symposium "Multiferroic Materials"**	Tue	14:30–17:30	HSZ 04	

Annual General Meeting of the Section Dielectric Materials

Wed 17:30–18:30 MÜL Elch

(For members only)
Tagesordnung

1. Zur Arbeit des Fachverbandes
2. Vorbereitung der 71. Jahrestagung der DPG
3. Verschiedenes

Sessions

– Invited, Contributed Talks and Posters –

DF 1 Internal Symposium "Integrated Electroceramic Functional Structures"

Time: Monday 09:30–13:10 Room: MÜL Elch

Invited Talk DF 1.1 Mon 09:30 MÜL Elch

Barium Strontium Titanate Thin Film for RF Applications — •Ulrich Böttger — RWTH Aachen, Insititut für Werkstoffe der Elektrotechnik II, Sommerfeldstr. 24, 52074 Aachen

Ferroelectric thin films are being intensively studied for wireless communication applications in voltage tunable RF and microwave devices. Tunable circuits like phase shifters, filters or matching networks offer the flexibility to adapt to changes in operating conditions, such as frequency, impedance environment or RF drive level. Key issues for the use of ferroelectric materials in such devices are high tunability, low dielectric losses, temperature stability and reliability, even with respect to alternative technologies based on semiconductor varactor diodes or MEMS (micro electro-mechanical systems). Much emphasis has been placed on thin film ferroelectric material barium strontium titanate, $Ba_{1-x}Sr_xTiO_3$ because of its promising high-frequency dielectric properties and its ability to device integration.

This talk reviews the properties of thin film $Ba_{1-x}Sr_xTiO_3$ and discuss the potential physical models of the origin of the tunability and of the correlated losses. Further, basic tunable devices are presented. Simulation results and measurements from such circuits are also given.

DF 1.2 Mon 10:10 MÜL Elch

Electronic structures and mechanical stabilities of coherent and semi-coherent perovskite interfaces from first-principles — •Christian Elsässer[1], Jan-Michael Albina[1], Matous Mrovec[1], and Bernd Meyer[2] — [1]Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany — [2]Ruhr-Universität Bochum, Bochum, Germany

Electroceramic thin-film heterostructures made of perovskite-type metal oxides are promising as alternatives to silicon-based components in microelectronics. The function and stability of such thin-film components are determined by the structure and chemistry of the few nm thin films and their contacts to substrates or electrodes. For the predictive development of electroceramic devices with desired functions, e.g., for dielectric or ferroelectric data storage, useful microscopic information about interfacial electronic structures and mechanical stabilities can be obtained from first-principles density functional theory. Calculations using the mixed-basis pseudopotential method were carried out for electronic energy barriers and mechanical separation energies of (001)-oriented interface models with $SrTiO_3$ in contact to three different perovskites: coherent $SrTiO_3/LaAlO_3$ with $LaAlO_3$ as an insulating substrate, coherent $SrTiO_3/SrRuO_3$ with $SrRuO_3$ as a conducting electrode, and semi-coherent $SrTiO_3/SrZrO_3$. For the latter system, with interfacial mismatch of 6%, a semi-coherent interface model with localized misfit dislocations separated by coherent regions was employed to estimate the influence of dislocation cores on electronic energy barriers and on mechanical separation energies.

DF 1.3 Mon 10:30 MÜL Elch

Multifunctional materials on the basis of oxidic thin films — •Matthias Opel[1], Karl-Wilhelm Nielsen[1], Stephan Geprägs[1], Sebastian T.B. Goennenwein[1], Rudolf Gross[1], Wentao Yu[2], Jürgen Simon[2], and Werner Mader[2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Str. 8, 85748 Garching — [2]Institut für Anorganische Chemie, Universität Bonn, Römerstr. 164, 53117 Bonn

Transition metal oxides can show very different properties, e.g. superconductivity, semiconductivity, ferromagnetism, and/or ferroelectricity. Due to the enormous progress in thin film deposition technology, these properties can be integrated in oxidic heterostructures, resulting in novel functionalities.

In this contribution, we discuss the state of the art in pulsed laser deposition for the growth of thin oxide films. Taking ferromagnetic materials such as $Zn_{1-x}Co_xO$, Sr_2CrWO_6, Fe_3O_4, and $BiMO_3$ (M = Fe, Cr) as an example, we report on the influence of strain and crystal orientation on the magnetic properties. We furthermore address multifunctional heterostructures consisting of ferromagnet/semiconductor multilayers, as well as the possibility to realize (multiferroic) ferromagnetic/ferroelectric multilayers. High-resolution transmission electron microscopy and electron energy loss spectroscopy give important insight into the role of defects and inhomogeneities in the layers and at the interfaces.

DF 1.4 Mon 10:50 MÜL Elch

Inorganic and organic layers for high-k and organic memory applications — •Karsten Henkel, Mohmaed Torche, Carola Schwiertz, Ioanna Paloumpa, Rakesh Sohal, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, 03013 Cottbus, P.O. Box 101344, Germany

We report about organic and inorganic MIS stacks for new possibilities for high frequency and high power applications as well as for non volatile memory cell. The organic stack contains a ferroelectric polymer as the functional layer.

Poly[vinylidene fluoride trifluoroethylene] (P[VDF/TrFE]) is spin coated from a solution onto oxidised silicon substrates. We report on the polarisation induced flatband voltage shifts.

For the inorganic stack our attempt is to combine higk-k dielectrics with high band gap semiconductors (SiC). Praseodymium oxide layers are prepared by electron beam evaporation from Pr_6O_{11} powder and in situ controlling of interface and volume composition (XPS). Praseodymium silicate layers were prepared either by metal evaporation onto a thin oxide on top of the semiconductor and following annealing steps or by a wet chemical process out of aqueous $Pr(NO_3)_3$ solutions. Using spectroscopic characterisation we investigate the stability of the various interfaces within the stacks as well as the reactivity of the metal electrodes on thin Pr_2O_3. We report the results of electrical characterisation consisting of permittivity values, leakage current and density of interface states.

DF 1.5 Mon 11:10 MÜL Elch

Resistive Switching in Pt/TiO2/Pt Thin Film Capacitors for Non-volatile Memory Applications. — •Doo Seok Jeong and Herbert Schroeder — IEM / IFF and CNI, Forschungszentrum Jülich GmbH, Germany.

Non-volatile memory (NVM) devices such as switchable resistors (ReRAM) are discussed for future ultra-large scale-integrated memory chips in cross-bar architecture because of their simple geometry. Among the large variety of candidates under discussion are ferroelectric and paraelectric oxides. We have produced metal/insulator/metal (MIM) capacitor structure with sputtered TiO2 thin films between platinum electrodes showing resistive memory switching. The DC electrical properties were measured in dependence of applied voltage or current, temperature and sample geometry. The main results are: a) All produced titanium oxide films are insulating and amorphous with stoichiometry close to TiO2. b) The films had to be electroformed at 5 to 8 V to show resistive switching. A current compliance between 1 and 10 mA had to be applied to induce the electroforming successfully, but not to degrade the film completely (permanent dielectric breakdown). c) The *Reset* voltage to the higher resistance state (*Off*-state) was 0.7 +/- 0.1 V. The resistance ratio between *On*- and *Off*-state was of the order of 1000. The set voltage for inducing the *On*-state again showed larger variations, 1.5 +/- 0.25 V, with a similar current compliance. The results will be discussed in the light of common mechanisms for resistive switching.

DF 1.6 Mon 11:30 MÜL Elch

Correlations between Microstructural Changes and Resistive Switching: An Approach by In-situ TEM Investigations — •Herbert Schroeder and Doo Seok Jeong — IEM / IFF and CNI, Forschungszentrum Jülich GmbH, Germany.

Among the material candidates for resistive non-volatile memories are functional oxides, e.g. ferroelectric and paraelectric oxide thin films. There are numerous experimental (leakage) current data published for each material class demonstrating the switchable memory effect but there is no agreement on the working mechanism. To a large extent this is due to the lack of microstructural information on the changes during formation and switching of the devices. If these effects are connected with microstructural changes these may be observable in a transmission electron microscope (TEM). Therefore, in this contribution we present a rather seldom used approach for a TEM experiment to observe the microstructure of a metal/insulator/metal (MIM) capacitor structure before and after (ex-situ) as well as during (in-situ) resistive switching due to an applied external voltage or current. We use a special TEM sample holder allowing controlled application of temperature (RT to 300°C) with a heating stage and of voltage (current) as a part of a 4-point resistance measurement set-up for ex- and in-situ experiments. This is combined with a special TEM sample preparation method, the so-called window-technique. Special electrode configurations have been designed to allow nearly undisturbed TEM observation of the switching insulator. Examples for first observations in a (Pt/amorphous TiO2 thin film/Pt) stack on the resistive switching will be presented.

DF 1.7 Mon 11:50 MÜL Elch

Domain structure of ferroelectric nanograins by piezoelectric force microscopy — •Serge Röhrig[1], Frank Peter[1], Andreas Rüdiger[1], Sven Clemens[2], Theo Schneller[2], and Rainer Waser[1,2] — [1]Center of Nanoelectronic Systems for Information Technology, Research Center Jülich, 52425 Jülich, Germany — [2]Institut für Werkstoffe der Elektrontechnik 2, RWTH Aachen, Sommerfeld Str. 24, 52074

Piezoelectric force microscopy in vertical and lateral operation has made tremendous progress in the characterization of ferroelectric nanostructures. We discuss some of our latest findings in laterally confined ferroelectrics of $BaTiO_3$ on $SrRuO_3$ and $PbTiO_3$ on Pt. Special attention is devoted to the sample-tip interaction as lateral PFM picks up signals that are prohibited by symmetry in an otherwise ideal c-axis oriented system. Lead titanate nanograins are fabricated by chemical solution deposition and post-treated by chemical mechanical polishing to modify their size distribution. Their ferroelectric functionality is proven by inversion of the piezoelectric tensor. We give an outlook to an upcoming new technique of tip-enhanced Raman spectroscopy on ferroelectric nanoislands and discuss some key issues like heat dissipation and the detection of soft-modes.

DF 1.8 Mon 12:10 MÜL Elch

Polarisation-induced Functionality at Ferroelectric Surfaces — •Sibylle Gemming, Walter Alsheimer, Regina Ermrich, and Gotthard Seifert — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden.

Density-functional investigations on titanate-based ceramics have confirmed that the rich defect chemistry of these materials strongly influences the structural, electronic, and elastic properties of the bulk phases and at surfaces. Strong structural relaxations at stepped titanate (10n) surfaces were obtained, which can compete with the ferroelectric distortion. The electronic structure does not differ quantitatively from the bulk properties, and no edge-specific states inside the band gap of the bulk compound are induced. On the other hand, the electric field above a stepped surface differs from the one above a planar surface at distances, which are typical in adsorbate-substrate systems. Thus, the prereqisites for a polarisation-driven self-organisation of field-sensitive molecules on polar surfaces are given. A screening of several molecule classes revealed the thiophene series as promising candidates.

DF 1.9 Mon 12:30 MÜL Elch

Optical waveguides in single-crystalline LiNbO3 films — •Carsten Dubs[1,2], Andreas Lorenz[1,2], Matthias Will[2], Jens-Peter Ruske[2,3], and Andreas Tünnermann[2] — [1]INNOVENT e.V., Prüssingstr. 27B, D-07745 Jena — [2]Institut für Angewandte Physik, Friedrich-Schiller-Universität, Max-Wien Platz 1, D-07743 Jena — [3]Guided Color Technologies GmbH, Göschwitzer Str. 25, D-07745 Jena

Lithium Niobate (LiNbO3) is one of the most extensively used dielectric material for optical waveguides at telecommunication wavelengths around 1.5 mm. Commonly LiNbO3 integrated optical devices for optical switches, modulators, second harmonic generation devices were fabricated by a combination of microfabrication techniques and metal diffusion (e.g. Ti) or ion-exchange (H+-ions) processes. Because of the considerably light-induced refractive index changes in the visible as well as at high power densities in the near-infrared spectral range only (damage-resistant) substituted LiNbO3 materials of reproducible high quality are usable for optical components exhibiting a well-defined performance. We prepared planar waveguides based on epitaxially grown zinc-substituted LiNbO3 by liquid phase epitaxy technology. We will report about film properties like surface morphology, crystalline perfection, homogeneity as well as about optical properties of the so obtained planar waveguides. Beside investigation of the film microstructure and waveguide properties results of ridge waveguide fabrication for the visible wavelength range and for application at high power densities will be reported. *

DF 1.10 Mon 12:50 MÜL Elch

Simulation of electronic transport in nanoscale ferroelectric tunnel junctions — •Klaus Michael Indlekofer[1] and Hermann Kohlstedt[2] — [1]Institute of Thin Films and Interfaces (ISG-1) and Center of Nanoelectronic Systems for Information Technology (CNI), Research Centre Jülich GmbH, D-52425 Jülich, Germany — [2]Institute for Solid State Research (IFF) and Center of Nanoelectronic Systems for Information Technology (CNI), Research Centre Jülich GmbH, D-52425 Jülich, Germany

The usage of nanoscale ferroelectric films as tunnel barriers in electronic devices offers a unique possibility to study the physics of ultra-thin ferroelectric materials by means of electronic transport. By use of a nonequilibrium Green's function approach in combination with a self-consistent Hartree potential we have simulated the current-voltage characteristics of a metal-ferroelectric-metal tunnel junction. Such an approach offers a consistent treatment of quantum interference und tunnel effects under the influence of ferroelectric polarization charges.

In this presentation, we discuss the role of quantum effects (such as Friedel oscillations) and depletion regions, which lead to deviations from the conventional semiclassical description of contacts in such a tunneling structure. In the simulated I-V characteristics we observe a well-pronounced bistable resistive switching effect, depending on the polarization state of the ferroelectric tunnel barrier. Ferroelectric tunnel junctions in general might be a first step into a new class of application-relevant tunnel systems. [1]

[1] K. M. Indlekofer and H. Kohlstedt, Europhys. Lett. 72, 282 (2005)

DF 2 Dielectric and Ferroelectric Thin Films and Nanostructures I

Time: Monday 14:30–17:30 Room: MÜL Elch

Invited Talk DF 2.1 Mon 14:30 MÜL Elch

Size effects in ferroelectric nanostructures — •Andreas Rüdiger — Center of Nanoelectronic Systems for Information Technology, Institute of Solid State Research, Research Center Jülich, 52425 Jülich, Germany

Ferroelectrics are among the most advanced candidates for non-volatile memory applications. They are also widely used in pyroelectric sensors and piezoelectric actuators. As current integration techniques are driving the dimensions towards 10nm lateral extension and only a few unit cells height, the analogy to ferromagnetism raises the question if a lower size limit also exists for ferroelectrics. Earlier studies on free particles neglected electromechanical constraints imposed by conductive substrates and rather determined a pyroelectric limit (i.e. the size-driven transition into a centrosymmetric phase). Our results of piezoelectric force microscopy on e.g. ferroelectric $BaTiO_3$ nanoislands indicate structural and functional integrity well below the critical volume of free particles. So far, there is no evidence of a size limit in ferroelectric nanoparticles

on conducting substrates. We highlight the impact of the aforementioned electromechanical boundary conditions on ferroelectricity and discuss composition and time-scale as possible origins of a critical size below 10 nm.

DF 2.2 Mon 15:10 MÜL Elch

Towards Ferroelectric Tunnel Junctions — •Alexander Kaiser, Adrian Petraru, Ulrich Poppe, Nicholas Pertsev, Hermann Kohlstedt, and Rainer Waser — Institut für Festkörperforschung (IFF-IEM) and Center of Nanoelectronic Systems for Information Technology (CNI), Forschungszentrum Jülich, 52425 Jülich

Experimental results showed evidence that ferroelectric phase is maintained even in a few nanometers thick ferroelectric films. If such an ultra-thin ferroelectric film is placed in between two electrodes, a so-called *ferroelectric tunnel junction* (FTJ) is obtained. Recent theories predict that the direct electron tunneling current through these ultra-thin ferroelectric films may be modified by the polarization state of the ferroelectric [1]. The piezoelectric effect, interface effects and the depolarization field may lead to a giant electroresistance (GER) [2] switching effect. For studying this behaviour we deposited $SrRuO_3$ (electrode)/$BaTiO_3$ (ferroelectric)/$SrRuO_3$ on $SrTiO_3$ (001) substrates by high-pressure sputtering. The film thickness of the ferroelectric $BaTiO_3$ was varied between 200 nm and 3 nm. AFM, XRD and TEM measurements show high cristalline quality with clear epitaxial $BaTiO_3/SrRuO_3$ interfaces. P−V and C−V measurements demonstrate ferroelectricity down to $BaTiO_3$ thickness of 5 nm. Tunnel junctions were fabricated in a four point geometry and I-V characteristics were measured between 300 K and 4.2 K. The I−V curves will be discussed in the framework of the I−V characteristics predicted by theory.

