Section Dielectric Solids
Fachverband Dünne Schichten (DF)

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Overview of Invited Talks and Sessions

(lecture rooms H11 and H48; Poster C)

Invited Talks

DF 2.1	Mon	10:00–10:40	H11	**Steuerung von Licht durch nichtlineare Brechungsindexänderungen - Perspektiven für den photonischen Chip** — •Cornelia Denz, Bernd Terhalle, Christoph Bersch, Philip Jander, Jörg Imbrock
DF 3.1	Mon	14:30–15:10	H11	**Investigation of relaxor ferroelectrics by piezoresponse force microscopy** — •Vladimir Shvartsman, Wolfgang Kleemann
DF 4.1	Tue	10:00–10:40	H11	**Intrinsically Heterogeneous Ferroelectrics: Origins and Consequences** — •A. R. Bishop
DF 4.7	Tue	12:20–13:00	H11	**Order - disorder versus displacive behaviour of ferroelectric perovskites** — •Robert Blinc
DF 7.1	Tue	14:30–15:10	H11	**Nanosized ferroelectrics** — •Izabela Szafraniak
DF 8.1	Wed	14:30–15:10	H11	**Piezoelectricity and pyroelectricity in amorphous perovskite thin films** — •Alexander K. Tagantsev, Vera Lyahovitsky, David Ehre, Ellen Wachtel, Sidney R. Cohen, Konstantin Gartsman, Igor Lubomirsky
DF 9.1	Thu	10:00–10:40	H48	**Electric Field Induced Critical Points and Electromechanical Response in Relaxor Ferroelectrics** — •Zdravko Kutnjak, Robert Blinc, Jan Petzelt, Stanislav Kamba
DF 12.1	Fri	10:30–11:10	H11	**Piezoelektrische Gradientenkeramik – Herstellung und Charakterisierung** — •Ralf Steinhausen

Invited talks of the joint symposium SYSE

See SYSE for the full program of the Symposium.

SYSE 1.1	Mon	14:30–15:00	H1	**Wavy and Buckled Nanoribbons and Nanotubes: Mechanics and Applications** — •John Rogers
SYSE 2.1	Mon	16:15–16:45	H1	**Enhancing Ferroelectrics and Multiferroics using Strain** — •D.G. Schlom, M.D. Biegalski, A. Soukiassian, J.H. Haeni, J.H. Lee, R.W. Ulbricht, C.M. Brooks, Y. Jia, V. Vaithyanathan, W. Tian, X. Ke, D.A. Tenne, A.V. Rao, A. Kumar, L. Tian, A. Sharan, S. Choudhury, Y.L. Li, P. Schiffer, S. Trolier-McKinstry, X.X. Xi, V. Gopalan, L.Q. Chen, K.J. Choi, D.M. Kim, C.B. Eom, Y.B. Chen, H.P. Sun, X.Q. Pan, D.D. Fong, M.A. Zurbuchen, J.A. Eastman, P.H. Fuoss, S.K. Streiffer, P. Irvin, J. Levy, W. Chang, S.W. Kirchoefer, T. Heeg, J. Schubert, A. Bruchhausen, N.D. Lanzillotti-Kimura, A. Fainstein, R.S. Katiyar, A. Cantarero, M.E. Hawley, Q.X. Jia, C.J. Fennie, S.M. Nakhmanson, K.M. Rabe, A.K. Tagantsev, B. Velickov, R. Uecker, P. Reiche
SYSE 2.3	Mon	17:00–17:30	H1	**Patterning ferroelectric nanostructures by epitaxial strain** — •Ho Nyung Lee, Matthew Chisholm
SYSE 2.4	Mon	17:30–18:00	H1	**Curl in Photonic Crystals Induced by Drying Stresses upon Sol-Gel Infiltration** — •Vladimir Kitaev, Evangellos Vekris, Geoffrey Ozin

Sessions

DF 1.1–1.3	Sun	14:00–17:00	H11	**Tutorial "Basics of Dielectric Solids"**
DF 2.1–2.8	Mon	10:00–13:00	H11	**Internal Symposium "Nonlinearities of Photonic Materials"**
DF 3.1–3.8	Mon	14:30–17:30	H11	**Relaxor Ferroelectrics**
DF 4.1–4.7	Tue	10:00–13:00	H11	**Internal Symposium "Order/Disorder versus/with Displacive Behaviour"**
DF 5.1–5.11	Tue	10:00–13:00	H23	**Glass I (joint session with DY)**
DF 6.1–6.10	Tue	14:30–17:50	H23	**Glass II (joint session with DY)**
DF 7.1–7.9	Tue	14:30–17:50	H11	**Dielectric and Ferroelectric Thin Films and Nanostructures I**
DF 8.1–8.7	Wed	14:30–17:10	H11	**Dielectric and Ferroelectric Thin Films and Nanostructures II**
DF 9.1–9.8	Thu	10:00–13:00	H48	**Electric, Electromechanical and Optical Properties I**
DF 10.1–10.10	Thu	14:30–17:50	H48	**Dielectric and Ferroelectric Thin Films and Nanostructures III**
DF 11.1–11.31	Thu	14:30–18:00	Poster C	**Poster Session**
DF 12.1–12.6	Fri	10:30–12:50	H11	**Electric, Electromechanical and Optical Properties II**

Symposium Strain-Engineering for New Functional Structures (SYSE)

SYSE 1.1–1.4	Mon	14:30–15:45	H1	**Strain engineering in semiconductors**
SYSE 2.1–2.4	Mon	16:15–18:00	H1	**Strain engineering in ferroics and photonics**

Annual General Meeting of the Section Dielectric Solids (for members only)

We 17:30–18:30 H11

1. Zur Arbeit des Fachverbandes
2. Vorbereitung der 72. Jahrestagung der DPG
3. Wahl des Vorstandes
4. Verschiedenes

DF 1: Tutorial "Basics of Dielectric Solids"

Time: Sunday 14:00–17:00 Location: H11

Tutorial DF 1.1 Sun 14:00 H11

Fundamentals of dielectric solids — •Horst Beige — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Physik ferroischer Materialien, Friedemann-Bach-Platz 6, 06108 Halle/S.

Dielectric solids have received increasing attention in recent years, both from a fundamental perspective and from a novel applications viewpoint. There are three major trends which led to this emphasis.

One trend concerns the fact that advanced functional components are made of material systems rather than of discrete materials. Material integration issues play an increasing important role driven by the interest in integrating functions of dielectric solids into conventional semiconductor chips as well as for the evolution of multifunctional components and systems.

A second trend is the scaling of the structure size into the sub 100nm regime.

A third trend concerns the role of theory and modeling. The materials and device design are more and more accompanied and guided by modeling, e.g. by thermodynamics, finite-element methods, and ab-initio calculations.

This lecture gives an introduction to basic principles of symmetry classification, dielectric polarization, elastic, dielectric and electromechanical properties. The Landau-Ginzburg-Devonshire theory and the soft mode concept for the phase transition from an unpolar to a polar phase are also topics of this paper.

Tutorial DF 1.2 Sun 15:00 H11

Experimental determination of linear and nonlinear material properties of dielectric solids — •Martin Diestelhorst — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Friedemann-Bach-Platz 6, 06108 Halle

Dielectrics are interesting for many applications due to their elastic, electromechanic and dielectric properties. Often it is sufficient to know the linear coefficients like elastic compliance, piezoelectric coefficient and dielectric permittivity. A wide variety of experimental methods exist to determine these linear properties. Increasing the accuracy of measurements it becomes obvious that all of these properties are nonlinear. They depend on the amplitudes of external influences, e.g. the dielectric permittivity depends on the amplitude of the external electric field as well as on the external elastic stress. These higher order coefficients may be measured applying high electric fields or/and high elastic stresses to the samples under test. Additionally the progressive miniaturization often causes nonlinear behaviour, since e.g. even a small voltage applied to a dielectric film of few nanometers thickness corresponds to a high electric field strength along this direction. In practice nonlinear properties may be undesirable for many applications, but on the other hand there are special applications which could not be realized without these nonlinearities. Therefore it is necessary to characterize dielectric materials both concerning their linear and their nonlinear properties. The talk presents some experimental methods to allow for the determination of linear and nonlinear elastic, electromechanic and dielectric properties.

Tutorial DF 1.3 Sun 16:00 H11

Nanoscale dielectrics: Preparation, microstructure, properties — •Dietrich Hesse and Marin Alexe — Max Planck Institute of Microstructure Physics Halle, Germany

Nanoscale dielectrics, i.e. thin films, multilayers, and artificial superlattices of individual layer thicknesses in the sub-100 nm range, and small dielectric objects laterally structurized down to sub-100 nm lateral dimensions (e.g. nanowires and nanotubes, or regular arrays of nanostructures) are in the center of research due to their interesting properties, which are relevant under both fundamental and application aspects. Due to the large interface-to-volume ratio in such nanoscale structures, the properties of nanoscale dielectrics are particularly sensitive to the preparation method, and also to microstructural details like lattice defects. Thus interrelations between preparation, microstructure, and properties need particular attention and are currently a subject of intensive research. Relations of this type will be highlighted on the example of various dielectric, in particular ferroelectric, nanostructures and nano-objects, like pulsed-laser deposited thin films, superlattices, and nanostructure arrays, epitaxial nano-islands grown by chemical solution deposition, and ferroelectric nanotubes prepared using negative or positive templates. The role of interfaces and lattice defects for the properties, possible origins of ferroelectric size and imprint effects, and the influence of the crystallographic orientation will be demonstrated. The problem of distinguishing between intrinsic (material-related) and extrinsic (defect- and microstructure-related) properties of nanoscale dielectrics will be discussed.