[1] Kohlstedt *et al.*, Phys. Rev. B **72**, 125341 (2005)
[2] Zhuravlev *et al.*, Phys. Rev. Lett. **94**, 246802 (2005)

DF 2.3 Mon 15:30 MÜL Elch

GROWTH, MICROSTRUCTURE AND PROPERTIES OF EPITAXIAL, ANTIFERROELECTRIC $PbZrO_3$ FILMS ON $SrRuO_3$ - COVERED $SrTiO_3$ SINGLE-CRYSTAL SUBSTRATES — •Ksenia Boldyreva, Ionela Vrejoiu, Gwenael LeRhun, Lucian Pintilie, Nikolai Zakharov, Marin Alexe, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

Epitaxial, antiferroelectric $PbZrO_3$ (PZO) films have been grown by pulsed laser deposition on $SrRuO_3$-covered $SrTiO_3$ (STO) single crystal substrates. Due to its good lattice match with the STO substrate and due to the possibility to obtain atomically flat surfaces by a layer-by-layer growth mode, epitaxial $SrRuO_3$ was used as bottom electrode allowing electrical measurements. XRD analyses and TEM, HRTEM and SAED investigations revealed a (120) preferred orientation of the PZO films. Since the films were grown above the nominal antiferroelectric Curie temperature of 230°C (to let cubic PZO grow epitaxially on cubic SRO/STO), the cooling after deposition leads to the spontaneous formation of crystallographic domains during the phase transition. As shown by XRD pole figures and TEM images, there are four kinds of domains in the orthorhombic PZO film. These domains also have the character of antiferroelectric domains. The antiferroelectric properties of the films are under study by piezoresponse scanning force microscopy and by macroscopic ferroelectric measurements.

DF 2.4 Mon 15:50 MÜL Elch

GROWTH-MICROSTRUCTURE-PROPERTY RELATIONS IN EPITAXIAL FERROELECTRIC PbZr0.2Ti0.8O3 FILMS — •Ionela Vrejoiu, Gwenael Le Rhun, Lucian Pintilie, Nikolai Zakharov, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D 06120, Halle

Epitaxial PbZr0.2Ti0.8O3 (PZT) films were grown by pulsed laser deposition (PLD) onto vicinal SrTiO3 (001) (STO) single crystal substrates. Step flow-grown SrRuO3 (SRO) fabricated by PLD was employed as bottom electrode, to allow for electrical characterization of the PZT films. The atomically flat surface of the SRO layer may act as a template for layer-by-layer growth of the subsequent layers. It may thus result in very smooth and defect-free PZT layers with remnant polarization values of up to Pr= 1 C/m2. The influence of defects such as threading and misfit dislocations along with formation of 90° domains on the ferroelectric and switching properties of the films is also discussed.

DF 2.5 Mon 16:10 MÜL Elch

Nonlinear phenomena in ferroelectric thin films — •Kay Barz[1], M. Diestelhorst[1], H. Beige[1], M. Alexe[2], and D. Hesse[2] — [1]Martin Luther-Universität Halle-Wittenberg, Germany — [2]Max Planck Institute of Microstructure Physics, Germany

Ferroelectric thin films have proven to be an interesting subject to investigate into numerous nonlinear effects. Some of these effects are discussed based on experimental data from a $Bi_4Ti_3O_{12}$ Metal-Ferroelectric-Semiconductor (MFS) structure. Firstly the high frequency capacitance-voltage characteristic is compared with simple model derived from a conventional MOS (Metal-Oxide-Semiconductor) structure. From this one can conclude to the influence of interface trap density when measuring a MFS at high frequencies. Secondly the MFS structure is used as capacitor in a LCR resonance circuit. Increasing the driving voltage of the circuit shifts the resonance frequency according to the nonlinearity of the MFS. Finally the investigated specimen shows a torus doubling bifurcation. This nonlinear phenomenon is seldom observable in experiments. A comparison with the behaviour of Metal-Ferroelectric-Metal structures may clarify which of these effects originate from the ferroelectric layer or MOS-typical behavior, respectively.

DF 2.6 Mon 16:30 MÜL Elch

Influence of layer defects in ferroelectric thin films — •Thomas Michael[1], Julia Wesselinowa[2], and Steffen Trimper[1] — [1]Fachbereich Physik, Martin-Luther-Universität, Friedemann-Bach-Platz, 06108 Halle — [2]University of Sofia, Department of Physics, Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria

Based on a modified Ising model in a transverse field we demonstrate that defect layers in ferroelectric thin films, originated by layers with impurities, vacancies or dislocations, are able to induce a strong increase or decrease of the polarization. The change is affected strongly by the variation of the exchange interaction within the defect layers. The applied Greens function methods enables us to calculate the polarization, the excitation energy and the critical temperature of the material with structural defects. Moreover, we find likewise the damping of the elementary excitation. The damping is increased due to interaction. The results are in qualitatively good agreement with experimental data for ferroelectric thin films. The model can be modified to discuss the polarization of ferroelectric nanoparticles. The nanoparticle is composed of layers with spherical and cylindrical geometry.

J. M. Wesselinowa, S.Trimper, and K.Zabrocki: Impact of layer defects in ferroelectric thin films, J.Phys.: Condens. Matter 17, 4687 (2005). J.M Wesselinowa,T.Michael,S.Trimper,and K.Zabrocki: Influence of layer defects on the damping in ferroelectric thin films, Phys. Lett.A in press. T.Michael, J.M.Wesselinowa, and S.Trimper: Ferroelectric nanoparticles (in preparation)

DF 2.7 Mon 16:50 MÜL Elch

Praseodymium silicate high-k dielectric layers on Si(100) — •Grzegorz Lupina, Thomas Schroeder, Jarek Dabrowski, Christian Wenger, Anil Mane, Gunther Lippert, and Hans-Joachim Müssig — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder)

Praseodymium silicate dielectrics were investigated as potential replacement for SiO_2 gate insulator in complementary metal-oxide-semiconductor (CMOS) applications. Physical characterization by applying TEM and SR-XPS indicate that the prepared dielectrics have a bilayer structure: an SiO_2-rich Pr silicate at the interface to Si substrate and an SiO_2-poor Pr silicate on top of the dielectric stack. Photoemission studies point to a reasonably high valence and conduction band offsets of $\sim$ 3 eV and $\sim$ 2 eV, respectively. Electrical characterization of the dielectrics was accomplished by capacitance-voltage and current-voltage measurements providing insight into the interface state density, fixed charge concentration, and the dominating conduction mechanisms. Based on the results of ab-initio calculations, the most probable fixed charge formation mechanisms in Pr silicates are discussed. Thermal treatments prove that Pr silicate / Si (100) system is compatible with the conventional CMOS processing.

DF 2.8 Mon 17:10 MÜL Elch

Intrinsic tunneling in perovskite derivatives: switching of resistive states and negative differential resistance — •P. Müller[1], F. Chowdhury[1], Y. Koval[1], V. Dremov[1], F. Lichtenberg[2], and J. Mannhart[2] — [1]Physikalisches Institut III der Universität Erlangen-Nürnberg, Erwin-Rommel Str. 1, 91058 Erlangen, Germany — [2]Experimentalphysik VI der Universität Augsburg, 86135 Augsburg, Germany

In many cases, perovskite related compounds with excess of oxygen can be described as materials with alternating conducting and insulating layers. Electric transport across these layers can be considered as tunneling between the conducting layers. We investigated several materials of the family $A_nB_nO_{3n+2}$, like $LaTiO_{3.41}$ and $SrNbO_{3.41}$, which can be considered as a stacking of blocks consisting of 5 perovskite layers. We measured I-V characteristics at different temperatures. Switching between different resistive states has been found in some of these materials. The resistive states have long-term stability, which makes them interesting for memory applications. Furthermore, our materials show negative differential resistance at low temperatures. We present a summary of our recent results.

DF 3 Poster Session

Time: Monday 09:30–17:00 Room: P1

DF 3.1 Mon 09:30 P1

Domain structures, grain boundaries and PTCR effect of ferroelectric barium titanate ceramics — •Michael Roessel, Mihail Dan Croitoru, David Moser, and Oliver Eibl — Institut fuer Angewandte Physik, Eberhard Karls Universitaet Tuebingen, Auf der Morgenstelle 10, D-72076 Tuebingen, Germany

Perovskite materials such as barium titanate have many applications as electronic devices. During the cubic to tetragonal phase transition at Tc (393K) BaTiO3 exhibits a strong non-linear change of the electrical resistivity (PTCR effect) caused by grain boundaries. The PTCR effect appears in semiconducting barium titanate and is determined by the microstructure of the material. The Heywang model explains the PTCR jump by the existence of a Schottky barrier at the grain boundaries. This model assumes 180° domains, compensating space charges at the grain boundaries. Our TEM studies by diffraction contrast under two-beam and many beam diffraction conditions show irregularly arranged 90° domains. For the analysis of the grain boundaries we concentrate on grains that are close to a pseudocubic [100] orientation. So far 180° domains were not observed experimentally. Compressive stresses in curved sections of the grain boundaries yield a sub-μm domain structure. The appearance of such domain structures might be explained by compensating mechanical stresses during the cubic to tetragonal phase transition. Therefore, Heywangs model is an oversimplification and does not contain a realistic structural model for explaining the electrical resistivity of barium titanate. The goal of our work is a better understanding of the PTCR effect based on an improved grain boundary structure model.

DF 3.2 Mon 09:30 P1

Thickness dependend dielectric properties of epitaxial $Ba_{0.7}Sr_{0.3}TiO_3$ thin film capacitors — •Regina Dittmann[1], Rafael Plonka[2], Nikolay Pertsev[1], and Rainer Waser[1,2] — [1]Institut für Festkörperforschung and Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich — [2]Institut für Werkstoffe der Elektrotechnik, RWTH Aachen University of Technology, 52056 Aachen

Single-crystalline all-perovskite $SrRuO_3\backslash Ba_{0.7}Sr_{0.3}TiO_3$ (BST) $\backslash SrRuO_3$ heterostructures have been grown epitaxially on $SrTiO_3$ by pulsed laser deposition. The samples exhibit a sharp paraelectric-to-ferroelectric phase transition with a maximum permittivity of about 6660. This value is comparable to that of bulk ceramics and exceeds by several times the highest values reported for BST thin film capacitors. At room temperature, the weak decrease of the permittivity with the BST thickness decreasing from 200 to 10 nm can be explained solely by the thickness-dependent strain relaxation in epitaxial films without assuming the presence of low-permittivity layers at the film/electrode interfaces. Furthermore, the ferroelectric-to-paraelectric phase transition temperature shifts to lower temperatures with decreasing film thickness. As a result, in the low temperature regime, where all samples are in the ferroelectric state, the permittivity increases with decreasing film thickness. This effect is analyzed with the aid of a thermodynamic theory and can be attributed to the influence of the depolarizing field originating from the incomplete screening of the SRO electrodes.

DF 3.3 Mon 09:30 P1

Ferroelectric Polarization as the Gradient of Phase Shift in Electron Holography at Atomic Resolution — •Christopher Matzeck, Hannes Lichte, and Marianne Reibold — Dresden University, Inst. of Structure Physics, Zellescher Weg 16, 01069 Dresden, Germany

The transferred electron wave in Transmission Electron Microscopy is strongly influenced in phase by ferroelectric specimen. This gradient of the phase shift is directly proportional to the projected electric polarization within the sample [1]. Since Electron Holography allows measuring the phase modulation of an object wave, it is also capable of deducing the projected polarization in principle.Discovering ferroelectric dipoles in the phase images of Barium Titanate by means of Electron Holography [2] has opened quantitative characterization of single dipoles and nanodomains directly from phase images. The gradient can be determined numerically by the calculation of the differential quotient of the image data and displayed as a vector plot. This technique shows ferroelectric nanodomains in the range of only a few unit cells.

References:

[1] H. Lichte, M. Reibold, K. Vogel, M. Lehmann, Ultramicroscopy 93 (2002) 1999

[2] H. Lichte, M. Reibold, K. Vogel, M. Lehmann, D. Geiger, R. Goldberg, Proc. EMC 2004 (Vol. II), Antwerp, Belgium, 491-492

[3] The financial support from the Deutsche Forschungsgemeinschaft for the Research Group on Ferroic Functional Components FOR520 is gratefully acknowledged

DF 3.4 Mon 09:30 P1

Computer simulation of nanoporous dielectrics — •Antje Elsner[1,2], Helmut Hermann[1], and Dietrich Stoyan[2] — [1]Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institute of Stochastics, Freiberg University of Mining and Technology, D-09596 Freiberg, Germany

New dielectric materials for future semiconducting circuits are needed to compensate the increasing capacity due to decreasing dimensions of interconnects. One promising way to get dielectrics with very low k-values is to use nanoporous material. Porous dielectric materials are simulated by dense random packings assuming a nearly spherical shape of pores. The pores are approximated by spheres whereas the material is represented by the space around. By extending the algorithm to arbitrary continous diameter distributions it is possible to optimise such structures with respect to maximum porosity and adequate machanical stability. Basic parameters of the material can be calculated, such as elastic constants and estimations of k-value. Some parameters of the simulated sphere packings can be used to characterize porous media, for example contact number, local density, specific surface area and diameter distribution.

DF 3.5 Mon 09:30 P1

Theoretical investigation of fullerene-based ultralow-k dielectrics — •Yuekui Wang[1], Gotthard Seifert[1], and Helmut Hermann[2] — [1]TU Dresden, Institute for Physical Chemistry and Electrochemistry, Bergstr. 66b, D-01062 Dresden — [2]IFW Dresden, P.O.Box 27 01 16, D-01171 Dresden

It is one of the urgent problems in microelectronics to develop insulating materials with dielectric constants of less than 2 for future application in semiconducting circuits. Networks of fullerenes connected by bridge molecules are a new class of hypothetical insulating materials with very low static dielectric constant k. It is shown that it is possible to design such materials with k-values of about 1.5. The results are obtained combining total energy and structure optimization calculations.

DF 3.6 Mon 09:30 P1

Thickness dependence of specific dc-conductivity of thin-film-ion-conductors — •M. Sh. Abouzari, Frank Berkemeier, Tobias Stockhoff, and Guido Schmitz — Westfälische Wilhelms- Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str.10, 48149 Münster

Ion-conducting, amorphous thin films with a thickness of 50-1000 nm are prepared by ion beam sputtering using a glass target of composition 0.2 Li2O 0.8 B2O3. The glass layers are deposited on a silicon substrate between two sputtered electrodes of an Al-Li alloy. Temperature-dependent impedance spectroscopy allows determining the specific dc-conductivities. Recent research work has concentrated on the dependence of the conductivities on the thickness of the films. The conductivity increases significantly with decreasing of film thickness. Close to room temperature, the conductivity of 50 nm thick films exceeds that of 1000 nm thick films by at least one order of magnitude.

DF 3.7 Mon 09:30 P1

DFT investigation of stepped titanate surfaces — •Walter Alsheimer, Sibylle Gemming, and Gotthard Seifert — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden.

The structural and electronic properties of vicinal (10n) surfaces of barium titanate were investigated by density-functional band-structure calculations. A plane-wave pseudopotential technique was employed for the (10n) surfaces with $n < 5$, and systems with larger terraces were studied with a density-functional-based tight-binding method. For the small system sizes, both methods yield considerable structure changes compared with the bulk geometry. These changes are mostly confined to the step edge and the two unit cells adjacent to it, thus from n=4 on the interaction between two adjacent step edges decreases. The density of electronic states exhibits only minor changes due to the deviations from the nominal stoichiometry at the step. The electric field far above the surface follows the nominal (10n) termination plane. Close to the step edge stronger local variations of the field occur, which may influence the adsorption geometry of polar or polarisable molecules.

DF 3.8 Mon 09:30 P1

Ferroelectric properties of Langmuir-Blodgett PVDF-Copolymer films — •Raphael Tadros-Morgane and Herbert Kliem — Institute of Electrical Engineering Physics, Saarland University, D66123 Saarbruecken Campus, Germany

Langmuir-Blodgett films are designed as a stack of mono-molecular layers piled up sequentially onto a solid substrate. These layers are transferred from surface active agents trapped at the interface between two dissimilar phases, either liquid-liquid or liquid-gas [1]. However, the P(VDF-TrFE) copolymer is not well suited to this technique. Nevertheless, it is possible to realize ferroelectric thin films using this method. To reach this goal, transfers on a glass substrate were realized for a surface pressure of the interface ranging from 0.5 mN/mm to 5 mN/mm and for concentrations of the copolymer from 0.1 g/l to 0.0001 g/l. For a given number of transfers, here 30, the optimal pressure is about 3mN/mm with a concentration of 0.01 g/l. These samples show true ferroelectric properties like hysteresis loops and switching of the polarization. Films of P(VDF-TrFE) with thicknesses ranging from 2.7 nm to 64 nm prepared by a Langmuir-Blodgett technique at the Institute of Crystallography in Moscow, were electrically characterized. It is found that the coercive fields increase with decreasing sample thickness following a power law. The switching of the polarization yields stretched exponential functions with time constants t dependent on thickness and temperature. t increases with decreasing thickness and is thermally activated [2]. Also the initial polarization curves obtained from the unpolarized state are thickness and temperature dependent.