DF 2: Internal Symposium "Nonlinearities of Photonic Materials"

Time: Monday 10:00–13:00 Location: H11

Invited Talk DF 2.1 Mon 10:00 H11

Steuerung von Licht durch nichtlineare Brechungsindexänderungen - Perspektiven für den photonischen Chip — •Cornelia Denz, Bernd Terhalle, Christoph Bersch, Philip Jander und Jörg Imbrock — Institut für Angewandte Physik, Westfälische Wilhelm-Universität Münster

Die Optik bietet durch ihre inhärente Parallelität und höchste Ausbreitungsgeschwindigkeit bereits zahlreiche Vorteile in der Informationsverarbeitung. Die Realisierung vieler Funktionen verlangt jedoch Elemente, die Licht direkt schalten und parallel verarbeiten können. Nichtlineare optische Effekte können solche Funktionen durch die Wechselwirkung von Licht mit Materie erzeugen, ohne zusätzliche Umwandlung in elektronische Signale zu benötigen. So kann Licht sich selbst führen, speichern oder manipulieren und damit adaptive Komponenten erzeugen - eine viel versprechende Perspektive für komplexe photonische Systeme bis hin zur der Realisierung des optischen Chips.

Insbesondere das Potential zahlreicher nichtlinearer optischer Materialien, den Brechungsindex entsprechend der einfallenden Lichtverteilung zu ändern, bietet hier die Möglichkeit, bei geringsten Lichtleistungen Material bereits derart zu strukturieren, dass adaptive Wellenleiter, optische Schaltelemente oder optisch induzierte photonische Kristalle entstehen. Im Vortrag werden die Grundlagen zur Erzeugung dieser Elemente auf der Basis photorefraktiver solitärer Strukturen sowie die Erzeugung dieser Elemente und deren Steuerung und Kontrolle durch Lichtmodulation dargestellt.

DF 2.2 Mon 10:40 H11

Holographic polymer-dispersed liquid crystals for neutron optics — •Martin Fally[1], Irena Drevenšek-Olenik[2], Mostafa Ellabban[1], Klaus Pranzas[3], and Jürgen Vollbrandt[3] — [1]Fakultät für Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Österreich — [2]Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19 und and J. Stefan Institute, Jamova 39, SI 1001 Ljubljana, Slovenia — [3]GKSS Forschungszentrum, D-21502 Geesthacht, Germany

Holographic polymer-dispersed liquid crystals (H-PDLC) are electrically switchable photonic media with large potential for optical applications.

Here, we demonstrate that H-PDLC are not only interesting for nonlinear light optics but also for neutron optics. We report strong diffraction of cold neutrons from an only 30 micrometer thick holographic polymer-dispersed liquid crystal transmission grating [1]. The nonlinearty mechanism of this photonic material and the diffraction are discussed and compared to light optical experiments performed on the same sample[2]. We finally argue, why H-PDLCs are promising candidates for fabricating not only photonic crystals but also electrically switchable neutron-optical devices.

[1] M. Fally, I. Drevenšek-Olenik, M. A. Ellabban, K. P. Pranzas, and J. Vollbrandt, Phys. Rev. Lett. **97**, 167803 (2006)

[2] I. Drevenšek-Olenik, M. Fally, and M. Ellabban, Phys. Rev. E **74**, 021707 (2006)

DF 2.3 Mon 11:00 H11

Mechanisms of holographic grating formation in silver nanoparticle suspensions * — •Helge Eggert[1], James 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 metal nanoparticles have interesting thermal and nonlinear-optical properties. The high third-order nonlinearity of metal nanoparticles at wavelengths close to the surface plasmon resonance makes such suspensions attractive, e.g., for optical switching applications. However, the optical response of these materials is still not completely understood, especially on the nanosecond time scale. To study silver nanoparticle suspensions, holographic experiments are conducted: Holographic gratings are recorded utilizing interfering nanosecond pulses. The diffraction efficiency is measured with continuous-wave light. 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 duration. 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 ms for grating spacings of several micrometers. This are indications for thermal gratings.

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

DF 2.4 Mon 11:20 H11

On the way to μJ THz pulses by optical rectification — •Eberhard Riedle[1], Balázs Bartal[2], Ida Z. Kozma[1], Andrei Stepanov[3], Gábor Almási[4], Jürgen Kuhl[5], and János Hebling[2] — [1]LMU München, Germany — [2]Dept. of Exp. Physics, Univ. of Pécs, Hungary — [3]Inst. of Spectroscopy, Russian Acad. of Science, Troitsk, Russia — [4]Dept. of Informatics in Physics, Univ. of Pécs, Hungary — [5]MPI for Solid State Research, Stuttgart, Germany

We investigate the energy scaling of sub-ps THz pulses generated by tilted pulse front excitation. With 150fs-long 500μJ pump pulses at 800nm THz energies up to 240nJ were achieved [1]. For a 1.2mm^2 pump area, the conversion efficiency of pump to THz energy had a maximum of 5x10^{-4} at 300μJ pump energy. This amounts already to a quantum efficiency of above 10%. For comparison, the maximum attainable THz pulse energy was limited to 2.1nJ at 32μJ pump energy in a line focusing geometry. To illustrate the very different type of development of the THz pulse inside the electro-optical crystal, model calculations were performed for both geometries and found to be in good agreement with the experiments. Comprehensive simulations predict that the tilted pulse front excitation allows further up-scaling of the THz pulse energy by using a larger pump spot size, still stronger pump pulses and cooling of the nonlinear crystal [2]. These measures should increase the THz energy into the μJ regime and the quantum efficiency to 50%. We also find an optimal pulse duration and crystal length for maximum resulting electric field and the potential for simple tuning of the THz center frequency.

[1] A. G. Stepanov, et al. Opt. Express 13, 5762-5768 (2005).
[2] B. Bartal et al., Appl. Phys. B (2006) DOI: 10.1007/s00340-006-2512-7

DF 2.5 Mon 11:40 H11

Optical excitation of space-charge waves in semi-insulating materials — •Mikhail Petrov[1], Valeriy Bryksin[1], Michaela Lemmer[2], and Mirco Imlau[2] — [1]Ioffe Physico-Technical Institute, St. Peterburg, Russia — [2]Department of Physics, University of Osnabrück, Germany

The application of an electric field to a semi-insulating (SI) crystal can create conditions for the existence of definite space-charge wave eigenmodes. Specific properties of these waves (dispersion law, quality factor) depend on intrinsic properties of the SI material (carrier mobility and lifetime, trap concentration, Maxwell relaxation time). Because these materials are typically good photoconductors, a proper illumination of the crystal can generate the desired space-charge waves with corresponding wave vector and eigenfrequency. This report is devoted to the discussion of a broad spectrum of the effects caused by optical excitation of space-charge waves. Some of these effects have direct analogs in nonlinear optics (for instance, complete rectification of space-charge waves reminds of optical rectification in nonlinear optics). The experiments have been performed in photorefractive crystals of the sillenite family (BSO, BTO, BGO) and SI semiconductors (CdTe:Ge, SiC, InP:Fe). New prospects of the investigations are discussed. They are the interaction of optically generated space-charge waves with magnetic field and investigation of space-charge waves in pseudo-two-dimensional structures when a crystal is illuminated with light that is absorbed in a thin surface layer of the crystal.

Supported by the DFG (projects GRK 695 and 436 RUS 17/15/07)

DF 2.6 Mon 12:00 H11

Hybrid materials with nonlinear optical properties — •Dominik Schaniel[1], Susanne Lisinski[2], Lorenz Ratke[2], and Theo Woike[3] — [1]I. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln — [2]Institut für Materialphysik im Weltraum, DLR, Linder Höhe, 51170 Köln — [3]Institut für Mineralogie, Universität zu Köln, Zülpicher Strasse 49b, 50674 Köln

Aerogels and xerogels are used as host matrices for a variety of guest materials. Due to their broad transparency range of 350-2500 nm they are especially interesting for the design of novel nonlinear photonic materials. E.g., silica-aerogels are synthesized in a sol-gel process leading to a porous network of SiO_2 particles with diameters of 3-5 nm and pore sizes in the range of 10 nm. Embedding micro- to nanoparticles of oxidic electrooptic materials or single photoactive molecules novel hybrid materials with nonlinear optical properties can be produced. We show first results on silica aerogels with embedded $KNbO_3$ and $BaTiO_3$ particles, where we investigated the efficiency of second harmonic generation as a function of particle size and particle density. Further prospects of such hybrid materials are discussed.

DF 2.7 Mon 12:20 H11

Bound soliton pairs in photonic crystal fiber — •Przemyslaw Szarniak, Alexander Podlipensky, Nicolas Joly, Chris Poulton, and Philip Russell — Max-Planck Research Group (IOIP), University of Erlangen-Nuremberg, Guenther-Scharowsky Str. 1/Bau 24, 91058 Erlangen, Germany

We demonstrate experimentally, for the first time to our knowledge, the formation of bound pairs of solitons in highly nonlinear PCF. The pairs are generated by break-up of higher order solitons, and each member of each pair experiences a different soliton self-frequency shift (SSFS), leading to a decrease in the temporal and spectral spacing between the soliton pair as the input power increases. This eventually results in the formation of a trapped pair of solitons when the spacing becomes sufficiently small. We observe that the trapped soliton pair continues to propagate along the PCF with constant frequency spacing and time delay, while the central frequency of the pair shifts to lower frequencies due to the SSFS. We also present the results of numerical calculations that confirm the experimental observations.