DF 3.9 Mon 09:30 P1

Optimization of sol-gel preparation and physical properties of multiferroic $BiFeO_3$ thin films — •Salah Habouti, Claus-Henning Solterbeck, Shiva Kumar Rudra, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences, Kiel, Germany

Compared to other deposition techniques, chemical solution deposited $BiFeO_3$ thin films show lower polarization values. To overcome this problem and optimize the films, influences of various parameters were investigated, like precursor solutions, annealing, temperatures and times, atmosphere etc. Their influence on crystallization, grain growth and microstructure were determined by x-ray diffractometry ($\theta - 2\theta$, grazing incidence), electron microscopy, and atomic force microscopy. The effects on the physical properties were investigated by macroscopical measurements of polarization, hysteresis, leakage current, impedance, and piezoelectric activity. Microstructural effects on local electrical properties were studied by means of electrical force microscopy. As a first success the dielectric strength was increased by a factor of 8.

Magnetic properties were measured by a vibrating sample magnetometer and by a scanning magneto-optical Kerr-effect device.

DF 3.10 Mon 09:30 P1

Interfacial properties of $Pb(Zr_{0.52}Ti_{0.48})O_3$ on $Pt(111)/Ti/SiO_2/Si$ heterostructure — •Shiva Kumar Rudra[1], Salah Habouti[1], Claus-Henning Solterbeck[1], Mohammed Es-Souni[1], Vladimir Zaporojtchenko[2], Michael Scharnberg[2], and Franz Faupel[2] — [1]Institute for Materials and Surface Technology, University of Applied Sciences, Kiel, Germany — [2]Technical Faculty, Chair of Multicomponent Materials, Christian-Albrechts-University, Kiel, Germany

$Pb(Zr_{0.52}Ti_{0.48})O_3 (PZT)$ thin films were processed by sol-gel method on $Pt(111)/Ti/SiO_2/Si$ substrate heterostructure. Interfacial composition and structure were investigated by means of X-ray photoelectron spectroscopy (XPS) in combination with depth profiling, and grazing incidence X-ray diffraction (GI-XRD). The surface roughness was measured by AFM. Ellipsometric studies as function of depth profiling are also reported. Various annealing temperatures such as 700°C, 650°C and 600°C were considered. Deposited thin films were single layered PZT with 10% Pb excess of the precursor solution. It is shown that with increasing sputtering time the refractive index increases. XPS results show that prior to sputtering there is an enrichment of Pb on the surface as well as higher Zr/(Zr+Ti) ratio in comparison to nominal composition. The AFM studies show no difference between the as processed and sputtered samples. XPS and XRD results point to the formation of a Pt_3Ti intermetallic layer at the PZT/Substrate interface.

DF 3.11 Mon 09:30 P1

CONDUCTIVITY OF NANOSTRUCTURED MESOPOROUS MCM-41 MOLECULAR SIEVE MATERIALS — •Martynas Kinka, Juras Banys, Jan Macutkevic, and Agnius Meskauskas — Faculty of Physics, Vilnius University, Sauletekio 9, 2040 Vilnius, Lithuania

Dielectric response of water confined in MCM-41 molecular sieve materials showed a power law dispersion, which was assigned to ac conductivity. This process, which occurs at temperatures close to room temperature, was found in all our investigated samples with the pore diameters ranging from 2.0 nm to 3.7 nm. Obtained values of the imaginary part of the complex dielectric permittivity were much larger than that of the bulk water. Such a phenomenon can be explained by the electrical response characteristic of the microstructural electrical network formed by water and hosting mesoporous silica material. The real part of conductivity has been calculated, and the influence of the pores size to electric conductivity and its mechanisms is discussed.

DF 3.12 Mon 09:30 P1

Phase and microstructure evolution during $BaTiO_3$ formation by solid state reactions on rutile single crystals — •Andriy Lotnyk, Stephan Senz, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

During the synthesis of $BaTiO_3$ ceramics out of a stoichiometric $BaCO_3$-TiO_2 mixture the evolution of different intermediate phases can generally be observed. These intermediate products are Ba_2TiO_4 and Ti-rich phases. Using micro chemically designed core shell powders the sequence of forming phases changes. To understand this behavior model experiments are performed using rutile (TiO_2) single crystals. The solid state reactions of TiO_2 with $BaCO_3$ (solid and vapour, respectively) are studied. A $BaCO_3$ target was electron beam evaporated in a high vacuum system with $P_{O2}=1\times10^{-2}$ Pa. The substrates were heated in a tube furnace at T=300-500°C during deposition, followed by a solid-solid reaction at 575-1100°C in vacuum or in air; for the gas-solid reaction, the substrates were heated at T=575-1100°C directly during deposition. The reaction products were investigated by XRD and TEM. The solid-solid reaction at 600°C for 30 min under vacuum produced the metastable intermediate Ba_2TiO_4 phase while the reaction in air resulted in the formation of $BaTiO_3$. Well-oriented products are formed on (110), (100), (101) TiO_2 and polycrystalline phases were identified on (001) TiO_2.

DF 3.13 Mon 09:30 P1

Investigation of Li diffusion in spinel-type structured $Li_4Ti_5O_{12}$ by means of solid state NMR and impedance spectroscopy — •M. Wilkening, W. Iwaniak, R. Amade, and P. Heitjans — Hannover University, Institute of Physical Chemistry andElectrochemistry, D-30167 Hannover

The cubic spinel oxides $Li_{1+x}Ti_{2-x}O_4$ ($0 \leq x \leq \frac{1}{3}$, space group Fd3m) are promising anode materials for lithium-ion rechargeable batteries. The end member of the Li-Ti-O series, $Li_4Ti_5O_{12}$, can accommodate Li ions up to the composition $Li_7Ti_5O_{12}$. Whereas a number of studies focus on the electrochemical behaviour of Li insertion into and Li diffusion in the Li intercalated material, only few investigations of Li dynamics in the non-intercalated host material $Li_4Ti_5O_{12}$ are reported so far. Here, the Li diffusion in pure-phase microcrystalline $Li_4Ti_5O_{12}$ with an average particle size in the μm range was probed by ^{7}Li solid state NMR spectroscopy using spin-alignment echo (SAE) and spin-lattice relaxation (SLR) measurements. Between $T = 295$ K and 400 K extremely slow Li jump rates $1/\tau$ ranging from 1 s^{-1} to 1000 s^{-1} were directly obtained by recording the decay of spin-alignment echoes at a Larmor frequency of 155 MHz as a function of mixing time and constant evolution time. $1/\tau(1/T)$ follows Arrhenius behaviour with an activation energy E_A^{SAE} of about 0.85 eV. Interestingly, E_A^{SAE} is comparable to activation energies deduced from conductivity measurements rather than from SLR-measurements, $E_A^{SLR} \approx 0.28$ eV.

DF 3.14 Mon 09:30 P1

Effect of anion substitution on Li diffusion in $Li_xTiS_{2-y}Se_y$: Solid state NMR results — •M. Wilkening[1], S. Indris[1], P. Heitjans[1], J. Wontcheu[2], W. Bensch[2], T. Bredow[3], and M. Binnewies[4] — [1]Hannover University, Institute of Physical Chemistry and Electrochemistry, D-30167Hannover — [2]University of Kiel, Institute of Inorganic Chemistry, D-24098 Kiel — [3]Hannover University,Theoretical Chemistry, D-30167 Hannover — [4]Hannover University, Institute of Inorganic Chemistry, D-30167Hannover

Li intercalated TiS_2 is known as a fast two-dimensional ionic conductor. At 298 K the diffusion coefficient D_{Li} turns out to be about 10^{-14} m^2s^{-1} and the corresponding Li residence time is of the order of 1 μs. It is of general interest to explore a possible effect of anion substitution on diffusion of small cations. The system $Li_xTiS_{2-y}Se_y$ is stable over the whole intercalation range ($0 \leq x \leq 1$) and shows a single-phase structure for all compositions. Due to these properties it represents a singularly well-defined series of materials to investigate whether Li diffusion is influenced by the substitution of selenium anions for sulfur anions having nearly the same ionic radii. Li diffusion in $Li_xTiS_{2-y}Se_y$ was studied by means of ^{7}Li solid state NMR. First lineshape analyses of data at a Larmor frequency of 78 MHz and temperatures between 140 K and 450 K indicate, that the Li mobility is slower in, e. g., $Li_{0.7}TiSSe$ than in the pure end member $Li_{0.7}TiS_2$. Supported by the DFG (SPP 1136).

DF 3.15 Mon 09:30 P1

Phonon modes of monoclinic BiB_3O_6 — •Th. Möller[1], A. Gössling[1], W.-D. Stein[1], P. Becker[2], L. Bohatý[2], and M. Grüninger[3] — [1]2nd Physical Institute, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Institute of Crystallography, University of Cologne, Zülpicher Str. 49b, 50674 Cologne, Germany — [3]2nd Physical Institute, RWTH Aachen, Huyskensweg, 52056 Aachen, Germany

The large optical nonlinearities of BiB_3O_6, a polar, non-ferroelectric crystal, open up a rich field of applications for frequency conversion of laser light via $\chi^{(2)}$ and $\chi^{(3)}$ processes, e.g. phase-matched second harmonic generation (SHG) or optical parametric oscillation (OPO) and stimulated Raman scattering (SRS). The exceptional optical nonlinearities of BiB_3O_6 have been attributed to the hyperpolarisabilities of the $[BO_3]$ structural units and the $[BiO_6]$ units with a lone electron pair. Lattice dynamics studies are required for a quantitative description of the crystal structure and are the basis for an interpretation of the nonlinear optical interaction. We present a detailed study of the phonon modes of this monoclinic compound based on polarized reflectivity measurements on single crystals. The spectra are analysed by means of a generalized Drude-Lorentz model, which allows us to resolve the modes of A and B symmetry.

DF 3.16 Mon 09:30 P1

Electronic structure and optical properties of sodium titanium diphosphate crystals — •Oleksandr Oliynyk[1], Yuriy Hizhnyi[1], Sergiy Nedilko[1], Volodymyr Bojko[2], Pavlo Nagornyi[1], and Mykola Slobodyanik[1] — [1]Kyiv National Taras Shevchenko University, 2, block 1, Hlushkova av., 03680, Kyiv, Ukraine — [2]National Agriculture University, Geroiv Oborony st., 03041, Kyiv, Ukraine

Sodium titanium diphosphate crystals $NaTiP_2O_7$ belong to the family of the complex phosphates of the alkaline and polyvalent metals. $NaTiP_2O_7$ can be considered as the base for development of new crystallophosphors. Such new materials can be designed by making the solid state solutions on the base of sodium titanium diphosphate matrixes.

Both experimental and theoretical investigations of $NaTiP_2O_7$ optical properties are carried out. Luminescence spectra are measured in 350 - 850 nm spectral region in temperature range 4.2 - 300 K. Several bands of luminescence in blue-green and orange-red region were found in the spectra. The electronic structure of $NaTiP_2O_7$ is calculated by full potential Linear Augmented Plane Wave (FLAPW) method implemented in WIEN2k program code [1]. The structures of the electronic bands, the energy dependencies of the components of dielectric tensor, reflection and absorption spectra of $NaTiP_2O_7$ are calculated. Results of the calculations are compared with experimental data and with results of the electronic structure calculations of several other complex phosphates. The origin of the $NaTiP_2O_7$ luminescence bands is discussed.

[1] P. Blaha, et. al., 2001, ISBN 3-9501031-1-2

DF 3.17 Mon 09:30 P1

Muon spin rotation studies of hydrogen-bonded ferroelectrics and antiferroelectrics — •Elvezio Morenzoni, Hubertus Luetkens, Andreas Suter, Dimitry Eshchenko, Alex Amato, Thomas Prokscha, and Robert Scheuermann — Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

We present muon spin rotation and relaxation measurements in hydrogen bonded systems of the KDP family. The positive muon and muonium behave like light proton and hydrogen isotopes and can be used to study stability and defect reactions of positive and neutral hydrogen interstitials in these ferroelectric or antiferroelectric materials, where hydrogen point defects are believed to affect the optical-absorption properties. A substantial fraction of the muons implanted into the crystals appear as neutral interstitial not reacting with the host. The hyperfine structure shows a slight axial anisotropy but is otherwise similar to that of free muonium. In the positively charged state, part of the muons form a hydrogen bond with an oxygen. In the ferroelectric KH_2PO_4 as well as in the antiferroelectric $NH_4H_2PO_4$ we observe spontaneous precession of the muon spin in the nuclear dipolar field of the proton of the O-H bond. The temperature dependence of this frequency exhibits a marked shift at the phase transition. Our results suggest that it is possible to use this and other parameters (such as the width of the local static dipolar field) as a microscopic measure of the order parameter of the phase transition. This is interesting especially for the study of proton and deuteron glasses where the order parameter characterizing the glass transition is not accompanied by a macroscopic field.

DF 3.18 Mon 09:30 P1

Effect of anion substitution on Li diffusion in $Li_xTiS_{2-y}Se_y$: Quantum-chemical calculations — •T. Bredow[1], M. Wilkening[2], S. Indris[2], P. Heitjans[2], J. Wontcheu[3], and W. Bensch[3] — [1]Hannover University, Theoretical Chemistry, D-30167 Hannover — [2]Hannover University, Institute of Physical Chemistry and Electrochemistry, D-30167 Hannover — [3]University of Kiel, Institute of Inorganic Chemistry, D-24098 Kiel

The Li intercalation of titanium chalcogenides TiS_2, TiSSe and $TiSe_2$ is investigated quantum-chemically at density functional level in combination with a crystalline orbital approach based on atom-centered basis functions. Periodic supercells are used to model the $Li_xTiS_{2-y}Se_y$ system. The electronic structure of the intercalation compounds, the electric field gradients at the Li lattice positions, and the activation barriers for elementary steps of the Li ion migration are calculated and compared to experimental results obtained by NMR spectroscopy. A strong dependence of both electric field gradient and migration barrier on the local environment of the Li ions is observed. The activation energy is similar for TiS_2 and $TiSe_2$ host systems but differs for TiSSe. Supported by the DFG (SPP 1136).

DF 3.19 Mon 09:30 P1

Fabrication and characterization of the electrical and dielectrical properties of thin insulating films for the application in superconducting devices — •Veit Grosse[1], Ralf Bechstein[1], Robert Pietzcker[1], Frank Schmidl[1], Ingo Uschmann[2], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena — [2]Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena

Thin dielectric films of strontium titanate (STO) as well as zinc oxide (ZnO) were deposited on $YBa_2Cu_3O_{7-x}$-layers on STO-substrates by Pulsed Laser Deposition. In the case of STO, X-Ray investigations showed good crystalline quality and orientation in c-direction due to the good match of the lattice parameter. First results to the epitaxial growth of ZnO will be presented. With regard to the application in superconducting devices the electrical and dielectrical properties of these films were investigated on capacitor-like structures. The time of oxygen annealing after deposition and the material of the top electrode (e.g. YBCO, Au) were varied to analyse the influence of these factors on the conduction process. We also investigated the dependence of the dielectric permittivity on temperature in the range from 300 to 4.2 K and on a electric bias field. We compare these results with measurements on amorphous insulating films (e.g. SiO_2, CeO_X) in Au/isulator/Au-systems.

DF 3.20 Mon 09:30 P1

Electrical, photoelectrical and optical properties of Ru-doped $Bi_{12}M(Si,Ti)O_{20}$ crystals — •Vera Marinova[1], S. H. Lin[2], K. Y. Hsu[2], Boriana Mihailova[1], and Ulrich Bismayer[1] — [1]Universität Hamburg, Mineralogisch-Petrographisches Institut, Grindelallee 48, D-20146 Hamburg — [2]Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu 30050, Taiwan

$Bi_{12}TiO_{20}$ (BTO) and $Bi_{12}SiO_{20}$ (BSO) sillenite-type crystals doped with different concentration of ruthenium are grown using the Top Seeded Solution Growth method (TSSG) and by the Czochralski technique, respectively. The addition of ruthenium shifts the optical absorption to the red and to the near IR spectral range for BSO and BTO, respectively. It is found that the relaxation (dark decay) of the light induced absorption consists of fast (transient) and a slow (persistent) component, suggesting participation of shallow levels in a charge-transport mechanism. The dark conductivity follows the Arrhenius law. The Ru-doped BSO crystal shows very fast response time during holographic recording at 633 nm and 647 nm. The Ru-doped BTO possesses infrared sensitivity and photorefractive gratings are successfully recorded at 790 nm and 825 nm.

DF 3.21 Mon 09:30 P1

Thermal motion induced resonant *forbidden* reflections in Ge and ZnO — •Alexey Oreshko[1], Vladimir Dmitrienko[2], and Elena Ovchinnikova[1] — [1]M.V.Lomonosov Moscow State University, Physical Department, Moscow, Russia, 119992 — [2]V.A.Shubnikov Institute of Crystallography RAS, Moscow, Russia, 119333

In this report we discuss thermal-motion-induced (TMI) *forbidden* reflections. Atomic displacements can change the symmetry of an atomic site, and thus induce an additional anisotropy of the atomic scattering factor near an absorption edge and therefore give rise to Bragg reflections, otherwise forbidden. Since TMI scattering arises from the relative displacement of adjacent atoms, its strength depends crucially on the thermal population of optical phonons modes. The search for suitable materials in which to study this effect is therefore governed by the requirements for: (1) a suitable space group; (2) site symmetry; (3) an absorption edge resonance at a wave-length suitable for crystal diffraction; (4) a low-lying optical phonon mode; (5) a high quality single crystal sample. Ge, which crystallizes with the diamond structure, and w-ZnO, which crystallizes with the Wurtzite structure, satisfy the above conditions. Strongly temperature dependent TMI reflections were recently observed in Ge and w-ZnO. Owing to interference with the temperature-independent contribution, their intensities can increase and decrease with temperature. In this report we present ab initio simulations of the temperature dependence and diffraction spectra for Ge and w-ZnO.

DF 3.22 Mon 09:30 P1

Construction of a wavelength filter in Lithiumniobat by irradiation — •Stefanie Haubrich, Matz Haaks, Konrad Peithmann, and Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität zu Bonn, Nußallee 14-16, 53115 Bonn

Lithiumniobat ($LiNbO_3$) is an interesting ferroelectric material well suited for applications in holographic storage and integrated optics. Periodic structures in the refractive index in the propagation direction of the light generate a frequency sensitive filter. Recent experiments proofed that the refractive index of $LiNbO_3$ can be changed by irradiation with light high energy ions. [1] In a proof of principle we create a periodic pattern of the refractive index by irradiating a $LiNbO_3$ crystal with ^3He. Thereby the ion beam is shaded by a parallel array of thin Tantalum foils arranged with a distance of 3 μm. For an exact positioning of the array a 20 nm layer of Aluminum is deposited on the crystals surface and structured with parallel lines in 3 μm distance by laser ablation. The position can be controlled by interference between both line-structures.

[1] K. Peithmann et al., Appl. Phys. B, (2005), in press

DF 3.23 Mon 09:30 P1

Ultrasound Investigations of $BaTi_{1-x}Sn_xO_3$ Ceramics — •Ulrich Straube[1], Ludwig Geske[1], Ralf Steinhausen[1], Hans Theo Langhammer[1], Horst Beige[1], and Hans-Peter Abicht[2] — [1]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, Friedemann-Bach-Platz 6, D-06108 Halle/Saale (Germany) — [2]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Chemie, Karl-Mothes-Str. 2, D-06120 Halle/Saale (Germany)

$BaTi_{1-x}Sn_xO_3$ (BTS) ceramics can be interpreted as a system with more or less diffuse phase transition behaviour depending on the Sn content of the material. BTS belongs to the class of $BaTiO_3$ based environmental-friendly solid solutions, which possesses similar properties like the classical lead-containing relaxors and is becoming an interesting candidate for future applications. Its dielectric and electromechanical resonance properties were already reported in [1]. In the present study the elastic stiffness coefficients were determined by the ultrasound impulse overlap technique at a frequency of 5 MHz allowing the simultaneous determination of sound velocity and attenuation. Elastic properties in a broad temperature range with compositions of $x \leq 0.15$ were obtained. The cubic-tetragonal and the tetragonal-orthorhombic phase transitions are accompanied by anomalies of the sound velocities and the ultrasound attenuation. Sound velocities show minima whereas attenuation increases strongly especially near the cubic-tetragonal transition. Effects of the acoustic dispersion of the elastic data of BTS are discussed.

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DF 3.24 Mon 09:30 P1

Growth, structural, electrical and optical properties of complex perovskite-type $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ single crystals — •Vera Marinova[1], Boriana Mihailova[1], Dimitrina Petrova[2], Thomas Malcherek[1], and Ulrich Bismayer[1] — [1]Universität Hamburg, Mineralogisch-Petrographisches Institut, Grindelallee 48, D-20146 Hamburg — [2]South-West University Neofit Rilski, 2700 Blagoevgrad, Bulgaria

$Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST) single crystals are prepared by the High Temperature Solution Growth (HTSG) method using a flux solution with composition $PbO : PbF_{0.2} : B_2O_3 = 0.75 : 0.23 : 0.2$. The growth conditions for a solid-state phase synthesis were established. The growing process was performed in platinum crucibles in temperature range 1430-1193 K with cooling velocity of 0.5 deg/h. The obtained crystals are cubic-shaped with approximately 1 cm^3 of size. X-ray diffraction data revealed a doubled perovskite-type structure for this newly synthesized compound. The PBST sample was analysed by electrical, optical, and inelastic light scattering measurements. The phase transition was studied by dielectric measurements in the temperature interval from 77 K to 400 K.

DF 3.25 Mon 09:30 P1

Temperature evolution of the phonon anomalies in relaxor ferroelectic $PbSc_{0.5}(Nb,Ta)_{0.5}O_3$ — •Boriana Mihailova[1], Ulrich Bismayer[1], Bernd Güttler[2], Rainer Stosch[2], and Marin Gospodinov[3] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [3]Institute of Solid State Physics - Bulgarian Academy of Sciences, Blvd. Tzarigradsko Chausee 72, 1784 Sofia, Bulgaria

Single crystals of stoichiometric $PbSc_{0.5}Ta_{0.5}O_3$ (PST) and $PbSc_{0.5}Nb_{0.5}O_3$ (PSN) as well as mixed $PbSc_{0.5}(Nb_xTa_{1-x})_{0.5}O_3$ compounds are investigated by Raman scattering and X-ray diffraction. The temperature dependence of the polarized Raman spectra reveals different preferred ferroic species in PST and PSN. Near the dielectric constant maximum cooperative shifts of Pb atoms in respect to the oxygen sheets perpendicular to the cubic body diagonal occur in larger spatial regions for PST than for PSN. On cooling down this structural modification becomes preferential for PST, thus giving rise to highly anisotropic ferroelectric domains. In PSN the temperature decrease favours B-cation deviations from the BO_6-octahedral centres, which leads to formation of small-sized polar clusters distributed in the isotropic matrix. Near 180 K PST undergoes an additional phase transition, which involves reduction of the rotation symmetry. The loading of Nb into PST affects strongly the nanoscale domain texture and the structural transformations that occur on cooling down.

DF 3.26 Mon 09:30 P1

Dielectric properties of BT-LMT mixed ceramics — •Povilas Keburis[1], Juras Banys[1], Algirdas Brilingas[1], Andrei Salak[2], and Victor M. Ferreira[3] — [1]Department of Radiophysics, Vilnius University, Lithuania — [2]Department of Ceramics and Glass Engineering/CICECO, University of Aveiro, Portugal — [3]Department of Civil Engineering/CICECO, University of Aveiro, 3810-193 Aveiro, Portugal

Ceramics of (1-x)$BaTiO_3$-x$La(Mg_{1/2}Ti_{1/2})O_3$ with x=0.025 (0.975BT-0.025LMT) were dielectrically investigated over the extended frequency range. Dielectric studies have been performed at 20 Hz to 3 GHz within the temperature interval of 100 K - 500 K. Apparent relaxor behaviour was revealed to set in when the BT-type three phase transitions become diffuse and merge at low temperatures. Maximums of both imaginary and real parts of the dielectric permittivity are shifted to lower temperatures comparing to pure BT and in the temperature ranges close to phase transitions show strong frequency-dependent behaviour, typical for relaxors. Dynamics of the phase transitions are discussed.

DF 3.27 Mon 09:30 P1

Dielectric spectra of PMN-PSN-PZN ceramics — •Juras Banys[1], Jan Macutkevic[1], Algirdas Brilingas[1], Jonas Grigas[1], Andris Sternberg[2], Vismants Zauls[2], and Karlis Bormanis[2] — [1]Department of Radiophysics, Faculty of Physics, Vilnius University, Lithuania — [2]Institute of Solid State Physics University of Latvia, Latvia

The dielectric dispersion of various ceramics $PbSc_{1/2}Nb_{1/2}O_3$-$PbZn_{1/3}Nb_{2/3}O_3$-$PbMg_{1/3}Nb_{2/3}O_3$ (PSN-PMN-PZN) was measured in very wide frequency range and analyzed in terms of distributions of relaxations times, using Tichonov regularization method. Symmetric and narrow distribution of relaxation times is obtained at higher temperature. On cooling the distribution function becomes asymmetrically shaped and second maximum appears. The longest relaxation times diverge according to Vogel-Fulcher law, however the most probable relaxation time diverges according to Arrhenius law. Enough high activation energy (0.5-0.2 eV) of most probable relaxation times show that in both parts of distribution of relaxation times dominate strongly correlated relaxation. The freezing of dynamics of polar nano regions in PMN-PSN-PZN ceramics must understood as uninterrupted process on cooling from T$_0$ to 0 K. Only at very low temperatures (T<50 K) the contribution of polar nano region becomes enough small, so that the contribution of non-polar matrix can be clearly resolved. The obtained activation energy of fluctuations in non-polar matrix is much smaller as activation energy of most probable relaxation times.

DF 3.28 Mon 09:30 P1

Broadband dielectric spectroscopy of PSN ceramics — •Robertas Grigalaitis[1], Juras Banys[1], Algirdas Brilingas[1], Andris Sternberg[2], Vismants Zauls[2], and Karlis Bormanis[2] — [1]Faculty of Physics, Vilnius University, 9 Sauletekio str., 10222 Vilnius, Lithuania — [2]Institute of Solid State Physic, University of Latvia, 8 Kengaraga str., 1063 Riga, Latvia

One of relaxor materials is $PbSc_{1/2}Nb_{1/2}O_3$ (PSN). In this material the spontaneous transition to ferroelectric phase and also the drastical change in dielectric properties due to the ordering of B' and B"cations was observed [1]. As is known that relaxors exhibit broad frequency dispersion and huge distribution of relaxation times we have studied the dielectric properties of PSN ceramics in the frequency range from 20 Hz to 3 GHz because no data about dielectric permittivity measurements above 1 MHz was found. The obtained results show a high diffusive peak of the dielectric permittivity and behaviour typical to ferroelectric relaxors above 360 K. In order to deal about the dielectric properties and relaxation processes in PSN in more detail we calculated the relaxation time distribution in these ceramics according to the methodology adopted in [2] and compared with PMN relaxation time distribution [3].

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DF 3.29 Mon 09:30 P1

Metastable polar structures in the uniaxial relaxor $Sr_{0.61}Ba_{0.39}Nb_2O_6$:Ce studied by piezoresponse force microscopy — •Vladimir V. Shvartsman and Wolfgang Kleemann — Angewandte Physik, Universität Duisburg-Essen, 47048 Duisburg

Strontium-barium titanate $Sr_xBa_{1-x}Nb_2O_6$ (SBN) based materials comprise a special group of relaxor ferroelectrics, which belong to the random-field Ising model (RFIM) universality class [1]. In accordance with the theory of 3D RFIM systems a metastable multidomain state appears on cooling through T_c, which is expected to relax slowly in time towards the single domain state [2]. We present the results of studies of the polar structures in a SBN single crystal doped with cerium (SBN:Ce) by piezoresponse force microscopy. The appearance of fractal-like nanodomains was found on cooling from the paraelectric state. These nanodomains are metastable and grow slowly in the course of time according to a logarithmic law as predicted [2]. At elevated temperatures the decay of the nanodomains takes place, but even above T_c areas of correlated polarization were observed. We suggest that they correspond to agglomerates of polar nanoregions formed via the ferroelectric mean-field of the system.

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DF 4 Internal Symposium "Ferroelectric Materials for Smart Structures"

Time: Tuesday 09:30–12:50 Room: KÖN Farb

Invited Talk DF 4.1 Tue 09:30 KÖN Farb

Piezoelectric composite materials for smart structures applications — •Andreas Schönecker — Fraunhofer IKTS, Winterbergstr. 28 , 01277 Dresden

Lightweight design in various industrial branches, like for example traffic technology and mechanical engineering, has become very important, mainly to reduce the effects of accelerated mass. However lightweight structures often suffer from vibrational sensitivity, tendency to buckling, and low damage tolerance, which desires active control of structural dynamics, as well as health monitoring and diagnostics to assure safety and reliability. A promising way to solve these problems is expected by using smart materials. Critical deformations, accelerations or other physical quantities can be detected by integrated sensors and in combination with suitable real-time controllers these impacts can be eliminated by driving structural conformable embedded or applied actuators. This paper will discuss the relevance of ferroelectric materials for smart structures, the issues of integration and the expectations on the progress in material sci-

ence, system design and technology. For example, composite materials based on PZT fibres, thick and thin films are considered.

DF 4.2 Tue 10:10 KÖN Farb

Using ferro-electrical material for biometrical application — •Rainer Schmitt — 86 Ironwood Way, Palm Beach Gardens, FL 33418, USA

The matrix structure of 1-3 piezo composite consisting ferro-electrical pzt-pillars, spaced 120 microns apart in a polymer matrix has successfully been utilized for fingerprinting. For this application the pillars are driven in serial resonance mode exhibiting a different electrical impedance when exposed to the very different acoustic load of a finger tip structure, which is 1.5 Mrayls for a ridge and only 350 rayls for a valley. Individual pillars are addressed by a cross-hatched electrode structure on the top and the bottom of the sensor. Under typical material choices (pzt, polymer, electrodes and low acoustical impedance substrate as well as pillar pitches ranging from 50 - 150 microns the variation in the electrical pillar impedances is approx. 1: 4 for the ridge and valley, providing sufficient discrimination for fingerprinting. Since the sensor can be produced inexpensively using soft mold technology, developed by Fraunhofer IKTS large scale application for cell phone, car, computer access are expected. This principle of acoustical impediography, verified at a resolution of 250 dpi is now being expanded to a resolution of 500 dpi by developing the appropriate 1-3 composite with a pillar pitch of 50 microns.

DF 4.3 Tue 10:30 KÖN Farb

Nonlinear constitutive modeling of ferroelectric ceramics: the role of thermally activated processes — •A.Yu. Belov and W.S. Kreher — Institut für Werkstoffwissenschaft, TU Dresden, Hallwachsstr. 3, 01062 Dresden, Germany

The microscopic parameters characterising the interaction between domain walls and short-range obstacles in ferroelectric ceramics are assessed from the experimental data on the temperature dependence of the polarization hysteresis. The approach used is based on a nonlinear constitutive model, which accounts for thermally activated processes assisting the domain walls to overcome the energy barriers of the obstacles. Within the framework of the model the microstructure of ceramics is described effectively, employing the volume fractions of ferroelectric domains with different polarization orientations as structural variables, and its evolution is given in terms of rate equations for these variables. The average polycrystal properties are computed using a discrete orientations approximation (a set of representative orientations) for the distribution function of grain orientations. Assuming that the domain wall mobility depends on temperature according to the Arrhenius law, the microscopic parameters of the model, including the obstacle strength and activation energy, are extracted from the temperature dependence of the coercive field. The analysis of the experimental data for doped lead zirconate titanate (PZT) ceramics shows that for both soft and hard PZT compositions the domain wall motion near the coercive field is essentially thermally activated.

This work has been supported by the Deutsche Forschungsgemeinschaft.

DF 4.4 Tue 10:50 KÖN Farb

Templated grain growth of lead zirconate titanate — •Thomas Richter[1], Morgane Radanielina[1], Carsten Schuh[1], Reinhard Krüger[2], Dieter Sporn[2], Christoph Pientschke[3], Horst Beige[3], Gennadij Lissatschenko[4], and Hugo Schlich[4] — [1]Siemens AG; Corporate Technology, Ceramics Department; Otto-Hahn-Ring 6; 81739 Munich, Germany — [2]Fraunhofer Institut Silicatforschung — [3]Universität Halle-Wittenberg — [4]MaTecK GmbH

For maximising the piezoelectric performance of lead zirconate titanate (PZT) textured polycrystalline ceramics or even single crystals would be advantageous. However, PZT single-crystal growth from melt is impossible due to the incongruent melting behaviour. So, the PZT is to be texturised by secondary recrystallisation of introduced seeds in a fine-grained matrix. By the texturising of electrical ceramics the dielectric and the piezoelectric characteristics can be increased up to 80% of those of single crystals. In the present work growth ability was first studied by very coarse-grained PZT fibres in a fine-grained PZT matrix. The sintering took place both statically in a chamber furnace and dynamically in a temperature gradient furnace. The aim of these results is to develop an understanding for the growth of those seeds. The maximum in growth distance between the original fibre boundary and the boundary between the grown region and the matrix (average grain size about 6 micrometer) was measured at 45 micrometer. The most important parameters for recrystallisation were the temperature gradient of the temperature gradient furnace and the PbO excess of the samples.