DF 2.8 Mon 12:40 H11

Measurement of linear and nonlinear band structures of 1D photonic crystals — •Detlef Kip, Jürgen Wisniewski, and Christian Rüter — Institut für Physik und Physikalische Technologien, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld

Arrays consisting of parallel aligned optical channel waveguides that are evanescently coupled due to the overlap of guided modes are an example of one dimensional photonic crystals. As such they can be analysed using the Floquet-Bloch approach. Due to the periodicity the linear transmission spectrum is split into bands of allowed extended Floquet-Bloch modes divided by forbidden gaps. In a nonlinear array the propagation dynamics may be altered, and nonlinear effects like modulational instabilities of Floquet-Bloch modes and energy localization, i.e., the formation of discrete solitons, occurs. So far nonlinear one dimensional waveguide arrays have been fabricated using various materials including polymers, III/IV semiconductors, or LiNbO3 and considerable work has been accomplished to study the linear and nonlinear light propagation in these systems. Recently we demonstrated that a prism coupling method can be used to measure the linear band structure and to excite pure Floquet-Bloch modes of a one dimensional periodic medium. Here we show that in a nonlinear waveguide array this method can be applied to study the temporal evolution of the propagation constant of an excited Floquet-Bloch mode and to directly measure the band structure modified by the induced nonlinear index changes.

DF 3: Relaxor Ferroelectrics

Time: Monday 14:30–17:30 Location: H11

Invited Talk DF 3.1 Mon 14:30 H11

Investigation of relaxor ferroelectrics by piezoresponse force microscopy — •Vladimir Shvartsman and Wolfgang Kleemann — Angewandte Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany

Relaxor ferroelectrics (relaxors) belong to a special group of polar oxides. In contrast to normal ferroelectrics, dynamic polar nanometer-sized regions (PNRs) appear in these materials deep in the nominally paraelectric state. On cooling a transition either into a short-range ordered clusterglass-like state or into a long-range ordered domain state occurs. In spite of numerous intense investigations the information about the evolution of the PNRs, in particular in the vicinity of the transition temperature, is still insufficient. New information about the polar structure of relaxors may be obtained by piezoresponse force microscopy (PFM). We present results of PFM studies done both on uniaxial relaxors $Sr_{1-x}Ba_xNb_2O_6$ (SBN) and on cubic relaxors $Pb[Mg_{1/3}Nb_{2/3}]_{1-x}Ti_xO_3$ (PMN-PT). Peculiarities of the polar structures below the transition temperature are analyzed. Quasi-static polar regions are revealed in a certain temperature range above T_C. In both cases the sizes of the observed clusters are much larger than expected for PNRs. The temperature dependence of the observed structures was investigated. The origin of these mesoscale polar regions, their relationship with the PNRs and their role in the phase transition are discussed.

DF 3.2 Mon 15:10 H11

Electric-field induced phase transition in near-electrode region of PbMg0.33Nb0.67O3 - 28% PbTiO3 relaxor - ferroelectric (001) single-crystal wafer — •Alexander A. Levin, Anja I. Pommrich, Torsten Weissbach, and Dirk C. Meyer — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

A (001) single-crystal PbMg0.33Nb0.67O3 - 28% PbTiO3 (PMN - 28% PT) wafer was investigated by means of Wide-Angle X-ray Scattering (WAXS) techniques in situ under the influence of an external static unipolar electric field (field strength E up to 13 kV/cm). Changes of profiles of X-ray 001 reflections of 1st and 3d orders and their rocking curves were recorded under applying the electric field along the [001] direction of the single-crystal plate. Evidences of a reversible phase transition between ferroelectric modifications of PMN-PT in a near-electrode region of about 1 micrometer depth are found. Under the influence of the static electric field, a part of the near-electrode layer (of about 5 vol. % and 15 vol. % at E = 4.5 kV/cm and 13 kV/cm, respectively) transforms from initially rhombohedral type of the structure (R, space group R3m) to another one (most probably, monoclinic Mb (space group Cm)).The transition is manifestated by change of the phase lattice constant (a = 4.0227(1) Å and c = 4.016(1) Å according to interpolation to E = 0 kV/cm for R and Mb phases, resp.), piezoelectric coefficient (d33 = 1092(14) pC/N (R) and 1735(248) pC/N (Mb), resp.) and the profile shape of the rocking curves. Financial support by the DFG research unit FOR 520 is gratefully acknowledged.

DF 3.3 Mon 15:30 H11

Relaxor ferroelectrics: ferroic clustering and phonon anomalies — •Boriana Mihailova[1], Anna-Maria Welsch[1], Bernd Guettler[2], Marin Gospodinov[3], and Ulrich Bismayer[1] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg — [2]PTB, Bundesallee 10, D-38116 Braunschweig — [3]ISSP-BAS, Blvd. Tzarigradsko Chausse 72, 1784 Sofia

Relaxor ferroelectrics are among the key materials in modern solid-state science due to their outstanding dielectric, electro-optic, and electro-elastic properties. Because of their complex local structure studies on the relaxor structure require the application of fine-scale structure-sensitive methods as inelastic light scattering, in addition to the conventional diffraction methods. Here we report on the relationship between the observed phonon anomalies and the local atomic arrangements in Pb-based perovskite-type relaxors studied on the basis of model representative lead scandium tanatalates/niobates doped with various elements. It is shown that the ferroic clustering and the development of ferroelectric state can be followed by analysing quantitatively the intensity ratios of the Raman scattering arising from the corresponding local structural distortions. The presence of point defects such as oxygen vacancies and incorporation of additional elements in the cation positions heavily influences the incipient ferroic species and suppresses the formation of proper ferroelectric state, thus favouring the non-ergodic state.

DF 3.4 Mon 15:50 H11

Crystal structure of the relaxor ferroelectric $PbSc_{0.5}Ta_{0.5}O_3$ from 300 K to 20 K — •Bernd Maier[1], Jörg Ihringer[1], Boriana Mihailova[2], and Ulrich Bismayer[2] — [1]Institut für Angewandte Physik, auf der Morgenstelle 10, 72076 Tübingen — [2]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, 20146 Hamburg

High resolution X-ray powder data of $PbSc_{0.5}Ta_{0.5}O_3$ (PST) collected an $20 < T < 300\,K$ with a modified image plate Camera (Huber) in Guinier geometry exhibits diffuse phase transitions from the cubic ($Pm3m$) paraelectric state to the rhombohedral ferroelectric state. Small domains of Sc/Ta-ordering lead to an doubled unit cell ($Fm3m$) which gives weak and broad reflections. Also, the thermal dependence of lattice constants will be given.
Changes in behaviour due to Ba doping at the Pb sites and Ru doping at the Sc/Ta sites will be discussed.

DF 3.5 Mon 16:10 H11

Defect structure in acceptor- and donor-doped PZT compounds — •Ruediger-A. Eichel — Edurad-Zintl-Institut, TU Darmstadt

The macroscopic properties of functional PZT compounds may considerably be modified by doping with rare-earth or transition-metal ions. High-frequency and multi-pulse EPR provides a local probe to characterize functional centers and defect states in acceptor- and donor-doped PZT ceramics.

In hard-doped Fe^{3+}:$PbTiO_3$, high-frequency EPR prooved the existence of an iron-oxygen vacancy defect associate - the orientation of this defect dipole being oriented persistently along the crystallographic c-axis and anti-parallel with respect to the orientation of spontaneous polarization. For the other end-member composition Fe^{3+}:$PbZrO_3$, again the creation of defect associates was observed. However, there is no persistent orientation of the corresponding defect dipole, but rather a 'multi-site* situation that is characterized in a way that the compensating oxygen vacancy may be localized at any of the six possible neighbour oxygen sites.

In contrast, acceptor-type Cu^{2+}:PZT modifications show no association of the Cu^{2+} functional centers to charge-compensating oxygen vacancies. This conclusion is based on the observation of an orientation-independent, quasi-isotropic ^{207}Pb-hyperfine coupling. As a consequence, considering the EPR results it could be predicted the Cu^{2+}-modifications induce an ionic conductivity in PZT compounds.

DF 3.6 Mon 16:30 H11

Surface barrier layer contacts and colossal dielectric constants in calcium-copper-titanate — •Stephan Krohns[1], Peter Lunkenheimer[1], Stefan Ebbinghaus[2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany — [2]Solid State Chemnistry, Universitiy of Augsburg, 86135 Augsburg, Germany

For tomorrows energy-storage technologies and wireless electronics, materials with high dielectric constants are in great demand. A prominent example for this kind of materials is the perovskite-related $CaCu_3Ti_4O_{12}$ (CCTO) [1]. It shows dielectric constants up to 10^5 being constant over a relatively broad temperature range. The origin of the colossal dielectric constant in CCTO is controversially debated and ascribed to internal barriers (e.g. grain boundaries) or external surface effects (e.g. electrode polarisation) [2,3]. A variety of single and polycrystalline samples, subjected to different treatments, like annealing, surface polishing and surface metallization, are investigated by broadband dielectric spectroscopy. There are at least two relaxations in CCTO, the second one being connected to even higher absolute values than the first one. From our experiments we obtain strong indications for a surface related origin of both relaxation modes and the colossal dielectric constants in CCTO.