DF 4.5 Tue 11:10 KÖN Farb

Point defects and pinning centres in acceptor- and donor-doped ferroelectrics — •Rüdiger-A. Eichel — TU Darmstadt, Eduard-Zintl Inst., Petersenstr. 20, 64287 Darmstadt

Point defects in ferroelectric oxides play an important role for tailoring device properties. In particular, if the pinning of mobile oxygen vacancies is considered that drastically may influence the ability of ionic conductivity in such compounds. On the other hand, quasi-immobile lead vacancies promote domain switching.

High-frequency and multi-pulse electron paramagnetic resonance (EPR) is used in order to study the role of aliovalent functional centres and their impact on lattice vacancies in $PbZr_xTi_{1-x}O_3$.

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DF 4.6 Tue 11:30 KÖN Farb

Pore network analysis of ceramic foams by means of synchrotron tomography — •A. Haibel[1], H. Freidank[1], and A. Berthold[2] — [1]Hahn-Meitner Institute Berlin — [2]Technical University Berlin

Due to their interconnected pore structure ceramic foams emulate well the natural configuration of human bones. In this talk we present protein based prepared ceramic foams. Biopolymers and ceramic powder mixed to a ceramic foam suspension generate a foam structure in a microwave reactor. Subsequent to the microwave coagulation the foams sinter at 1600°C. These foams act as substrates for the cultivation of stem cells. By means of high resolved synchrotron tomography experiments we investigated the effect of the different preparation techniques on the pore accruement and growth of such ceramic foams. By 3D image analysis of the tomographic images we analyzed the influence of coagulation and sintering on the pore size and shape, e. g. the influence of the different dispersing agents on the pores, the diameters of interconnections, and the wall and vessel thicknesses. The knowledge of this parameters allows the realization of ideal cell growth conditions at the artificial environment.

DF 4.7 Tue 11:50 KÖN Farb

Micro-mechanics of multi-variant and multi-phase ferroelectric domain structures — •Johannes Rödel — TU Dresden, Institut für Werkstoffwissenschaft

High-strain piezoelectric materials are often ceramics with a complicated constitution. In particular, PZT, but also PMN-PT and PZN-PT, are used with compositions near to a so-called morphotropic phase boundary, where not only different variants of the same phase (domains), but different phases may coexist. Micro-mechanical models for ferroelectric ceramics would be much more realistic, if these effects could be incorporated.

We consider the conditions of mechanical and electrical compatibility of ferroelectric domain structures. One result are the well known crystallographic relationships between domains of the same phase for various phases. Furthermore we are able to address the question of coexistence of different crystallographic phases within the very same crystallite. In general, the spontaneous strain and spontaneous polarization of a tetragonal and a rhombohedral ferroelecctric domain are not compatible. The internal fields which are caused by this incompatibility, and the associated energy contributions, can be calculated using distributed crystal defects and charge models. We can also show that this internal fields and energies can be decreased by an intermediate, e.g. monoclinic, phase.

The outlined approach can be used to model the overall behavior of multi-variant and multi-phase crystallites with certain, simplified geometrical arrangements of the constituents.

DF 4.8 Tue 12:10 KÖN Farb

Fullerene-based hypothetical ultra-low k dielectrics for microelectronic application — •Kostyantyn Zagorodniy, Manfred Taut, Helmut Hermann, and Klaus Wetzig — Institute for Solid State and Materials Research, IFW Dresden, PF 270116, D-01171 Dresden

Fullerene-based structures are shown to be good candidates for materials with very low dielectric constant. It is our idea to use the C60 fullerene as structural unit and to connect neighbouring C60 molecules by other molecules which have approximately linear shape (for example CnH2n). Such units are the base for the generation of a 3D network with low density and high mechanical stability. The introduction of bridge molecules can be understood as the creation of pores in the fullerene lattice on the 1nm scale. This results in a considerable decrease of the macroscopic polarizability of the material. In this study we analyze the influence of the length of the CnH2n bridge molecules on the properties of the material and the influence of adding fluorine to the C60 molecules. The electronic properties and the local polarizability of the structural units is expected to be changed by fluorination of the fullerenes. Quantum chemical methods are applied to calculate the local polarizability of fluorinated fullerenes. Possible improvements and the limitations are discussed.

DF 4.9 Tue 12:30 KÖN Farb

Electron Holography for ferroelectric characterization — •Hannes Lichte, Marianne Reibold, Karin Vogel, Christopher Matzeck, and Michael Lehmann — Institute for Structure Physics, Technische Universität Dresden, Dresden, Germany

Electron holography in a Transmission Electron Microscope gives quantitative access to magnetic and electric fields by evaluating their phase shifting effect on the electron wave. Electric fields stemming from the ferroelectric polarisation have been identified and analyzed by means of electron holography showing domain structures in sub-micron dimensions. Furthermore, at atomic dimensions, dipole-like structures are found in the holographic phase images of unit cells of BaTiO3, which strongly resemble the assumed atomic dipoles. The found ordering of these dipoles suggests that nano-domains exist which are only several unit cells wide.

DF 5 Glass I (together with division 'Dynamics and Statistical Physics' [DY])

Time: Tuesday 09:30–12:10 Room: MÜL Elch

Invited Talk DF 5.1 Tue 09:30 MÜL Elch

Towards a Statistical Mechanics for Network Glasses — •Reimer Kühn[1], Jort M. van Mourik[2], Martin Weigt[3], and Annette Zippelius[4] — [1]King's College London, UK — [2]Aston University, Birmingham, UK — [3]Institute for Scientific Interchange, Torino, Italy — [4]Universität Göttingen, Germany

We introduce models of heterogeneous systems with finite connectivity defined on random graphs, to capture effects of finite coordination characteristic of finite dimensional systems. Our models use a description in terms of small deviations from a set of reference positions, appropriate for the description of low-temperature phenomena. A Born-von-Karman type expansion with random coefficients is used to model glassy systems. Gel-phases can be described when anharmonicities are absent. The key quantity in the theoretical analysis is a distribution of effective single-site potentials. For gels, where anharmonicities are absent in the interactions, the single-site potentials are harmonic as well, and their distribution is equivalent to the distribution of localization lengths used earlier for the description of such systems. With frustration in the interactions and anharmonicities present, the systems develop glassy phases at low temperature, characterized by an ensemble of single- and double-well potentials, the latter with a broad spectrum of barrier heights and asymmetries. The double well potentials are responsible for the universal glassy low-temperature anomalies, as previously described for fully connected systems

DF 5.2 Tue 10:10 MÜL Elch

Nanostructured Solid Electrolytes analyzed by Time-Domain Electostatic Force Spectroscopy — •Ahmet Taskiran[1], Andre Schirmeisen[1], Harald Fuchs[1], Bernhard Roling[2], Hartmut Bracht[3], Frank Natrup[2], and Sevi Murugavel[2] — [1]Physikalisches Institut, Wilhelm-Klemm-Str.10, 48149 Münster, Gemany — [2]Institut für Physikalische Chemie, Corrensstr..30, 48149 Münster, Gemany — [3]Institut für Materialphysik, Wilhelm-Klemm-Str.10, 48149 Münster, Gemany

Ion conducting solid materials are widely used as solid electrolytes in, e.g,. batteries. An important prerequisite for further progress in this field is a better understanding of ion transport mechanisms on nanoscopic length scales. We are using an atomic force microscope (AFM) operated in the non-contact mode for electrostatic force spectroscopy to measure the ion conductivity in nanoscale volumes of homogeneous and heterogeneous solid electrolytes. The measurements are carried out at sample temperatures ranging from 200 K to 675 K and at different positions on the sample. The relaxation times at different temperatures follow the Arrhenius model,which yield the activation energy of the ion hopping processes [1]. Furthermore the local variation of the relaxation strength provides us with information on the different phases and interfaces in the sample. In our work we focus on nanostructured solid electrolytes. We find that the activation energies for the ions in the nanocrystallites and in the glass regions are different, in agreement with macroscopic results [2]. [1] Schirmeisen et al., Appl.Phys.Lett. 85,2053 [2] Roling et al., Phys.Chem.Chem.Phys. 7,1472

DF 5.3 Tue 10:30 MÜL Elch

Ionic Motion in Ion Beam Sputtered Borate Glasses — •Frank Berkemeier, Reza Abouzari, Tobias Stockhoff, and Guido Schmitz — Westfälische Wilhelms-Universität, Institut für Materialphysik, Wilhelm-Klemm Straße 10, 48149 Münster

Ion-conducting, amorphous thin films with a thickness of $20 - 500\,\mathrm{nm}$ are prepared by ion beam sputtering using glass targets of the compositions $0.2\,A_2O \cdot 0.8\,B_2O_3$, with A = Li, Na, Rb. The glass layers are deposited on a silicon substrate between two sputtered electrodes of Ag, Al, or Al-Li alloy. TEM cross-section investigations show a homogeneous thickness and a homogeneous, amorphous structure of the films. Chemical analysis, performed by EELS, gives alkali oxide concentrations comparable to those of the target material. Temperature-dependent impedance spectroscopy allows to differentiate between different electrical properties of the samples and to determine the specific dc-conductivities of the glass layers. Layers thicker than 100 nm show dc-conductivities which are about one order of magnitude higher than those of the target materials and activation enthalpies about $20\,\mathrm{kJ\,mol^{-1}}$ less compared to the targets. Additionally, layers thinner than 100 nm show a non-trivial increase in dc-conductivity with decreasing film thickness, which we attribute to the increasing influence of the glass-electrode interfaces.

DF 5.4 Tue 10:50 MÜL Elch

Theoretical model of the conductivity of alkali glasses — •Joachim Sohns and Michael Schulz — Abteilung theoretische Physik, Albert-Einstein-Allee 11, 89069 Ulm

Our aim is to formulate a model of the conductivity of glasses which reproduces the mixed alkali effect. Therefore we analyze the conductivity of an ensemble of charged particles in a random environment. As in a former model this environment was static, the model proposed here includes the dynamics of the glass environment. The memory effects are described by the mode-coupling theory. A nonequilibrium Green function determines the properties of the alkali system. Finally the conductivity of the system is calculated. Furthermore, we give some ideas how feedback mechanisms between the ions and the glass environment may be included in the theoretical description.

DF 5.5 Tue 11:10 MÜL Elch

Glasses, Clusters, and Philosophy — •Andreas Reiser, Gernot Kasper, Siegfried Hunklinger, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric relaxation studies can reveal information on structural or chemical processes in liquids, soft matter, and partly crystalline or amorphous solids. Glass formers can belong to all of these groups, depending on the external control parameters temperature, pressure, and more gen-

erally on the thermodynamic present and history. We have measured the dielectric permittivity of several prototypical organic glass formers as a function of frequency, temperature, and pressure. Isobaric, isothermal and isochoric routes in the temperature-pressure plane were taken. We show basic scaling properties of the dielectric function. For data interpretation a cluster-based approach is discussed with respect to crystallization.

DF 5.6 Tue 11:30 MÜL Elch

Collective Single Particle Jumps Below The Glass Transition — •Katharina Vollmayr-Lee — Institut für Theoretische Physik, Universität Göttingen,Friedrich-Hund-Platz 1, D-37077 Göttingen,Germany

We study a binary Lennard-Jones mixture below the glass transition via molecular dynamics simulations. To investigate the dynamics of the system we define single particle jumps via their single particle trajectories. To study how the single particle jumps are correlated in time and space we investigate (I) clusters of simultaneously jumping particles and (II) temporally extended clusters, i.e. clusters of jump events for which the jumping particles are spatially nearby and the jumps occur at consecutive times. We find highly collective jump processes. The distribution of cluster sizes $P(s)$ is independent of temperature and follows a power law $P(s) \sim s^{-\tau}$ with $\tau \approx 2.7$ in case (I) and $\tau \approx 2.2$ in case (II). By studying the average coordination number within the clusters as a function of the cluster size, we find that the shape of the clusters is string-like.

We thank K. Binder, A. Zippelius, J. Horbach, and B. Vollmayr-Lee, and we gratefully acknowledge financial support from SFB 262 and DFG Grant No. Zi 209/6-1.

DF 5.7 Tue 11:50 MÜL Elch

Optical Properties of Colloidal Suspension of Silver Nanoparticles* — •Helge A. Eggert[1], Jim R. Adleman[2], Demetri Psaltis[2], and Karsten Buse[1] — [1]Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn — [2]Department of Electrical Engineering, California Institute of Technology, Pasadena, CA 91125

Colloidal suspensions of silver nanoparticles are an interesting optical material because of homogeneity, stability, and tailored absorption properties. To understand the thermal and nonlinear-optical response, holographic gratings are recorded in such colloidal suspensions of silver nanoparticles utilizing interfering nanosecond pulses (wavlength λ=532 nm, puls duration 6 ns, intensity 10 GW/m^2). The diffraction efficiency is measured with continuous-wave light (λ=633 nm). An instantaneous response together with a longer lasting but also transient grating are observed: The nanoparticles absorb the pump light and heat up, which yields a response on the time scale of the laser pulse. Heat is transferred to the solvent, and a delayed thermal grating appears. The final decay time constant of this grating depends quadratically on the period length of the interference pattern and has a typical value of 1 μs for grating spacings of several micrometers.

*Financial support by the DFG (BU 913/17) and by the Deutsche Telekom AG is gratefully acknowledged.

Prize Talk

The prize talk (Max-Planck-Medaille) by Prof. Götze takes place Tuesday, 13:15, HSZ 04. The title of the talk is "Glassy Relaxation: a Paradigm for Condensed-Matter Dynamics". See the plenary section for the abstract.

DF 6 Glass II (together with division 'Dynamics and Statistical Physics' [DY])

Time: Tuesday 14:30–16:10 Room: MÜL Elch

DF 6.1 Tue 14:30 MÜL Elch

Indications for a slow β-relaxation by mechanical spectroscopy of a strong and a fragile metallic glass — •Jörg Hachenberg, Annelen Kahl, and Konrad Samwer — 1. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Mechanical spectroscopy is used to investigate the elastic properties of the strong metallic glass former $Zr_{65}Al_{7.5}Cu_{27.5}$ and the fragile $Pd_{77}Cu_6Si_{17}$. The dynamic mechanical analyser is used to measure the complex elastic modulus of melt spun bands in the low Hz regime while the double-paddle oscillator is applied for thin films at 5.4 kHz. In the vicinity of glass-transition, the α-relaxation is fitted using a Havriliak-Negami function in temperature domain. The measured data clearly deviate from the model for both metallic glasses. An explicit misfit on the low temperature flank, also termed excess wing, is interpreted as an underlying, merged slow β-relaxation. Our experimental results provide evidence that this secondary relaxation, existing in both strong and fragile amorphous metals, can be regarded as a universal property of glasses and is compared with recent MD-simulations by H. Teichler et al.

This work is supported by the Deutsche Forschungsgemeinschaft, Graduiertenkolleg 782 and SFB 602, TP B8.

DF 6.2 Tue 14:50 MÜL Elch

Sculpting the free energy landscape — •Timo Aspelmeier[1], R. A. Blythe[2], A. J. Bray[3], and M. A. Moore[3] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]School of Physics, University of Edinburgh, UK — [3]School of Physics and Astronomy, University of Manchester, UK

The free energy landscape of the Ising spin glass is analysed using the TAP equations. It is found that local minima of the free energy and saddles always occur in pairs, and that the saddles always have exactly one unstable direction. We show that local minima, which are usually very hard to find numerically, can be found in abundance using an iterative algorithm which operates "on the edge of chaos". We compare these results with the free energy landscape generated by the naive mean field equations of the spin glass and show that despite identical groundstates the free energy landscape at finite temperatures is fundamentally different from the TAP landscape.

DF 6.3 Tue 15:10 MÜL Elch

Dynamic critical behaviour in Ising spin glasses — •Michel Pleimling[1], Malte Henkel[2], and Ian Campbell[3] — [1]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — [2]Laboratoire de Physique des Matériaux, Université Henri Poincaré Nancy I, France — [3]Laboratoire des Colloïdes, Verres et Nanomatériaux, Université Montpellier II, France

The non-equilibrium ageing behaviour of critical Ising spin glasses with Bimodal, Gaussian, and Laplacian interaction distributions is studied numerically in three and four dimensions. The same phenomenology of the time-dependent scaling as in non-disordered magnets is found. Our data strongly indicate that the values of the non-equilibrium exponents and of the critical limit fluctuation-dissipation ratio depend on the distribution of the coupling constants.