[1] C.C. Homes, T.Vogt, S.M. Shapiro, S. Wakimoto, and A.P.

Ramirez, Science 293, 673 (2001). [2] P. Lunkenheimer, et al., Phys. Rev. B 66, 052105 (2002). [3] P. Lunkenheimer, et al., Phys. Rev. B 70, 172102 (2004).

DF 3.7 Mon 16:50 H11

Characterization of piezo ceramics on the nanoscale by Conducting AFM — Yue Hou, •Andrei Andreev, and Christian Teichert — Institute for Physics, University of Leoben, Franz-Josef-Str., 18, A-8700 Leoben, Austria

The Conducting Atomic-Force Microscope (C-AFM) is a conventional AFM working in contact mode, where the usual AFM tip is replaced by a conductive tip. Between the tip and the sample a voltage is applied and the resulting current is measured using a special amplification circuit. The C-AFM is well known as a valuable tool for nanometer scale electric characterization of very thin oxide layers [1,2].

In this work we demonstrate the analytical capabilities of C-AFM technique for spatially resolved electrical investigations of cross sectional piezo ceramic samples (PZT). The applicability of C-AFM for the characterization (2D lateral current mapping and local I-V curves) of such complex nanostructures is presented and discussed in terms of electrical active grain boundaries in the ceramic matrix in the vicinity of the metal electrodes.

[1] S. Kremmer, S. Peissl, C. Teichert, F. Kuchar, H. Hofer, Mat. Sci. Eng. B102 (2003), 88.

[2] S. Kremmer, H. Wurmbauer, C. Teichert, G. Tallarida, S. Spiga, C. Wiemer, M. Fanciulli, J. Appl. Phys. 97/7 (2005), 74315-1-7.

DF 3.8 Mon 17:10 H11

Stability of polypropylene ferroelectrets against ionizing alpha-radiation — •Mario Dansachmüller, Ivan Minev, Francisco Camacho-Gonzalez, Simona Bauer-Gogonea, Reinhard Schwödiauer, and Siegfried Bauer — Soft Matter Physics, Johannes-Kepler University, Altenbergerstraße 69, 4040 Linz, Austria

Cellular polypropylene (cPP), a thin foil containing flat lens-like voids displays similarities to ferroelectric materials, after internally charging the surfaces of the voids, hence cPP is called a ferroelectret. The piezoelectric coefficient of charged cPP is proportional to the effective surface charge on the voids. By analyzing the nonlinearities in the current response of a charged cPP capacitor upon application of a sinusoidally varying ac-voltage, the piezoelectric response of cPP is directly determined from an electrical measurement alone. Samples of cPP with a density of 330 kg/m* were irradiated by ionizing alpha-radiation of a Ra-226 (4.87 MeV) or an Am-241 (5.64 MeV) source for several hours corresponding to doses of up to 2000 Gy or 20 000 rad. The charge decay was measured in-situ during the irradiation by continuously recording the first and second harmonic contribution of the current response, by means of digital lock-in amplifiers. A decay of the relative surface charge of 5 % was observed for a dose of 50 Gy. The smallest resolvable dose in a temperature controlled measurement was found to be 1.4 Gy.

DF 4: Internal Symposium "Order/Disorder versus/with Displacive Behaviour"

Time: Tuesday 10:00–13:00 Location: H11

Invited Talk DF 4.1 Tue 10:00 H11

Intrinsically Heterogeneous Ferroelectrics: Origins and Consequences — •A. R. Bishop — Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

We describe expectations of intrinsic heterogeneity and coexistence of phases in some classes of ferroelectric materials. Understanding such behavior is essential to rationalize and motivate experiments, and to optimize materials for applications. We emphasize ferroelectrics as highly anisotropic, polarizable materials. We suggest modeling approaches based on coexisting anisotropic short- and long-range interactions arising from the coupling of spin, charge and lattice (strain) in multi-orbital situations, and the sympathetic proximity of solid-solid structural phase transitions with extended multiscale precursor regimes of twinning, tweed,etc.

DF 4.2 Tue 10:40 H11

High resolution NMR of phase transitions: experimental criteria for order/disorder vs. displacive behaviour — •Naresh Dalal — Florida State University and National High Magnetic Field Laboratory

Traditionally, phase transitions have been classified as of either 'order-disorder' or 'displacive' type. Recently, however, there has been increasing evidence that this classification should be reexamined, and that many systems that were considered as proto-types of order-disorder type, actually exhibit strong features indicating the role of 'displacive' mechanism as well. We have found that among other techniques for probing this question, the modern high-field, high-resolution nuclear magnetic resonance (NMR) could prove to be perhaps the most sensitive and easily accessible method. This presentation will discuss the basics of this tenet, experimental details and recent data, with a conclusion that perhaps most such transitions involve both types of features, and should thus be reclassified as such.

DF 4.3 Tue 11:00 H11

Peculiarities in the dielectric and heat capacity responses of strontium barium niobate — •Jan Dec[1], Zdravko Kutnjak[2], Severyn Miga[1], Wolfgang Kleemann[3], George Cordoyiannis[2], Vladimir Shvartsman[3], Tadeusz Łukasiewicz[4], and Marek Świrkowicz[4] — [1]Institute of Physics, University of Silesia, Pl-40-007 Katowice, Poland — [2]Josef Stefan Institute, P. O. Box 3000, SV 1001 Ljubljana, Slovenia — [3]Angewandte Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [4]Institute of Electronics Materials Technology, Pl-01-919 Warsaw, Poland

The ferroelectric materials SrxBa1-xNb2O6 (SBN) are particular among ferroelectrics since investigations of the c-axis linear dielectric response of SBN single crystals with x = 0.40, 0.50, 0.61 and 0.75, (SBN40, SBN50, SBN61, SBN75) reveal a crossover from conventional ferroelectric (SBN40) to relaxor (SBN75). The temperature dependencies of the dielectric susceptibility were measured in the range 10-2 - 10-5 Hz. Analysis of the data shows that the Curie point TC of SBN40 lies on a linear extrapolation of the "estimated" TC*s of the other SBN crystals. Correspondingly, a change from "normal" domains (SBN40) to smaller ones with fractal-like boundaries was observed by piezoresponse microscopy. The estimated TC*s correspond with anomalies in heat capacity runs. A difference in these around TC shows a non-vanishing latent heat. This complies with the positive sign of the third order nonlinear dielectric susceptibility which decreases when increasing the amplitude of the probing field. Thus, the phase transition in SBN is first order and converts into critical at higher fields.

DF 4.4 Tue 11:20 H11

Is the observation of a soft mode sufficient to characterize a transition as displacive? The case of SrTi18O3 — •Annette Bussmann-Holder — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Deutschland

For many years it has been believed that ferroelectric phase transitions can be strictly classified as either being of displacive or of order / disorder type. First doubts about this clear cut distinction came from local probes like EPR and NMR, where evidence for order / disorder behaviour was obtained in systems exhibiting classical soft mode behaviour. A similar seemingly controversial situation is now also encountered in the isotope induced ferroelectric system SrTi18O3 where long wave length testing experiments reveal classical mode softening whereas NMR and nonlinear dielectric response support order / disorder dynamics. It is shown here that displacive and order / disorder dynamics coexist in SrTi18O3, however obeying different length and time scales. Far above the actual lattice instability self-induced polar nano-domains are formed which stem from optic-acoustic mode coupling and are characterized by order / disorder dynamics, whereas simultaneously a classical soft mode exists in the long wave length limit. The polar state is novel in this compound since an incomplete ferroelectric state forms below Tc.

DF 4.5 Tue 11:40 H11

Domain states and critical behaviour of random field Ising model systems — •Wolfgang Kleemann — Angewandte Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

The charge-disordered three-dimensional uniaxial relaxor ferroelectric Sr0.61Ba0.39Nb2O6 splits up into metastable polar nanoregions (PNRs) and paraelectric interfaces upon cooling from above Tc. The frozen PNRs are verified by piezoresponse force microscopy, respond domain-like to dynamic light scattering and dielectric excitation, reveal non-ergodicity at via global aging, and coalesce into polar nanodomains below Tc. Contrastingly, the percolating system of unperturbed interfaces becomes ferroelectric with two-dimensional Ising model-like non-asymptotic critical exponents, , and , as corroborated by ac calorimetry, second harmonic generation, and susceptometry, respectively [1,2]. Signatures of the crossover into the asymptotic critical behavior of the three-dimensional random-field Ising model (RFIM) will be discussed and compared to corresponding features of the dilute axial antiferromagnet in an external magnetic field (DAFF). [1] W. Kleemann, J. Dec, V. V. Shvartsman, Z. Kutnjak, Th. Braun, Phys. Rev. Lett. 97 (2006) 065702. [2] W. Kleemann, J. Phys.: Cond. Matter 18 (2006) L253.

DF 4.6 Tue 12:00 H11

Possible frustrated ferroelectricity and very high K of oxide perovskites — •Francois Gervais, Virginie Brizé, Cécile Autret, Jérôme Wolfman und Monique Gervais — LEMA UMR 6157 CNRS/CEA Universite François Rabelais Tours (France)

The integration of capacitors on silicon with the highest possible capacity per surface unit is a challenge of mobile microelectronics. One way to achieve this task is to use materials with very high dielectric constant. The origin of the dielectric constant in barium titanate takes place in displacive-order-disorder crossover mechanisms. CaCu3Ti4O12 (CCTO) opens a new way to still better properties with a dielectric constant in excess of 10,000 in the single crystal. In addition, the property little varies with temperature around room temperature. The observation of diffuse scattering in CCTO was recently observed and a frustrated ferroelectricity mechanism was proposed. When CCTO is substituted with only 0.5 % of transition metal element such as Fe or Mn, the permittivity drops down to 100, the contribution due to phonons. Electron spin resonance displays a rapid downshift of the resonance line of copper towards low magnetic field below 30 K when substituted, correlated with dielectric data. The downshift is the signature of local magnetic field. A possible multiferroic character is therefore evidenced. These results will be discussed in terms of frustrated ferroelectrics scenarios.

Invited Talk DF 4.7 Tue 12:20 H11

Order - disorder versus displacive behaviour of ferroelectric perovskites — •Robert Blinc — J. Stefan Institute, Ljubljana, Slovenia

Whereas the first microscopic theory of BaTiO3 was based on order-disorder behavior, later on BaTiO3 has been considered as a classiacal example of displacive soft mode transitions, which can be described by anharmonic lattice dynamics. Already more than twenty years ago, electron paramagnetic resonance (EPR) measurements performed on Mn4+, Cr3+, and Fe3+ doped BaTiO3 by Müller et. al. seriously questioned the pure displacive character of the phase transitions. Recently, the problem has been studied by quadrupole perturbed 47Ti and 49Ti NMR. It was clearly shown that the Ti sits off-center not only in the tetragonal but also in the cubic phase. This off-center scenario confirms theoretical studies which showed a combined displacive and order-disorder character of the transitions in BaTiO3. The model clearly shows the characteristics of a displacive transition, but with a simultaneous partial ordering of the Ti subsystem as an additional order-disorder feature. Similar results were obtained for SrTiO3 and 18O enriched SrTiO3. Here we present quadrupole perturbed 17O NMR data of both BaTiO3 and SrTiO3 which throw some new light on the role of the oxygen network as well as the A and B ions at the phase transitions in ABO3 perovskite lattices.

DF 5: Glass I (joint session with DY)

Time: Tuesday 10:00–13:00 Location: H23

DF 5.1 Tue 10:00 H23

Connection of the slow β-relaxation and physical aging in metallic glasses — •Jörg Hachenberg, Dennis Bedorf, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Metallic glasses are commonly used as model systems for glassy dynamics. This is due to the fact that their interactions can be simplified as such of hard spheres. Special attention has been attracted by recent experimental studies [1] and computer simulations [2] revealing the existence of a secondary, slow β-relaxation as a universal feature of the glass transition. Here, heat rate dependant mechanical spectroscopy is used to investigate the connection between this β-relaxation and physical aging, commonly described as a change in fictive temperature. The close dependence of both phenomena can be interpreted as a single relaxation showing up on two timescales (heating rate resp. spectroscopy frequency). It is proposed that both phenomena share a common origin.

This work is supported by DFG, Graduiertenkolleg 782 and SFB 602, TP B8.

[1] J. Hachenberg, K. Samwer, J. Non-Cryst. Sol. 352, 5110 (2006)
[2] H. Teichler, Phys. Rev. E 71, 031505 (2005)

DF 5.2 Tue 10:15 H23

Fast β-relaxation of Na in Na_2O-xB_2O_3 melts — •Florian Kargl[1], Andreas Meyer[2], and Michael Marek Koza[3] — [1]Physik Department E13, TU München, 85748 Garching, Present Address: Department of Applied Physics, Chalmers University of Technology, 41296 Göteborg, Schweden — [2]Physik Department E13, TU München, 85748 Garching, Permanent Address: Institut für Raumsimulation, DLR, 51147 Köln — [3]Institut Laue-Langevin, 38042 Grenoble, France

We report on a fast β-relaxation process in a network-glass forming system that is up to the melt a fast-ion conductor. The process is evidenced by means of quasielastic neutron scattering [1]. The data are analysed in the framework of the mode-coupling theory (MCT) of the liquid to glass transition [2]. It is shown that this fast β-relaxation process, that can consistently be described within the framework of this theory, prepares the α-relaxation of the fast diffusing Na ions. We discuss the q- and T-dependence of the relevant parameters of the β-scaling law of the MCT and its dependence on Na concentration.

[1] F. Kargl, A. Meyer, M. M. Koza (submitted).
[2] W. Götze, J. Phys.: Condens. Matter **2**, 8485 (1990).

DF 5.3 Tue 10:30 H23

Microscopic mechanism of the β-process in metallic glass formers: molecular dynamics results for NiZr — •Helmar Teichler — Inst. f. Materials Physics, University of Göttingen

For glass formers around and below the dynamical critical temperature Tc of mode coupling theory (MCT), the fluctuation spectrum shows the β-regime in the time domain as precursor of the final α-decay. Recently, the β-regime has re-attracted much interest due to observation of the β-excess wing in spectroscopic data of a metallic glass by Rösner, Samwer, and Lunkenheimer (Europhys. Lett. 92, 105701(2004)) and the evaluation of the interconnection between Cole-Cole peak and spectral properties of the β-regime in the MCT by Sperl (PRE, 74, 011503(2006)). Here we address the question of the microscopic mechanisms that take place in the corresponding frequency regime in metallic glasses. Regarding this, molecular dynamics simulation data of vitrifying Ni0.5Zr0.5 melts are investigated by studying their inherent structure dynamics in order to eliminate the masking, predominant effect of thermal single-particle vibrations. Analysis of the remaining dynamics by nearest neighbour correlation functions, aimed at identifying topological fluctuations of the system, yields reversible over-barrier transitions of correlated chains of atoms as source of a β-peak between single-particle vibrations and the α-decay.

DF 5.4 Tue 10:45 H23

Liquid-to-glass transition of bulk-glass forming Cu60Ti20Zr20 alloy by molecular dynamics simulations — •Xiujun Han[1,2] and Helmar Teichler[1] — [1]Inst. f. Materials Physics, University of Göttingen — [2]IFF, Forschungszentrum Jülich

The present work reports results from molecular dynamics studies about microscopic structure and dynamics of the ternary, bulk metallic

glass forming Cu60Ti20Zr20. In detail we consider nearest neighbour numbers, specific heat, simulated glass temperature, diffusion coefficients, and the incoherent intermediate scattering function (ISF). The applied atomic model reproduces well experimental X-ray data of total radial distribution function. It provides for Cu60Ti20Zr20 a structure with marked intermediate range order. The incoherent ISFs are analyzed within an extension of the mode coupling theory (MCT), where the memory kernel is evaluated from Laplace transform of the ISF. The dynamics of the system fulfils in most respects the predictions of the MCT, up to a suppression of the algebraic t^{-a}-decay in the early β-range, which is traced back to effects of single particle vibrations in the effective memory kernel that are not fully included in the MCT. As by-product, our investigation provides a method to re-construct, around the critical temperature, major parts of the memory kernel from λ and the plateau-value of the ISF.

DF 5.5 Tue 11:00 H23

Neutron scattering on levitated metallic droplets — •Andreas Meyer[1], Dirk Holland-Moritz[1], Sebastian Stueber[2], Thomas Hansen[3], and Tobias Unruh[4] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Physik Department E13, TU München — [3]ILL, Grenoble — [4]FRM-II, TU München

We report on first quasielastic neutron scattering experiments on metallic droplets using an electromagnetic levitation device on the neutron time of flight spectrometer ToF-ToF of the FRM-II. With this containerless processing undercoolings of the liquids up to 230K below the melting point were achieved. In binary ZrNi and ternary ZrNiAl glass forming melts the undercooling leads to a slowing down of the atomic mobility. The relation to the atomic dynamics in bulk glass forming metallic alloys in a Zr base will be discussed. We measured static structure factors of these systems on the neutron diffractometer D20 of the ILL. By isotopic substitution partial structure factors are accessible in liquid ZrNi. The partial structure factors also serve as an input for numerical mode coupling calculations.

15 min. break.

DF 5.6 Tue 11:30 H23

Understanding the fragility of supercooled liquids in terms of the properties of the potential energy landscape — •Andreas Heuer — Inst. f. Phys. Chemie, Corrensstr. 30, 48149 Münster

According to the Angell representation supercooled liquids are classified according to their fragility, i.e. the degree of non-Arrhenius behavior. Although in recent years fragility has been empirically correlated with different properties such as, e.g., mechanical behavior no microscopic understanding of the fragility exists. We report computer simulations of different glass-forming systems (silica, binary Lennard-Jones) where a detailed characterization of the potential energy landscape has been achieved. A crucial parameter is the crossover energy scale above which the local dynamics is fluid-like and below which it becomes activated. For these systems the macroscopic diffusion constant can be analytically expressed in terms of landscape parameters, reflecting its thermodynamic properties and its local dynamics. In this way we can show that the fragility strongly depends on the crossover energy scale and that for fragile systems the crossover to activated behavior only starts for very low-energy configurations. This result is interpreted in qualitative terms.