[1] M. Pleimling and M. Henkel, Europhys. Lett. 69, 524 (2005)
[2] M. Pleimling and I.A. Campbell, to appear in Phys. Rev. B (cond-mat/0506795)

DF 6.4 Tue 15:30 MÜL Elch

Dynamics of mobile particles in an immobile environment: Computer simulations of disparate-sized mixtures — •Jürgen Horbach and Norio Kikuchi — Insitut für Physik, Johannes-Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz

Molecular dynamics computer simulations are used to study transport properties of mobile particles in an immobile environment. To this end, we consider simple binary mixtures. The first system consists of small and big soft spheres in two dimensions where the big spheres are a factor of 5 bigger than the small ones. We discuss whether the transport properties are similar to those obtained from mode coupling theory [1]. The second system contains also small and big particles with a size–ratio 1:5. But now a three–dimensional system is considered where the particles interact via a screened Coulomb (or Yukawa) potential (note, that this system can be realized experimentally [2]). Here, a transition is observed where the big particles crystallize while the small particles remain in a kind of fluid phase. We study the activated transport of the small particles in the crystalline matrix.

[1] J. Bosse and Y. Kaneko, Prog. Theoret. Phys. Suppl. **126**, 13 (1997); Phys. Rev. Lett. **74**, 4023 (1995).
[2] A. Imhof and J.K.G. Dhont, Coll. Surf. A **122**, 53 (1997); Phys. Rev. E **52**, 6344 (1995); Phys. Rev. Lett. **75**, 1662 (1995).

DF 6.5 Tue 15:50 MÜL Elch

The m-component spin glass on the Bethe lattice — •Axel Braun and Timo Aspelmeier — Institut für theoretische Physik, Universität Göttingen

We investigate the m-component vector spin glass on the Bethe lattice in the limit $m \to \infty$. This is done analytically via the cavity method on a replica symmetric level. We exhibit a phase transition and calculate the critical temperature. Furthermore we confirm numerically the condensation of the lattice spins into a subspace in the groundstate (generalized Bose-Einstein condensation). The dimension n_0 of this subspace is proportional to N^μ, where N is the number of spins and μ is an exponent less than 2/5. This result is compared to the fully connected, the 2-d and the 3-d m-component spin glass.

DF 7 Dielectric and Ferroelectric Thin Films and Nanostructures II

Time: Wednesday 14:30–16:50 Room: KÖN Farb

DF 7.1 Wed 14:30 KÖN Farb

Temperature dependence of elastic electron tunnel currents through thin tantalum oxide films — •Yanka Jeliazova and Detlef Diesing — Institut für Physikalische Chemie, Universität Duisburg Essen

The tunnel process through thin tantalum oxide layers is investigated in tantalum–tantalumoxide–gold thin film tunnel devices. They consist of metal layers (30 nm tantalum, 15 nm gold) separated by a 3.5 nm thick oxide layer. Field strengths up to 1 GV / m were applied to the device and the tunnel current was measured from the 10 $\mathrm{pA \cdot cm^{-2}}$ to 10 $\mathrm{mA \cdot cm^{-2}}$. At tunnel voltages exceeding the barrier height ($\mathrm{e \cdot U_T} > \varphi_\mathrm{B}$) a clear fingerprint of the Fowler-Nordheim tunnel process should be expected in the current voltage plot. This can be barely seen in the experiment with a single current voltage plot at one dedicated temperature. Thereby the band structure of the devices has to be determined by another method. We recorded current voltage plots from 60 K to 500 K and evaluated the temperature dependence of the tunnel current for dedicated tunnel voltages. For tunnel voltages ($\mathrm{U_T} < 1$ V) only a weak increase of the tunnel current of 30 % could be observed while heating the sample from 60 K to 500 K . For tunnel voltages ($\mathrm{U_T} > 1.3$ V) a strong current increase about 4 orders of magnitude was detected. These experimental findings can be rationalized by a thermally induced increase of Fowler Nordheim tunneling processes through a tunnel barrier with 1.8 eV height.

DF 7.2 Wed 14:50 KÖN Farb

Charge states of native point defects in Pr-based high-k dielectrics — •Jarek Dabrowski[1], Andrzej Fleszar[2], Grzegorz Lupina[1], Gunther Lippert[1], Anil Mane[1], and Christian Wenger[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt(Oder), Germany — [2]Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

High-k dielectric films can trap electric charge, which aggravates their application in silicon technology as dielectrics in MOS transistors and MIM capacitors. On the basis of ab initio calculations for band offsets and defect formation energies we discuss the charge states of native point defects in Pr oxides and silicates. In particular, we find that oxygen vacancies in Pr_2O_3 introduce electron transition states at Fermi energies falling within the range of the Si substrate band gap. In thin films grown on Si, oxygen intersitials are always negatively charged in Pr_2O_3 (i.e., they act as negative fixed charges there) and always electrically neutral in PrO_2. In Pr silicates, a valence alternation defect consisting of a Si atom with a dangling bond interacting with an O atom from the silicate network is expected to be the source of a positive fixed charge.

DF 7.3 Wed 15:10 KÖN Farb

Impedance spectroscopy study of thin film capacitors with SrTiO(3) as dielectric — •Kesav Reddy[1], Dieter Mergel[1], and Werner Osswald[2] — [1]Thin film working group, Physics Department, University Duisburg-Essen, 45117 Essen — [2]Institute for Solid-State Chemistry, Chemistry Department, University Duisburg-Essen, 45117 Essen

Planar thin films capacitors with RuO(2) electrodes and SrTiO(3) as dielectric layer have been prepared by rf-magnetron sputtering. Substrate temperature (up to 700°C), oxygen content of the sputter gas and thickness of the dielectric layer have been varied.

The capacitors were investigated by x-ray diffraction and impedance spectroscopy in the range 10 Hz to 10 MHz and for temperatures from 20°C to 200°C. Contributions from the electrode-dielectric interface, grain boundaries and bulk grains could be distinguished by modelling the spectra with RC-elements. The conductivity and the dielectric permittivity of the bulk SrTiO(3) grains were extracted. The dielectric permittivity ranges from 150 to 350. Its temperature dependence shows Curie-Weiss behaviour with characteristic temperatures between 30 and 50 K.

DF 7.4 Wed 15:30 KÖN Farb

Optical Characterization of Suspensions of Lithium Niobate Nanoparticles* — •Judith Schwesyg, Helge A. Eggert, and Karsten Buse — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn

Using suspensions of ferroelectric nanoparticles in liquids one can combine the outstanding properties of the nanoparticles with the characteristics of fluids. Stable suspensions of lithium niobate nanocrystals in liquids are produced in a high-energy ball-milling process. The size of the particles is of the order of 20–50 nm. We present the details of the methods for producing such stable suspensions and for investigating the characteristic parameters of these liquids. Furthermore, we present data of absorption and scattering experiments. In addition one can apply external electric fields to measure the field-induced birefringence of the suspensions. Alignment of the nanocrystals breaks the inversion symmetry and should enable frequency conversion processes in suspensions of ferroelectric nanoparticles.

DF 7.5 Wed 15:50 KÖN Farb

DFT investigation of PZT bulk and surface properties — •Igor Chaplygin, Sibylle Gemming, and Gotthard Seifert — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden.

Density-functional investigations on the structural, electronic and elastic properties of lead zirconate titanate (PZT) were carried out, employing both an all-electron and a pseudopotential technique. The lead/zirconium distribution was studied with a supercell approach and with the random mixing provided by the CPA and the alchemical mixing scheme. All approaches yield a nearly linear dependence of the structural and eleastic properties of the Zr:Ti ratio. Only the character of the conduction band changes from Pb-based 6p states to Ti-3d states if the Ti content exceeds 50 Thus, the (001) surfaces of PZT were investigated with the alchemical mixing technique. All surfaces exhibit an inward relaxation of the termination plane and a less pronounced outward relaxation of the next lower plane. The strongest relaxations of up to 20 constant occur at the less densely packed PbO termination. Similarly, the relaxations of the Zr-rich systems are larger than the ones in the Ti-rich models. Thus, the slab thickness required to obtain stable bulk-type PZT in the centre of the slab varies between 1.6 to 2.4 nm.

DF 7.6 Wed 16:10 KÖN Farb

Computational investigations on the Kohlrausch relaxation law for interacting dipole systems — •Markus Kühn and Herbert Kliem — Saarland University, Institute of Electrical Engineering Physics, P.O. Box 151150, 66041 Saarbrücken, Germany

For an interacting system of permanent dipoles calculations of transient polarization relaxations show a pronounced Kohlrausch behaviour. It can be described in the time domain by stretched exponential functions or power laws. The model which is employed here is based on permanent dipoles which fluctuate thermally activated in double-well potentials. The dipoles are statistically distributed with respect to their centres and the direction of their axes. The long-range electrostatic dipole-dipole interaction strongly influences the local fields at the dipoles. The iterative algorithm mainly consists of two steps. For each current configuration the local electric fields at the dipoles are deterministically calculated. Then the transition times of the dipoles which depend on the local electric fields are computed in a following weighted probabilistic Monte Carlo step. Simulation results yield a strong dependence of the Kohlrausch be-

haviour on the dipole charge, the dipole length and the dipole density. Further calculations show the influence of the geometrical dimensions, the temperature, the intrinsic activation energy for a dipole flip and the external electric field.

DF 7.7 Wed 16:30 KÖN Farb

COMBINING HALF-METALS AND MULTIFERROICS FOR SPINTRONICS — •Hélène Béa[1], Manuel Bibes[2], Gervasi Herranz[1], Martin Sirena[1], Karim Bouzehouane[1], Stephane Fusil[3], Eric Jacquet[1], Jean-Pierre Contour[1], Patrycja Paruch[4], Matt Dawber[4], and Agnès Barthélémy[1] — [1]Unité Mixte de Physique CNRS-Thales, RD 128, 91767 Palaiseau, France — [2]Institut d'Electronique Fondamentale, Université Paris-Sud, 91405 Orsay, France — [3]Université d'Evry, Bât. des Sciences, rue du Père Jarlan, 91025 Evry, France — [4]Condensed Matter Physics Department, University of Geneva, 24 quai Ernest Ansermet, CH-1211 Geneva 4, Switzerland

Multiferroic materials possess simultaneously ferroelectric and ferro- or antiferromagnetic orders and a coupling between the two order parameters. A first step towards fabrication of magnetoelectric functional devices is to grow these materials as thin films. One of the best candidates is $BiFeO_3$ (BFO) which shows ordered states at high temperatures (it is antiferromagnetic below $T_N = 647$ K and ferroelectric below $T_C = 1043$ K). We have explored the influence of deposition pressure and temperature on the growth of BFO thin films by pulsed laser deposition onto (001)-oriented $SrTiO_3$ substrates. Single-phase BFO films are obtained in a narrow region close to 10^{-2} mbar and 580°C. We have characterized the structural and functional properties of BFO/$La_{2/3}Sr_{1/3}MnO_3$ (LSMO) bilayers. We show that the BFO layer has a ferroelectric tunnel barrier behavior. This would open a way to combine the half-metal properties of LSMO with the multiferroic properties of BFO in devices.

DF 8 Spectroscopy, Scanning and Diffraction Methods

Time: Wednesday 14:30–16:50 Room: MÜL Elch

Invited Talk DF 8.1 Wed 14:30 MÜL Elch

Phonons in multiferroics: BiFeO3 and related systems — •Jens Kreisel[1], Raphaël Haumont[1,2], Pierre Bouvier[3], and Françoise Hippert[1] — [1]ENS de Physique de Grenoble (F), CNRS — [2]Université d'Orsay (F) — [3]ENSEE Grenoble (F), CNRS

On the way towards a fundamental understanding of magnetoelectric multiferroics the experimental observation and understanding of the coupling mechanism between the ferroelectric and magnetic order are of great interest. Very little is currently known about the behavior of phonons in magnetoelectric multiferroics, and this although investigations of phonons have in the past played a crucial role in the understanding of classic ferroelectrics.

Motivated to determine and understand the role of phonons in multiferroics, we will discuss the phonon spectrum measured by Raman spectroscopy of the model system bismuth ferrite BiFeO3 (BFO). Further to the discussion of Raman spectra from BFO powder, single crystalline and thin film samples we will compare our results to those from similar but not multiferroic RFeO3 samples.

Key points that will be addressed are: 1) A paraelectric-to-ferroelectric phase transition which is not soft-mode-driven in BFO, 2) Colossal phonon anomalies for BFO around the Néel temperature for some particular phonons, while this is not observed for non multiferroic EuFeO3. The results are discussed in the context of spin-phonon coupling and interactions between magnetic and ferroelectric order parameters. 3) A significant difference in Raman spectra between bulk and thin film BFO samples illustrating the role of epitaxial strain.

DF 8.2 Wed 15:10 MÜL Elch

Luminescent spectroscopy of the RE ions incorporated in the lead tungstate crystals — •Oksana Chukova[1], Sergiy Nedilko[1], and Marian Pashkovskyi[2] — [1]Physics Faculty, Kyiv National Taras Shevchenko University 2, block 1, acad. Hlushkov Ave., 03680, Kyiv, Ukraine — [2]Physics Faculty, Lviv National Ivan Franko University, Lviv, Ukraine

The lead tungstate $PbWO_4$ (PWO) crystals are widely doped by various impurities, especially rare earth (RE) ions, in order to change characteristics of these crystals, e.g., significantly improve transmission and radiation hardness of the crystal. Spectral properties of the RE doped PWO crystals were studied formerly, but the investigations were directed mainly on spectroscopy of proper matrix emission of the pure and doped crystals. The present paper is concentrated on investigation of spectroscopy of RE ions in the PWO crystal matrix. Spectral properties of the Pr^{3+} and Eu^{3+} ions doped into the PWO crystal were studied at photo and synchrotron radiation excitation and analyzed on parameters of Stark splitting in the crystal field. Formation of at least two types of emission centers based on the RE ions in the PWO crystal lattice is shown and origin, structure and spectroscopy of these centers are investigated. Different site symmetry and oxygen coordination influence in different ways on probabilities of emission and excitation transitions as well as on shifts of lines and weight centers of manifolds for the both types of centers. Experiments with synchrotron excitation were performed at SUPERLUMI Station at HASYLAB, DESY, Hamburg.

DF 8.3 Wed 15:30 MÜL Elch

Rare-earth doped barium halide x-ray storage phosphors and scintillators — •Julia Selling and Stefan Schweizer — Department of Physics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Rare-earth (RE) doped orthorhombic BaX_2 (X = Cl, Br, I) single crystals were investigated for their properties as x-ray storage phosphors and as x-ray scintillators by means of photoluminescence (PL), photostimulated luminescence (PSL) and x-ray luminescence (XL). The investigation of the storage and read-out mechanism in these materials will help to optimise the PSL effect in Eu- or Ce-doped fluorozirconate-based glass ceramics containing PSL-active BaX_2 nanoparticles which are formed upon thermal processing of the glass [1, 2]. The PSL efficiency of the single crystals is comparable to that of Eu-doped BaFBr, which is used in commercial x-ray storage phosphor screens. The scintillation efficiency of the RE-doped barium halides investigated is compared to that of CWO ($CdWO_4$). Features like afterglow or radiation hardness have not been considered in our comparison. The influence of the anion-cation distance on the intensity ratio of the emission types is discussed.

[1] A. Edgar, J.-M. Spaeth, S. Schweizer, S. Assmann, P.J. Newman, and D.R. Macfarlane, Appl. Phys. Lett. **75** (1999) 2386.

[2] S. Schweizer, L.W. Hobbs, M. Secu, J.-M. Spaeth, A. Edgar, G.V.M. Williams, Appl. Phys. Lett. **83** (2003) 449.

DF 8.4 Wed 15:50 MÜL Elch

Luminescent oxygen-vacancy complex in Mn-doped $LiBaF_3$ investigated by optically detected magnetic resonance — •Bastian Henke[1], Uldis Rogulis[2], and Stefan Schweizer[1] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Institute of Solid State Physics, University of Latvia, Riga, Latvia

Upon ultraviolet photoexcitation, Mn-doped $LiBaF_3$ shows different luminescence bands in the visible range. The luminescence, which can be attributed to Mn^{2+}, is at 712 nm [1], whereas two additional bands appear at 423 and 480 nm. The peaks at 423 and 480 nm have completely different excitation spectra than the one for the 712 nm emission, which shows the typical Mn^{2+} excitation bands. Photoluminescence detected electron paramagnetic resonance measurements yielded that the bands at 423 and 480 nm can be attributed to an oxygen-vacancy complex. Its principal axis, z, of the fine structure tensor is aligned along a <110> direction. The Mn^{2+}-dopant can be found in the vicinity of this complex. We assume that Mn^{2+} substitutes for a Ba^{2+} ion.