DF 5.7 Tue 11:45 H23

Molecular dynamics of a bioprotective fluid confined to nanopores — •Nicolas Ubrig[1], Rémi Busselez[2], René Berwanger[1], Denis Morineau[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2, Experimentalphysik, Universität des Saarlandes, Postfach 151150, 66 041 Saarbrücken, Germany — [2]GMCM, campus de Beaulieu, 35042 Rennes Cedex, France

We study structure and molecular dynamics of a bioprotective fluid. This is a solution of glycerol and trehalose , the glass transition of which depends on the mixing ratio. The fluid is confined in parallel rodlike nanopores of a silicon matrix. Different techniques such as temperature dependent NMR, Raman-, infrared- and dielectric spectroscopy are applied in order to detect confinement-induced deviations from the bulk behavior.

DF 5.8 Tue 12:00 H23

Continuous Time Random Walk Description of the Dynamics of a Model Glass Former — •Oliver Rubner and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster

In this work we present an analysis of data obtained by simulations on a 65 particle binary Lennard-Jones Mixture (BMLJ65). We show that the dynamics of this system can be interpreted on the grounds of a Continuous Time Random Walk (CTRW) description. The basic assumptions of the CTRW model are well fulfilled and thus the picture of spatially and temporally independent jump processes between metabasins is supported.

Given the waiting time distribution of the jumps, it is then possible to deduce analytically some of the properties of the incoherent scattering function F(q,t). These predictions are compared to the numerical data and show very good agreement which supports strongly the notion of the BMLJ65-dynamics as a CTRW-process.

DF 5.9 Tue 12:15 H23

Complex Dynamics in a Binary Glass Former investigated by Dielectric Spectroscopy — •Philipp Gutfreund, Thomas Blochowicz, and Bernd Stühn — TU Darmstadt

Previous work on binary glass forming mixtures showed pronounced dynamic heterogeneities and a broad distribution of relaxation times of the smaller molecules in the mixture and in some cases even a distinct secondary relaxation peak was observed. It was also demonstrated that an additional power law contribution at the high frequency side of the main relaxation peak in neat glass-formers, called excess wing, can be separated as a distinct secondary relaxation peak if the molecule is contained in a slower matrix.

In the present work a mixture of Methyl-Tetrahydrofuran (M-THF) in Tristyrene was investigated by dielectric spectroscopy. The dielectric spectra are dominated by the smaller M-THF molecules due to the much stronger dipole moment. Calorimetry measurements show full miscibility in the whole concentration and temperature range. Pure M-THF is known to show a pronounced high frequency wing and a small secondary relaxation process, it is shown that in the mixtures several other processes emerge. The fastest of these processes seems to show certain typical signs of liquid dynamics far below T_G of the mixture. The fact of coexisting glassy and liquid states in a binary mixture below T_G was already shown in NMR measurements [1] and was previously anticipated by theoretical considerations [2].

[1] T. Blochowicz et al., J. Phys. Chem. B 103 (1999) 4032
[2] J. Bosse and Y. Kaneko, Phys. Rev. Lett. 74 (1995) 4023

DF 5.10 Tue 12:30 H23

Ab-inito calculations of atomic cluster configurations for ion conducting glasses — •Christian Müller and Philipp Maass — Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany

Ab-inito quantum mechanical simulations of atomic configurations are carried out in order to explore structural properties of ion conducting glasses and in order to develop effective pair potentials for molecular dynamics simulations. Such potentials are of crucial importance for the modelling of ionic transport properties, which require a realistic identification of ion-sites and diffusion pathways [1]. In previous work mostly small structural units of a glass with high symmetry were considered. The computational power nowadays allows one to simulate much larger clusters, and to take into account the medium range order by means of Hartree Fock and density functional theory calculations. We present calculations for lithium borate and lithium sulphate glasses. In particular a comparison of calculated and experimental infra-red and Raman spectra is shown, which allows to judge the quality of the energy-optimized disordered cluster configurations.

[1] C. Müller, E. Zienicke, St. Adams, J. Habasaki, P. Maass, Phys. Rev. B, in press; condmat/0607523

DF 5.11 Tue 12:45 H23

Evaluation of effective one-particle potentials for the identification of ion conduction pathways in glasses — •Egbert Zienicke, Christian Müller, and Philipp Maass — Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany

The energetic characteristics of sites and the topology of diffusion pathways of mobile ions in network glasses play a key role for the understanding ion transport in vitreous electrolytes [1], which are used in many different technological applications. In molecular dynamics simulations of such systems the sites and diffusion pathways can be identified from the local number density of mobile ions determined from their motion [2,3]. Here we study the possibility of determining them from

the time-averaged immobile network structure by applying an effective one-particle potential. To this end we compare the results of such analysis with those obtained from molecular dynamics simulations of lithium silicate glasses at various temperatures and compositions. In addition a comparison is made to results obtained from a bond valence analysis [3].

[1] W. Dieterich, P. Maass, Chem. Phys. **284**, 439 (2002).

[2] H. Lammert, M. Kunow, A. Heuer, Phys. Rev. Lett. **90**, 215901 (2003).

[3] C. Müller, E. Zienicke, St. Adams, J. Habasaki, P. Maass, Phys. Rev. B, in press; condmat/0607523.

DF 6: Glass II (joint session with DY)

Time: Tuesday 14:30–17:50 Location: H23

DF 6.1 Tue 14:30 H23

Mikrostrukturierung silbernanopartikelhaltiger Gläser durch elektrische Felder — •Stefan Wackerow[1], Amin Abdolvand[2], Gerhard Seifert[1] und Heinrich Graener[1] — [1]FG Optik, Institut f. Physik, MLU Halle-Wittenberg, Hoher Weg 8, 06120 Halle — [2]LPRC, University of Manchester, UK

Silbernanopartikel haben eine charakteristische Absorptionsbande im optischen Spektralbereich, die durch Oberflächenplasmonen hervorgerufen wird. Silberpartikel in Glas finden Anwendung als Farbfilter, bzw. in Form elliptischer Partikel als Polarisatoren. Mögliche neue Anwendungen sind mikroskopische optische Bauelemente, die die besonderen optischen Eigenschaften der Partikel ausnutzen.

Ein technisch einfacher Weg zur Erzeugung von Strukturen in silberpartikelhaltigen Gläsern ist die Auflösung von Partikeln in starken elektrischen Feldern. Dazu werden zwei Elektroden auf das Glas gepresst und bei einer Temperatur um $250°C$ an diese eine Spannung von etwa $1kV$ angelegt. Unter der Anode entsteht dadurch ein kationenarmer Bereich, der eine um mehrere Größenordnungen geringere Leitfähigkeit als das unveränderte Glas hat. Über diese wenige μm dicke Schicht fällt der größte Teil der anliegenden Spannung ab, wodurch Feldstärken um $10^8 V/m$ erreicht werden. Diese starken elektrischen Felder führen zur Ionisierung und Zerstörung der Partikel.

Benutzt man als Anode einen leitfähigen photonischen Kristall aus makroporösem Silizium, erhält man im Glas eine Partikelverteilung, die der inversen Struktur des photonischen Kristalls entspricht und die theoretisch eine photonische Bandlücke aufweisen kann.

DF 6.2 Tue 14:50 H23

Characterization of silver nanoparticles in glasses by X-ray absorption spectroscopy — •Jörg Haug, Manfred Dubiel, Holger Kruth, and Angelika Chassé — Department of Physics, Martin Luther University Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06108 Halle, Germany

Glasses containing metal nanoparticles are of interest because of their specific linear and non-linear optical properties. In the present work, there are represented structural investigations of Ag nanoparticles as well as of neighbourhood of Ag ions embedded in the glass matrix by means of EXAFS spectroscopy at the Ag K-edge. In a first step, EXAFS investigations are reported concerning the thermal expansion behaviour of bulk silver to test this method for investigations of nanoparticles. In a second step, in situ experiments at elevated temperatures of particle generation are described in order to evaluate the elementary processes of particle formation as well as the specific structure of nanoscaled particles.

DF 6.3 Tue 15:10 H23

Finite size effect of the conductivity of sputtered lithium-borate glasses — •Frank Berkemeier, Mohammad Reza Shoar Abouzari, and Guido Schmitz — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster

The specific dc-conductivity of ion-conducting, sputtered glass films of the compositions $x\,Li_2O \cdot (1-x)\,B_2O_3$, with $x = 0.15$, 0.20 and 0.35, are determined by temperature dependent impedance spectroscopy. The thickness of the films varies between 7 nm and 1000 nm. In the case of relatively thick glass films (> 100 nm) each glass composition shows a specific dc-conductivity independent of the film thickness. For glasses with less than 20% alkali oxide, a significant increase of the specific dc-conductivity of about three orders of magnitude is observed, when decreasing the film thickness down to some nanometers. Three different models are suggested to explain this non-trivial 'finite size effect': structural modifications at the interfaces between glass layer and metallic electrode, formation of space-charge regions at the interfaces, and the existence of ion-conducting pathways inside the glass layers. Computer simulations based on percolation theory are presented to show the link between the experimental data and the assumption of conducting clusters inside the glass films.