[1] B. Henke, M. Secu, U. Rogulis, S. Schweizer, J.-M. Spaeth, phys. stat. sol. (c) **2**, No. 1 (2005), 380

DF 8.5 Wed 16:10 MÜL Elch

Density-functional simulations for X-ray and Electron Holographic measurements of single crystal properties of tetragonal Bariumtitanate — •Axel Rother[1], Igor Chaplygin[2], Sibylle Gemming[2], Tillman Leisegang[1], Dirk Meyer[1], and Hannes Lichte[1] — [1]Institute of Structure Physics, Dresden University, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University, Germany

As a typical member of Ferroelectrics, tetragonal BaTiO3 reveals a lot of interesting properties such as the electric polarization along the tetragonal axis. Modern X-ray and Electron Holographic methods are able to measure these features by utilizing refinement with given theoretical models. Firstly, a single crystal X-ray reflection measurement was performed to obtain structural parameters and the electron density. Secondly, high resolution electron holography was utilized to measure the dipole character of the electric potential, and thirdly, different Density-functional simulations were carried out for a detailed comparison with the measured data. Furthermore we began to incorporate the theoretical calculations in the refinement models used in High Resolution Electron Holography.

[1] Support from DFG in the Framework of FOR 520 is gratefully acknowledged

DF 8.6 Wed 16:30 MÜL Elch

Density-functional simulations for X-ray and Electron Holographic measurements of single crystal properties of tetragonal Bariumtitanate — •Axel Rother[1], Igor Chaplygin[2], Sibylle Gemming[2], Tilmann Leisegang[1], Dirk Meyer[1], and Hannes Lichte[1] — [1]Institute of Structure Physics, Dresden University, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University, Dresden, Germany

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[1] Support from DFG in the Framework of FOR 520 is gratefully acknowledged

DF 9 Phase Transitions

Time: Thursday 09:30–12:30 Room: MÜL Elch

Invited Talk

DF 9.1 Thu 09:30 MÜL Elch

Driving a macroscopic state switching into materials with a laser pulse and probing atoms moving in real time with a X-ray pulse — •CAILLEAU Herve[1,2], COLLET Eric[1,2], BURON Marylise[1,2], LEMEE-CAILLEAU Marie-Helene[3], and KOSHIHARA Shin-ya[2,4] — [1]Groupe Matiere Condensee et Materiaux, Cnrs-Université Rennes 1, F 35042 Rennes Cedex, France — [2]ERATO, JST, Japan — [3]Institut Lauë-Langevin, Grenoble, France — [4]Tokyo Institute of Technology, Tokyo, Japan

The possibility of controlling with a single ultra-short laser pulse the coherent and cooperative transformation of the state of atoms or molecules in solid state opens new avenues in materials science. This challenge of driving a macroscopic state switching on an ultra-fast time scale, so realizing at the material level what has been done at the molecular level in femto-chemistry, goes beyond the current principles. Indeed, these new out-of-equilibrium processes are highly cooperative and highly non-linear. In other words, light can induce self-amplification and self-organization processes in the material, a so-called photoinduced phase transition. Molecular materials are particularly promising by virtue of light tuning of the charge state and/or spin state in molecules. Another new step is the recent possibly to directly observe in real time the assembly of molecules in a solid moving in a regimented way towards the new electronic and structural order by using the emerging ultra-fast X-ray diffraction. Reference: * Photoinduced Phase Transitions*, K. Nasu ed., World Scientific (2004).

Invited Talk

DF 9.2 Thu 10:10 MÜL Elch

Structural instabilities in Ferroelectric Aurivillius compounds — •J. Manuel PEREZ-MATO — Dept. Fisica Mat. Condensada, Fac. Ciencia y Tecnologia, Univ. del Pais Vasco, UPV/EHU, Apdo 644, 48080 Bilbao, Spain

The Aurivillius phases are layered bismuth oxides formed by the regular stacking of Bi2O2 slabs and perovskite-like blocks. Many are ferroelectric at room temperature and are of special technological interest. Apart from the polar distortive mode, other displacive modes at the Brillouin zone border are unstable and are frozen in the room temperature structure. The close interplay of these different instabilities situates these systems beyond the conventional framework for perovskite ferroelectrics. We present ab-initio calculations and thorough structural and symmetry analyses of two specific compounds, SrBi2Ta2O9 (SBT) [1], and Bi4Ti3O12 (BTO), which have respectively two and three layers of BO3 octhaedra within the perovskite blocks. The energy landscape around the parent tetragonal configuration has been explored analysing the possible existence of intermediate phases. The essential role of secondary hard modes for the stabilization of the ferroelectric phase is shown. Surprisingly, the rigid-like behaviour of the perovskite octahedra in BTO is the result of anharmonic couplings. Energy maps have been compared with empirical bond valence criteria with a striking agreement of both approaches [2].

[1]Perez-Mato et al., Phys. Rev. B (2004) 70, 214111
[2]Etxebarria et al., Phys. Rev. B (2005) 72, 174108

DF 9.3 Thu 10:50 MÜL Elch

Soliton Density in Incommensurate Thiourea — •Robert Blinc[1] and Tomaž Apih[2] — [1]J. Stefan Institute, Jamova 39, Ljubljana, Slovenia — [2]. Stefan Institute, Jamova 39, Ljubljana, Slovenia

Whereas soliton regimes have been reported in the past in type I incommensurate systems where the order parameter is at least two-dimensional and a Lifshitz invariant drives the system to a modulated incommensurate phase, this is not the case with type II incommensurate systems such as thiourea. Here there is no Lifshitz invariant and the order parameter is one-dimensional. It has been generally assumed until recently that the incommensurate modulation of type II systems is always of the plane wave type. Recent X-ray scattering results seem to show the appearance of soliton like modulation profiles close to the lock-in transition in thiourea. Perez - Mato provided a possible theoretical explanation of this situation. Here we show that the deuteron NMR spectra of thiourea exhibit a gradual change of the incommmensurate modulation wave from the plane wave to the soliton type. We determined the temperature dependence of the soliton density and compare the results with the theory of Perez - Mato. The obtained data support the above mentioned theoretical results and show that type II incommensurate systems can indeed exhibit a multi soliton lattice regime similar to that found in type I incommensurate systrems like RbZnCl4 and others.

DF 9.4 Thu 11:10 MÜL Elch

Poling Effect on the Ferroelectric and Transport Properties of Soft Piezoelectric PZT — •T.M. Kamel, F. X. N. M. Kools, and G. de With — Laboratory of Materials and Interface Chemistry, Eindhoven University of Technology, 5600 MB Eindhoven, the Netherlands

The properties of the piezoelectric ceramic materials are strongly dependent on the degree of polarization as set by the poling process. In the present work a soft piezoceramic PZT material was polarized at different poling conditions. Three different methods were used to evaluate the polarization state in the material. These are the polarization current, pyroelectric coefficient and the hysteresis loop measurements. The polarization current was monitored during the poling process at different applied electric fields, poling time and temperature. The pyroelectric coefficient and hence the polarization was calculated form the pyroelectric current vs. temperature. The hysteresis loop was displayed using

a home-made computerized Sawyer-Tower circuit. The dielectric, ferroelectric and piezoelectric properties were measured as a function of temperature and frequency after different poling conditions. The effects of the various poling conditions on the functional and physical properties of the soft PZT are presently discussed.

DF 9.5 Thu 11:30 MÜL Elch

Investigation of the relaxor system Strontium-Barium-Niobate by Second Harmonic Generation — •Uwe Voelker, Klaus Betzler, and Sergey Podlozhenov — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, D - 49069 Osnabrück, Germany

The relaxor phase transition in ferroelectrics is still not completely understood. In contrast to past investigations, we use second harmonic generation (SHG) as a tool to observe the behavior of the bulk of $Sr_{0.61}Ba_{0.39}Nb_2O_6$(SBN). Thus we are able to watch closely how particular classes of domains lose their spontaneous polarisation while passing through the phase transition without integrating over the whole crystal. We will present the concentration-dependence of the relaxor phase transition of SBN doped with rare earth-metals obtained by these measurements. Supported by DFG (project GRK 695).

DF 9.6 Thu 11:50 MÜL Elch

Non-ergodic behavior of polar state in Li-doped KTaO3 under an electric field — •Yoshiaki Uesu[1], Hiroko Yokota[1], Taeko Oyama[1], Charlotte Malibert[2], and Jean-Michel Kiat[2] — [1]Department of Physics, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan — [2]SPMS, Ecole Centrale Paris, Grande Voie des Vignes 9225 Chatenay-Malabry, France

Incipient ferroelectric KTaO3 doped with Li-3% was investigated in order to clarify the dipole state under electric field. Using optical second-harmonic generation (SHG) microscope, we observed a marked history dependence of SHG intensity through zero-field cooling (ZFC), zero-field heating (ZFH), field heating after ZFC (FH/ZFC) and FH after field cooling (FH/FC) for both crystals. At fixed temperature in FH/ZFC, the long relaxation process to the equilibrium state is observed dependent on temperature. In quite low temperature, the SHG does not develop under the electric field. This kind of non-ergodicity is known to be a character of inhomogeneous system. Further experiments are performed using precise X-ray diffraction method. It reveals that two-step transformation occurs: at 50K, remarkable field-induced SHG and photo-conductivity accompanied by tetragonal lattice strain occur, while at 90K, does only small lattice strain. The fact indicates that polar nano-regions generated at 90K in nonpolar cubic matrix are transformed into ferroelectric micro-domain state at 50K without field. Under an electric field, the micro-domain state is changed to macroscopic ferroelectric state.

DF 9.7 Thu 12:10 MÜL Elch

Mapping of Microwave-Induced Phonons by Mikro-Brillouin Spectroscopy: High Resolution Access To Acoustic Fields In Piezoelectric Materials — •Mathias Kolle, Jan Kristian Krüger, Brice Vincent, Roland Sanctuary, Laurent Le Brizoual, Omar Elmazria, Laurent Bouvot, Didier Rouxel, and Patrick Alnot — Laboratoire Européen de Recherche Universitaire : Saarland-Lorraine, Universität des Saarlandes, Bau E6.2, D-66041 Saarbrücken

Brillouin spectroscopy (BS) is a versatile technique to measure acoustic properties at hypersonic frequencies and has been proven to be capable to detect thermally excited surface- and guided acoustic waves at microwave frequencies. BS on microwave induced phonons, generated at the surface of piezoelectric crystals can be used to determine the sound velocity of surface acoustic waves as well as their hypersonic attenuation from the decay of the Stokes intensity of the BS. Only recently, BS was used for studying acoustic microscopy (BM). It turns out that this new technique is able to characterize the distribution of acoustic fields, generated by inter digital finger structures (IDTs) at microwave frequencies in piezoelectric materials. The aim of this talk is to elucidate the efficiency of the electro-acoustic generation of hypersonic waves in thin piezoelectric films including their field properties and especially their spatial decay within the film plane.

DF 10 Electric, Electromechanical and Optical Properties I

Time: Thursday 14:30–18:10 Room: MÜL Elch

Invited Talk DF 10.1 Thu 14:30 MÜL Elch

Broadband Dielectric Spectroscopy in Functional Transition-Metal Compounds — •Joachim Hemberger, Peter Lunkenheimer, Robert Fichtl, Stefan Weber, Torsten Rudolf, Franz Mayer, Andrei Pimenov, Vladimir Tsurkan, and Alois Loidl — Center for Electronic Correlation and Magnetism, University of Augsburg, D-85135 Augsburg, Germany

Transition-metal compounds offer an exceptional variety of functional properties with a broad range of application. In addition to the canonical dielectric oxides reaching from piezo-electric or ferroelectric to high-permittivity materials, compounds with complementary magnetic and electronic properties are currently more and more under focus. An example are multiferroic compounds combining ferroelectricity and ferromagnetism. However, the coexistence of magnetic spin, orbital or charge degrees of freedom requires the consideration of systems with partially filled d-shells in contrast to the usual dielectric d^0-systems. This is accompanied by an deterioration of the insulating properties. Non-d^0 systems commonly are "bad insulators", i.e. they posses smaller, correlation induced electronic gaps instead of the large band gaps of usual optically transparent dielectric materials. This leads to finite DC- and AC-contributions to the conductivity and to a finite charge carrier density in the conduction band. The talk will outline the potential as well as the difficulties of broadband dielectric spectroscopy to study complex transition-metal compounds and illustrate them discussing various examples like titanates, manganates or Cr-based thio-spinels.

This work was supported by BMBF (VDI/EKM 13N6917-A) and DFG (SFB 484).

DF 10.2 Thu 15:10 MÜL Elch

Structuring of ferroelectric volume domains in lithium niobate crystals by space charge fields — •Felix Kalkum, Helge A. Eggert, and Karsten Buse — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn

The controlled structuring of ferroelectric domains in lithium niobate crystals promises a variety of new optical applications, e.g., electrically switchable Bragg filters. The quality of domain structures made by conventional methods is not sufficient for most of these applications. Therefore the so-called method of electrical fixing was studied: After a space charge field is written in iron doped lithium niobate crystals by means of the photorefractive effect, an external electrical field is applied. Since the resulting electrical field is above the threshold field for ferroelectric domain inversion in some regions and below in others, domains can be structured. A stochastical description of domain inversion assumes that the electrical field increases the probability for inversion, but does not imply necessarily a domain inversion if it exceeds the coercive field. The stochastical approach explains the shape and the effective modulation degree of the domain patterns. *Financial support by the DFG (BU913/11) and by the Deutsche Telekom AG is gratefully acknowledged.

DF 10.3 Thu 15:30 MÜL Elch

Fabrication of embedded waveguides in $LiNbO_3$ by radiation damage — •K. Peithmann[1], M.-R. Zamani-Meymian[1], M. Haaks[1], K. Maier[1], B. Andreas[2], K. Buse[2], and H. Modrow[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, — [2]Physikalisches Institut, Bonn, Germany

Irradiation of $LiNbO_3$ with low-mass, high-energy ions as 40 MeV ^{3}He (range in $LiNbO_3 \approx 0.6$ mm) creates strong, permanent refractive-index changes: The ordinary refractive index n_o is decreased and the extraordinary refractive index n_e is increased in the regions where the ions are transmitted through the material. Characteristic dependences of these changes on the ion dose and their thermal stability are measured, and the feasibility of fabrication of embedded waveguides (size ≈ 30 μm) using spatially modulated ion distributions is demonstrated.
*Supported by the Deutsche Forschungsgemeinschaft (FOR 557)

DF 10.4 Thu 15:50 MÜL Elch

Photorefraction as a general property of light-induced metastable states in nitrosyl compounds — •Dominik Schaniel[1], Thomas Weisemoeller[1], Mirco Imlau[1], Theo Woike[2], Karl Krämer[3], and Hans-Ueli Güdel[3] — [1]Fachbereich Physik, Universität Osnabrück, Barbarstrasse 7, 49069 Osnabrück — [2]Institut für Mineralogie, Universität zu Köln, Zülpicherstrasse 49b, 50674 Köln — [3]Department of Chemistry and Biochemsitry, University of Bern, Freiestrasse 3, 3000 Bern 9

Photorefractive materials have a broad range of applications in the field of nonlinear optics and need often to be tailored to meet specific demands. In oxidic electro-optic materials or photorefractive polymers tuning is achieved by additional doping of charge carriers or application of external fields. We report on another class of photosensitive compounds containing molecules of type $[ML_5NO]^{n\pm}$ with M a transition metal, L a broad range of ligands, and n the formal charge of the anion/cation. In these compounds metastable states can be generated by light irradiation and tuning of the photorefractive response is achieved by selecting different molecules $[ML_5NO]^{n\pm}$, e.g., the lifetime and spectral sensitivity of the metastable states can be varied from 10^{-8}s to10^{1}s and from 300-1200 nm, while the size of the effect can be adjusted up to $\Delta n \sim 10^{-2}$. We show that photorefraction is a general property of the light-induced metastable states accessible in molecules of the type $[ML_5NO]^{n\pm}$ and thereby establish a new class of photorefractive compounds.

DF 10.5 Thu 16:10 MÜL Elch

Space-charge waves in silicon carbide — •M. Lemmer[1], M. Imlau[1], M. Petrov[2], V. Bryksin[2], and A. Lebedev[2] — [1]Department of Physics, University of Osnabrück — [2]Physico-Technical Institute, Russian Academy of Sciences, St. Petersburg

The non-linear phenomenon of space-charge waves (SCW) is investigated in single crystals of 4H-SiC polytype. By excitation with an oscillating interference pattern at $\lambda = 488$ nm and an externally applied electric field of $0 < E_0 \leq 10$ kV/cm spatial rectification (SR) is found. The amplitude and the frequency of the SR-resonance signal show relevant dependences on the applied electric field and the wave number K of the interference pattern. For instance the amplitude exhibits a pronounced maximum at low values of K of approximately $2 \cdot 10^3$ cm^{-1}. All results are successfully described by the generalized SCW-model, if the effect of trap saturation, caused by a limited trap density, is considered. This allows to determine important material parameters of 4H-SiC like the product of mobility and lifetime of the charge carriers $\mu\tau = (7.4 \pm 0.8) \cdot 10^{-7}$ cm^2/V, the Maxwell relaxation time $\tau_M = (5.3 \pm 0.6) \cdot 10^{-4}$ s, and the effective trap concentration $N_{\text{eff}} = (5 \pm 1) \cdot 10^{13}$ cm^{-3}.

Supported by the Deutsche Forschungsgemeinschaft (DFG, projects GRK 695 and 436 RUS 17/16/06).

DF 10.6 Thu 16:30 MÜL Elch

Dispersion of the electrooptic properties of Cerium-doped Strontium-Barium-Niobate — •K. Bastwöste[1], M. Imlau[1], and M. Goulkov[2] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück — [2]Institute of Physics, Kiev, Ukraine

The electrooptic coefficient r and the photorefractive trap density N_{eff} are determined as a function of the wavelength in Cerium-doped Strontium-Barium-Niobate (SBN:Ce) by applying the photorefractive method of photo-induced light scattering. A pronounced increase of r is found in the blue-green spectral range, which is described by a combination of the Sellmeier formulation and the polarization tensor concept. Thus, the strength and energy of the average dipole oscillator characterizing the optical interband transfer are estimated with $f_e = (2 \pm 0.5) \cdot 10^{31}$ s^{-2} and $E_e = (3.7 \pm 0.26)$ eV. The increase of r with decreasing wavelength equals to already reported results for electrooptic crystals. Nevertheless, the strong increase by more than a factor of two is remarkable compared to an increase of 16 % in $LiNbO_3$:Fe [1] and 38 % in $BaTiO_3$ [2]. The dispersive behavior of N_{eff} is discussed in the context of the results of undoped SBN and interband photorefraction [3].

Financial support from the Deutsche Forschungsgemeinschaft (DFG, project GRK 695).

[1] S. Fries, S. Bauschulte, Phys. Stat. Sol. **125**, 369 (1991).
[2] A. R. Johnston, J. Appl. Phys. **42**, 3501 (1971).
[3] M. D. Ewbank,R. R. Neurgaonkar, W. K. Cory, J. Feinberg, J. Appl. Phys **62**, 374 (1987).

DF 10.7 Thu 16:50 MÜL Elch

Ferroelectric domain gratings contributing to photo-induced polarization-anisotropic light scattering in $LiNbO_3$:Fe — •A. Selinger, U. Voelker, and M. Imlau — Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück

Only recently, the appearence of a bright polarization-anisotropic elliptical scattering pattern upon exposure to cw- and pulsed laser light has been discovered in thin Fe-doped $LiNbO_3$ crystals, i.e. in samples with thicknesses below 900 μm [1]. Our further investigations reveal that this phenomenon can be explained by the interplay of photo-induced refractive-index and ferroelectric-domain gratings. For example, the kinetics of the scattering intensity of the ellipse is found to be identical to the kinetics of the so called e-line, which is a scattering pattern originating solely from the photo-induced formation of microdomains. At the same time, the polarization-flip observed in the ellipse, comparable to that in the well-known anisotropic ring, gives rise to a contribution of photorefractive gratings via the electrooptic tensor element r_{42}. This approach is strongly supported by experimental studies of the influence of temperature towards appearence, stability and decay of the elliptical scattering pattern. An Ewald-construction, taking into account both photo-induced refractive-index and ferroelectric-domain gratings, is presented and allows to explain the specific shape of the ellipse.

Financial support by the Deutsche Forschungsgemeinschaft (DFG, project IM 37/2-1) is greatfully acknowledged.

[1] A. Selinger, U. Voelker, M. Imlau, OSA Trends in Optics and Photonics (TOPS), Vol. 99, pp. 61 -67

DF 10.8 Thu 17:10 MÜL Elch

Frequency mixing of photorefractive index gratings with ferroelectric domain gratings in lithium niobate crystals — •Ulrich Hartwig[1], Michael Kösters[1], Theo Woike[1], Karsten Buse[1], Alexander Shumelyuk[2], and Serguey Odoulov[2] — [1]Institute of Physics, University of Bonn, Wegelerstraße 8, 53115 Bonn, Germany — [2]Institute of Physics, National Academy of Sciences, 252650 Kiev, Ukraine

Copper-doped lithium niobate crystals are periodically poled. Afterwards holographic gratings are recorded into this material using only diffusion for charge redistribution. Readout reveals that the principal grating with grating vector $\mathbf{K}$ is strongly suppressed. At the same time sideband gratings with grating vectors $\mathbf{K} \pm \mathbf{G}$ appear, where $\mathbf{G}$ is the grating vector of the domain pattern. From the measurements the grating vector $\mathbf{G}$ and the duty cycle DC (ratio of the width of up- and down domains) of the domain pattern can be calculated. These values are important quality criteria of the periodic structure of the sample. The findings of this work enable nondestructive quality inspection of periodically-poled lithium niobate. Furthermore, conclusions can be drawn for applications involving both holographic gratings and periodic domain structures for, e.g., hybrid distributed-feedback optical parametric oscillators.

*Financial support from the DFG (FOR 557), the Alexander von Humboldt foundation (Research Award to Serguey Odoulov), and from the Deutsche Telekom AG is gratefully acknowledged.

DF 10.9 Thu 17:30 MÜL Elch

Light-induced changes of polarization dynamics in PLZT ceramics — •T. Granzow, A. Volkenborn, and J. Rödel — FB Material- und Geowissenschaften, TU Darmstadt

Due to their excellent electrooptical properties, PLZT ceramics have been investigated since the early days of electrooptics. Most investigations have focussed on the influence of electric fields on the optical properties. The opposite effect, the influence of illumination on the ferroelectric domain structure and hysteresis is still not entirely clear. It has been shown that there is an interplay between the nucleation of ferroelectric domains, motion of domain walls and light-induced free charge carriers, but there are contradictions both in theory and in experiments if free charge carriers will help or hinder ferroelectric polarization reversal.

In this talk, we will compare the polarization behavior in PLZT 8/65/35 and PLZT 9.5/65/35 with and without illumination in the visible spectral range. We will present the ferroelectric hysteresis detected by measuring the switching current as well as the integrated polarization. To obtain the domain dynamics, the development of P on a timescale between 1 μs and 10 s under a constant electric field is examined for various field amplitudes. It will be shown that, although the difference between the illuminated and unilluminated hysteresis measurement is rather small for frequencies up to 100 Hz, there is a notable decrease of the switch-

ing time constants in the ms range. This phenomenon will be discussed within the framework of conduction band electrons facilitating domain wall movement.

DF 10.10 Thu 17:50 MÜL Elch

Theoretical modelling of optical and luminescence processes in tungstate crystals — •Yuriy Hizhnyi and Sergiy Nedilko — Faculty of Physics, Kyiv National Taras Shevchenko University, 2, block 1, Hlushkova av., 03680, Kyiv, Ukraine

Tungstate crystals AWO_4 (A = Zn, Cd, Pb) are widely used as scintillation materials in various scientific and technical applications. Despite of intensive investigations of their optical and luminescent characteristics carried out in the last decade, there is no a commonly assumed view on the origin of luminescence processes in these crystals. Profound examinations of luminescence mechanisms in tungstate crystals can be done using theoretical calculations of their electronic structures.

In our study, we use a complex approach in calculations, which combines two different methods. The electronic and optical properties of perfect AWO_4 crystals are studied by full potential Linear Augmented Plane Wave (FLAPW) method [1]. The electronic structures of the lattice defects and impurities that in general determine the luminescence properties of AWO_4 crystals are examined in the molecular cluster approach. Several types of defects are modelled in clusters constructed from 12 - 110 atoms of the crystals. The electronic structures of the clusters are calculated by the Restricted Hartree-Fock (RHF) method [2].

Results of calculations are compared with corresponding experimental data. Schemes of possible luminescence processes in AWO_4 crystals are determined on the basis of the obtained results.

[1] P. Blaha, et al., 2001, ISBN 3-9501031-1-2
[2] Schmidt M.W., et al., J.Comput.Chem., 14, 1347, (1993)

DF 11 Electric, Electromechanical and Optical Properties II

Time: Friday 10:50–13:10 Room: MÜL Elch

Invited Talk DF 11.1 Fri 10:50 MÜL Elch

Universal domain wall dynamics in ferroics and relaxors — •Wolfgang Kleemann — Angewandte Physik, Universität Duisburg-Essen, Duisburg, Germany

Domain walls in random ferroic media reveal different dynamic modes. The complete series under external *ac* fields at decreasing frequencies, f, segmental relaxation, creep, slide and switching, is observed in quantum ferroelectric $SrTi^{18}O_3$ [1], superferromagnetic $CoFe/Al_2O_3$ multilayers [2], and ultrathin ferromagnetic trilayers Pt/Co/Pt [3]. Dynamic scaling explains the transition from Cole-Cole-type segmental relaxation to creep with inverse power law dispersion as observed in periodically-poled $KTiOPO_4$ at $f_m = f_{m0}\exp(-E/k_BT)$, $f_{m0} = 3\times10^9$ Hz and E = 0.6 eV [4]. Segmental relaxation and creep are also observed in the uniaxial relaxor $Sr_{0.61}Ba_{0.39}Nb_2O_6$ [5], where wall pinning due to charge disorder-induced random electric fields is also responsible for the occurrence of nanopolar regions in the paraelectric regime, $T > T_c \approx 350$ K. Their interfaces with the paraelectric environment reveal similar dynamic modes as pinned ferroic domain walls. [1] J. Dec *et al.*, Ferroelectrics **298** (2004) 163. [2] X. Chen *et al.*, Phys. Rev. Lett. **89** (2002) 137023. [3] O. Petracic *et al.*, unpublished. [4] Th. Braun *et al.*, Phys. Rev. Lett. **94** (2005) 117601. [5] W. Kleemann *et al.*, Phys. Rev. B **65** (2002) 220101.

DF 11.2 Fri 11:30 MÜL Elch

Characterization of Periodically-Poled Lithium Niobate Crystals using External Electric Fields* — •Michael Kösters[1], Ulrich Hartwig[1], Theo Woike[1], Karsten Buse[1], and Boris Sturman[2] — [1]Institute of Physics, University of Bonn, Wegelerstraße 8, D-53115 Bonn, Germany — [2]Institute of Automation and Electrometry, 630090 Novosibirsk, Russia

A nondestructive method for characterizing copper-doped periodically-poled lithium niobate crystals (PPLN) using external electric fields is presented. The samples are irradiated with a laser beam of the wavelength $\lambda = 633$ nm; simultaneously electric fields of up to 6 kV/mm are applied. The resulting refractive index pattern inside the crystal, which is not solely due to the electro-optic effect, but also due to effects at the domain walls, creates a diffraction pattern behind the crystal. The model used to describe this pattern allows to determine important properties of PPLN such as the duty cycle. It also gives information on properties of the domain walls. This is of great importance for applications using quasi phase-matching, e.g. second harmonic generation and optical parametrical oscillation.

*Financial support from the Deutsche Forschungsgemeinschaft (FOR 557) and from the Deutsche Telekom AG is gratefully acknowledged.

DF 11.3 Fri 11:50 MÜL Elch

Trapping and Manipulation of Micro- and Nanoparticles on the Surfaces of Lithium Niobate Crystals utilizing Light-Induced Electric Space Charge Fields* — •F.Y. Kuhnert[1], J. R. Adleman[2], H. A. Eggert[1], D. Psaltis[2], and K. Buse[1] — [1]Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn — [2]Department of Electrical Engineering, California Institute of Technology, Pasadena, CA 91125

The ability to trap and to manipulate inorganic particles and organic cells of micrometer and submicrometer size plays an important role in the field of Optofluidics. Optical tweezers are well known that use high intensity laser beams to trap particles due to the field gradient of a focused laser beam. Here we try a novel approach: Irradiating a lithium niobate crystal with an inhomogeneous light pattern leads to charge separation along the c-axis which causes electrical fields. As a result strong field gradients are present in proximity of the crystal surface. In contrast to optical tweezers, the strength of the electrical field depends only on the exposure i.e. on the product of intensity and time. With a laser beam we record space-charge and field patterns of circular shape as well as space-charge gratings with period length between 20 micron and 1000 micron into a lithium niobate crystal doped with 0.05 wt% Fe. Chalk particles (˜15 micron diameter) and silicon dioxide particles (80 nm diameter) in air as well as silicon carbide particles (130 nm diameter) in liquid are trapped and moved on the crystal surface. * Financial support by the DAAD, the DFG (BU 913/17), and the Deutsche Telekom AG is gratefully acknowledged.

DF 11.4 Fri 12:10 MÜL Elch

Recording and Readout of Spatial Gratings with Femtosecond Laser Pulses* — •Dominik Maxein[1], Peter Reckenthäler[1], Oliver Beyer[1], Karsten Buse[1], Boris Sturman[2], Hung Te Hsieh[3], and Demetri Psaltis[3] — [1]Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn — [2]Institute of Automation and Electrometry, Novosibirsk, Russia — [3]Department of Electrical Engineering, California Institute of Technology, Pasadena, USA

Employing the pump-and-probe technique with short laser pulses it is possible to investigate physical processes on very short time scales. With holographic methods, one can detect small absorption and refractive index changes. It is therefore desirable to combine both kinds of measurements for the investigation of light-induced processes in materials. However, while the well-known coupled wave equations are applicable for continuous-wave light and long pulses, new aspects like the short pulse duration and geometry have to be taken into account. We present results of theoretical studies on recording of spatial gratings with two femtosecond laser pulses. Time resolved read out of resulting gratings is performed with a Bragg matched pulse at another wavelength. Instantaneous effects (Kerr effect, two-photon absorption) are taken into consideration as well as longer-lasting changes of the material due to the exposure (excitation of charge carriers). The predictions of our model are compared with results of experiments utilizing lithium niobate and calcium fluoride crystals as the recording material.

* Financial support by the DFG (award BU 913 / 13) and the Deutsche Telekom AG is gratefully acknowledged.

DF 11.5 Fri 12:30 MÜL Elch

Holographic Investigation of Lithium Niobate Crystals with Femtosecond Laser Pulses* — •Peter Reckenthäler[1], Dominik Maxein[1], Oliver Beyer[1], Boris Sturman[2], and Karsten Buse[1] — [1]Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn — [2]Institute of Automation and Electrometry, Novosibirsk, Russia

Lithium niobate is an important material for nonlinear and photorefractive applications. For short light pulses high intensities occur, and

transient nonlinearities like the Kerr-effect and free charge-carriers, become increasingly important. These effects can be serious obstacles for applications. A profound understanding of the processes on the femtosecond-timescale is therefore indispensable. Holography with femtosecond laser pulses allows to investigate charge excitation and transport processes as well as other nonlinear effects with very high temporal resolution. Volume gratings are generated with two interfering pump pulses ($\lambda_p = 388$ nm, $t_p \simeq 200$ fs) in lithium niobate crystals, and time-resolved read out is performed using a probe pulse ($\lambda_r = 776$ nm, $t_r \simeq 200$ fs). The diffraction efficiency shows mainly two features: A sharp peak with a width of the order of the pump-probe-crosscorrelation, and a plateau which is constant on the picosecond timescale. Matching the Bragg condition for the 2K contribution to the grating allows to separate different transient effects. With further experiments, it is possible to extract information about the build up of photorefractive gratings and to learn about the dynamics of charge separation on the femtosecond time scale.

* Financial support by the DFG (award BU 913 / 13) and the Deutsche Telekom AG is gratefully acknowledged.

DF 11.6 Fri 12:50 MÜL Elch

Suppression of optical damage in lithium niobate crystalsby thermo-electic oxidization* — •Matthias Falk, Theo Woike, and Karsten Buse — Physikalisches Institut, Wegelerstr. 8, 53115 Bonn

Lithium niobate crystals are a promising material for nonlinear optics. For applications, e.g. frequency mixing, undesired refractive index changes caused by intense light are a serious problem ("optical damage"). This effect originates from a light-induced redistribution of electrons between defect centers, a build-up of space-charge electrical fields, and finally the electro-optic effect. A method to suppress the optical damage is to remove all electrons, that occupy impurity sites and crystal defects, i.e. a perfect oxidization of the crystal is needed. We discovered a thermo-electric treatment, that provides an extremely strong oxidization of the crystals. Quantitative measurements of the optical damage are performed. Thermo-electrically oxidized crystals are much more robust than untreated crystals.

*Financial support of the DFG (FOR 557) and the Deutsche Telekom AG is gratefully acknowledged.