DF 6.4 Tue 15:30 H23

Evidence for fast interfacial ion conduction in nanostructured solid electrolytes — •Ahmet Taskiran[1], Andre Schirmeisen[1], Harald Fuchs[1], Hartmut Bracht[2], and Bernhard Roling[3] — [1]Physikalisches Institut,Wilhelm-Klemm-Str.10,48149 Münster,Germany — [2]Institut für Materialphysik,Wilhelm-Klemm-Str.10,48149 Münster,Germany — [3]Intsitut für Physikalische Chemie,Hans-Meerwein-Str.,35032 Marburg,Germany

Solid ion conductors are used for applications like super-capacitors, high storage batteries and chemical sensors. Recent investigations have revealed that the overall conductivity can be enhanced by creating interfaces between different phases of the ion conductor. However, more detailed investigations have to be carried out on the nanoscopic length scale in order to understand the ion transport mechanism in the bulk and at the interface. We use electrostatic force microscopy (EFM) operating in the non-contact mode to measure the ionic conductivity in nanoscale volumes. In this method the temperature dependent ion conductivity was monitored in the range from 100 K to 675 K, yielding the activation energies of the ion hopping processes [1]. This work mainly focuses on the interfacial conductivity between the nanocrystallites and the glass phases of a partially crystal. LiAlSiO sample. Additionally to the activation energies found for the nanocrystallites and glass phase, which are in good agreement with macroscopic results [2], we identified a third activation energy, which can be attributed to the interfacial ion conductivity. [1] Schirmeisen et al., Appl. Phys. Lett. 85(2004)2053 [2] Roling et al., Phys.Chem.Chem.Phys. 7(2005)1472

DF 6.5 Tue 15:50 H23

Thickness-dependence of dc-conductivity in $Li_2O - B_2O_3$ Glasses — Mohammad Reza Shoar Abouzari, Frank Berkemeier, and •Guido Schmitz — Institut für Materialphysik, Universität Münster, Wilhelm-Klemm Str. 10, D-48149 Münster

Thin films of $(x)Li_2O \cdot (1-x)B_2O_3$ glasses with different concentrations of Li_2O, $0.15 < x < 0.35$, are prepared by ion-beam sputtering.The thickness of glass films vary from 1400 nm down to 7 nm. Thin metallic films of Al Li on each sides of glass film serving as metallic electrodes. To determine dc-conductivity of glass layers we used impedance spectroscopy at different temperatures. Considering the system of glass layer and electrodes as two parallel (R+CPE) circuits, the measured data are described by Nyquist diagrams and the specific dc-conductivities of the glass layers are determined. It is observed that the specific dc-conductivity depend significantly on the layer thickness. For x = 0.2, the specific dc-conductivity of layers with a thickness between 700 nm and 100 nm is constant, while it increases monotonously for thinner layers with a thickness of 100 nm down to 7 nm with decreasing of the thickness. The increase of dc-conductivity amounts to three orders of magnitude. The obtained result for x = 0.15 shows the thickness dependency of the dc-conductivity up to 300 nm. It seems that this peculiar behaviour of the glass films stems from finite size effects disappears with increasing of layer thickness.

DF 6.6 Tue 16:10 H23

A binary Yukawa mixture under shear: A computer simulation study — •Jochen Zausch and Jürgen Horbach — Inst. f. Physik, Universität Mainz, Staudinger Weg 7, 55099 Mainz

Extensive Non-Equilibrium Molecular Dynamics (NEMD) simulations are performed to investigate a binary mixture of like-charged colloids under shear. The interactions between the colloidal particles are mod-

elled by an effective screened Coulomb (Yukawa) potential, without considering explicitly any solvent degrees of freedom. The system is coupled to a DPD thermostat while determining dynamic properties in equilibrium. The DPD thermostat is also used for the NEMD runs where the system is sheared by means of Lees-Edwards boundary conditions. We investigate the dynamic properties in equilibrium and at different constant shear rates in steady state. Moreover, we study how the sheared system relaxes back to equilibrium when we suddenly switch off the shear. To this end, we consider a dynamic four-point susceptibility that measures fluctuations around the mean dynamics.

DF 6.7 Tue 16:30 H23

Free energy fluctuations in the Sherrington Kirkpatrick spin glass — •Martin Goethe and Timo Aspelmeier — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

A new numerical method of calculating the sample to sample fluctuations ΔF of the free energy in the Sherrington Kirkpatrick spin glass will be presented which is based on an interpolating Hamiltonian and works for all temperatures $0 < T < \infty$. By its use the scaling behaviour of ΔF in the spin glass phase is obtained. It strongly disagrees with previous numerical studies at zero temperature. Finally possible explanations for the difference and arising consequences will be discussed.

DF 6.8 Tue 16:50 H23

Free energy fluctuations and chaos in mean-field spin glasses — •Timo Aspelmeier — Institut für Theoretische Physik, Universität Göttingen

The sample-to-sample fluctuations ΔF of the free energy in the mean-field Ising spin glass are a long standing unsolved problem in spin glass physics. Here we show that ΔF is intimately connected to an apparently unrelated phenomenon, namely chaos in spin glasses. Chaos in spin glasses, first suggested within the droplet model for finite-dimensional spin glasses, also exists for the mean-field spin glass. This opens up a new way to calculate ΔF analytically. Since ΔF is related not only to chaos but also to domain wall energies in finite dimensional spin glasses, our results have direct bearing on spin glass physics in finite dimensions.

DF 6.9 Tue 17:10 H23

Long-time behavior of the velocity autocorrelation function in the overlapping Lorentz model — •Thomas Franosch and Felix Höfling — Arnold-Sommerfeld-Center for Theoretical Physics, LMU München, Germany

The long-time behavior of transport coefficients in the overlapping Lorentz model in two and three dimensions is investigated by means of extensive Molecular Dynamics simulations. The behavior of the velocity auto-correlation function can be rationalized in terms of a competition of the critical relaxation due to the underlying percolation transition and the hydrodynamic power-law anomalies. In two dimensions and in the absence of a diffusive mode, another power law anomaly due to trapping is found with an exponent -3 instead of -2. Further, the logarithmic divergence of the super Burnett coefficient is corroborated in the dilute limit; at finite density, however, it is dominated by a linear divergence.

DF 6.10 Tue 17:30 H23

The Jamming Transition in Granular Systems — •Matthias Sperl[1], Trushant Majmudar[1], Stefan Luding[2], and Robert Behringer[1] — [1]Duke University — [2]TU Delft

Recent simulations have predicted that near jamming for collections of spherical particles, there will be a discontinuous increase in the mean contact number, Z, at a critical volume fraction, ϕ_c. Above ϕ_c, Z and the pressure, P, are predicted to increase as power laws in $\phi - \phi_c$. In experiments using photoelastic disks we corroborate a rapid increase in Z at ϕ_c and power-law behavior above ϕ_c for Z and P. Specifically we find power-law increase as a function of $\phi - \phi_c$ for $Z - Z_c$ with an exponent beta around 0.5, and for P with an exponent ψ around 1.1.

DF 7: Dielectric and Ferroelectric Thin Films and Nanostructures I

Time: Tuesday 14:30–17:50 Location: H11

Invited Talk DF 7.1 Tue 14:30 H11

Nanosized ferroelectrics — •Izabela Szafraniak — Institute of Materials Science and Engineering, Poznan University of Technology, Poznan, Poland — Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland

Among functional materials ferroelectrics are expected to play an important role because they find various applications in a remarkably broad spectrum of advanced electronic, electromechanical and electro-optic components. Future applications require ferroelectric structures with lateral size well below 100 nm. It is well- known phenomena that many materials change or even lose their useful properties as soon as their sizes fall below a certain limit. The ferroelectric size limit has been very important subject of research during last decades. The recent achievements will be discussed. The special emphasis will be put on fabrication ferroelectric nanostructures (including nanowires and nanotubes), multiferroic materials and relations between nanostructure sizes and properties (including role of misfit dislocation on switching behaviour). Financial support: Polish Ministry of Sciences (3TO8A00527, PBZ-MIN-012/KBN/2004, 11/6.PRUE/2005/7).

DF 7.2 Tue 15:10 H11

Ferroelectric $PbZr_{0.4}Ti_{0.6}O_3$ / $PbZr_{0.6}Ti_{0.4}O_3$ superlattices grown on $SrTiO_3$ (001) by pulsed laser deposition — •Ionela Vrejoiu, Yinlian Zhu, Gwenael Le Rhun, Andreas Schubert, Dietrich Hesse, and Marin Alexe — Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle, Germany

Artificial heterostructures and superlattices (SLs) involving ferroelectric perovskites have been explored to achieve materials with potentially novel / improved physical properties. Ferroelectric epitaxial superlattices combining tetragonal $PbZr_{0.4}Ti_{0.6}O_3$ and rhombohedral $PbZr_{0.6}Ti_{0.4}O_3$ thin films were grown by pulsed laser deposition (PLD) onto vicinal $SrTiO_3$ (001) single crystal substrates. Step flow-grown $SrRuO_3$ layers fabricated also by PLD were employed as bottom electrodes, to allow for the electrical characterization of these PZT-based superlattices. The SLs were subjected to extensive structural characterization by means of (high resolution) transmission electron microscopy and x-ray diffraction, to atomic- and piezo-force microscopy and to macroscopic ferroelectric and dielectric measurements. The thickness of the individual PZT layers was found to play an important role for the structure adopted by the superlattices, which, in particular cases, grow with a uniform tetragonal structure and form 90° a-c domains.

DF 7.3 Tue 15:30 H11

The impact of interfaces and structural defects on the properties of tetragonal $Pb(Zr,Ti)O_3$ thin film heterostructures — •Ludwig Geske[1,2], Ionela Vrejoiu[1], Lucian Pintilie[1], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max-Planck-Institut für Mikrostrukturphysik Halle — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

During the deposition of films on substrates with different lattice parameters internal stresses arise. Above a critical thickness h_c dislocations will be introduced. While cooling down from the high deposition temperature, new stresses arise due to the different thermal expansion coefficients of film and substrate, and due to structural phase transitions in PZT. As soon as the temperature is too low to create further dislocations, twin domains will form if the film thickness is above a critical thickness $h_{c,do}$. Heterostructures consisting of bilayers or multilayers of tetragonal $Pb(Zr_{0.2}Ti_{0.8})O_3$ and $Pb(Zr_{0.4}Ti_{0.6})O_3$ thin films were layer-by-layer grown onto vicinal $SrTiO_3$ (001) single crystals by pulsed laser deposition. The thickness of the individual layers, that of the entire PZT structure, and the sequence of layers were varied, to induce or suppress the formation of dislocations and/or ferroelectric twin domains. The ferroelectric and dielectric properties of the samples were studied by the Aixacct TF Analyzer 2000 and by an impedance analyzer. Structural investigations comprising defect analysis were performed by TEM and by AFM. It turns out that the properties of the heterostructures, in particular the dielectric constant and the remanent polarization, are clearly influenced by the defect

contents.

DF 7.4 Tue 15:50 H11

Ferroelectric Thin Films used as Nonlinear Capacitors — •Kay Barz[1], Martin Diestelhorst[1], Horst Beige[1], Ludwig Geske[1,2], Marin Alexe[2], and Dietrich Hesse[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Max-Planck-Institut für Mikrostrukturphysik Halle

A simple serial resonance circuit with a ferroelectric bulk material used as capacitance can easily be driven into nonlinear regimes [1]. The response of such a circuit can be explained by the double well potential, introduced by the ferroelectric. Therefore the system can be described with 3 degrees of freedom, thus allowing it to pursue e.g. period doubling sequences into chaos. Recent experiences in ferroelectric thin films suggest, that even more degrees of freedom could be introduced by the semiconductor-like behaviour of ferroelectric thin film structures [2]. Hence, we deployed metal/ferroelectric/metal (MFM) and metal/ferroelectric/silicon (MFS) thin film structures as nonlinear capacitors in the resonance circuit. In the case of MFS, this led to the observation of a torus doubling bifurcation. As this phenomenon depends on the existence of a minimum set of 4 degrees of freedom it supports the previous made assumption. The talk will deal with the problem of separating nonlinear effects known from the pure ferroelectric (MFM and bulk, respectively) structures from those observable in ferroelectric/semiconductor heterostructures.

[1] Diestelhorst, *et al.* 1999 *Int. J. of Bifurcation and Chaos* **9**, 243-250.

[2] Pintillie *et al.* 2005 *Integrated Ferroelectrics* **73**, 37-48

DF 7.5 Tue 16:10 H11

Microstructure and properties of antiferroelectric/ferroelectric $PbZrO_3$/$Pb(Zr_xTi_{1-x})O_3$ epitaxial multilayers — •Ksenia Boldyreva, Eugene Pustovalov, Lucian Pintilie, Marin Alexe, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Antiferroelectric/ferroelectric multilayers and superstructures represent a topic of interest due to potential coupling phenomena and strain effects. Here, we investigate epitaxial multilayers consisting of alternating antiferroelectric $PbZrO_3$ (PZO) and ferroelectric $Pb(Zr_{80}Ti_{20})O_3$ (PZT80/20) layers. Rhombohedral PZT80/20 was chosen, because its ferroelectric axis lies along the pseudocubic (pc) $[111]_{pc}$-direction, corresponding to the $[111]_{pc}$-direction of the ferroelectric axis in the field-induced ferroelectric state of PZO. PZO/PZT80/20 multilayers were deposited onto STO (100) substrates by pulsed laser deposition (PLD) in oxygen atmosphere. To enable electrical measurements, epitaxial (100)-otiented $SrRuO_3$ (SRO) was used as bottom electrode, because of its atomically flat surface and the low STO/SRO lattice mismatch. SRO deposited on STO shows steps of single unit-cell height due to the layer-by-layer growth mode. XRD analyses and TEM, HRTEM and SAED investigations revealed the preferred $(120)_o$ orientation of the PZO layers and the $(001)_{rh}$ orientation of the PZT layers. (Index „o“ refers to orthorhombic, index „rh“ to rhombohedral indexing). The antiferroelectric properties of the films are under study by macroscopic ferroelectric measurements. Growth-structure-property relations of the PZO/PZT80/20 epitaxial multilayers will be discussed.

DF 7.6 Tue 16:30 H11

Resistive Switching in Ferroelectric Materials — •Hermann Kohlstedt[1], Adrian Petraru[1], Kristoff Szot[1], Valanoor Nagarajan[2], Ulrich Poppe[1], Wolgang Speier[1], and Rainer Waser[1] — [1]Institut für Festkörperforschung (IFF) and CNI, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]School of Materials Science and Engineering, UNSW, NSW 2052, Sydney

We investigated the resistive switching effect in SrRuO3/PbZr0.2Ti0.8O3/Pt ferroelectric capacitors. By using a conductive atomic force microscope the piezoelectric response, the capacitance as well as the resistive current vs. the applied bias voltage was simultaneously measured. The piezoelectric response and the capacitance butterfly loop showed clear indication that the PZT films were ferroelectric. We determined a coercive field of 167 kV/cm in 30 nm thick PZT films. By increasing the bias electric field approximately a factor two larger then the coercive field we observed an electric forming process, i.e. the resistance changed strongly. Hereafter the devices showed bipolar resistive switching. The simultaneously recorded piezoelectric response data showed that after the electric forming procedure the film was ferroelectric. The difference between the coercive field and the resistive switching voltage is explained on the basis of a filament model in which the resistive switching and ferroelectricity are considered as independent phenomena. This model is supported by measurements of the resistance times area (R x A) product. Parasitic effects during the measurements of the piezo response during I-V curve cycling will be discussed.

DF 7.7 Tue 16:50 H11

Impedance spectroscopy of thin ($d \approx 4\,(nm)$) tantalum oxide films: Temperature and Field dependence — •Katrin Bruder[1], Achim Walter Hassel[1], Beate Mildner[2], and Detlef Diesing[2] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf — [2]Institut für physikalische Chemie, Universität Duisburg-Essen, 45141 Essen

Impedance spectroscopy of tantalum oxide films was accomplished in thin film capacitors (tantalum–tantalum oxide–noble metal). With investigations from $f = 10^{-2}$ Hz to 10^{+6} Hz it is possible to determine the capacitance, the metals resistivities and the tunnel resistivity of the oxide. The latter one is a function of the bias voltage while the capacitance and the metals resistivities remain unchanged. The tunnel resistivity was found to have a maximum at a bias U_{max} slightly different from 0 V. Within single band tunneling models $U_{max} \equiv 0\,V$ is expected whereas two band tunneling models were found to deliver $U_{max} \neq 0$ V as function of the barrier asymmetry and the oxides band gap. For a further investigation the bias dependence of impedance spectra was characterised in the temperature range from $T = 58$ K to 350 K. U_{max} was found to vary with T. A comparison with theory points to a temperature dependent barrier asymmetry of the oxide.

DF 7.8 Tue 17:10 H11

Wachstum und elektrische Eigenschaften von dünnen $SrTiO_3$-Schichten auf $YBa_2Cu_3O_{7-x}$ — •Veit Grosse[1], Frank Schmidl[1], Ingo Uschmann[2] und 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

Dünne Strontiumtitanat (STO)-Schichten wurden mittels gepulster Laserdeposition (PLD) epitaktisch auf mit $YBa_2Cu_3O_{7-x}$ (YBCO) beschichteten STO-Einkristallen abgeschieden. Röntgen-Untersuchungen zeigen eine sehr gute (001)-Orientierung der YBCO- und STO-Schichten. Oberflächenrauhigkeiten von 10 nm (YBCO) bzw. 2 nm (STO) konnten erreicht werden.

Zur elektrischen Charakterisierung diente das YBCO als untere Elektrode. Die obere Elektrode bildete eine zusätzlich aufgesputterte Gold-Schicht. In diesem YBCO/STO/Au-System zeigt sich in Abhängigkeit von der Schichtdicke und Temperatur unterschiedliches Leitungsverhalten von Raumladungslimitierung, Variable Range Hopping bis hin zu resistiven Schalteffekten. Es werden Einflüsse der Sauerstoffstöchiometrie auf das Leitungsverhalten diskutiert. Weiterhin werden Ergebnisse zu den dielektrischen Eigenschaften in Abhängigkeit von der Temperatur, Schichtdicke und zusätzlichem elektrischen Feld vorgestellt.

DF 7.9 Tue 17:30 H11

Size and strain effects in ultrathin epitaxial $BaTiO_3$ films grown by high pressure sputtering — •Adrian Petraru[1], Hermann Kohlstedt[1], Nikolay Pertsev[1], Ulrich Poppe[1], Axel Solbach[2], Uwe Klemradt[2], and Rainer Waser[1] — [1]Institut für Festkoerperforschung and CNI, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, 52074 Aachen

High quality epitaxial $BaTiO_3$ films with thicknesses ranging from 2.8 nm to 175 nm were grown epitaxially on $SrRuO_3$-covered $SrTiO_3$ (001) substrates by high-pressure sputtering. The film structure was studied by conventional and synchrotron x-ray diffraction. The amount of the compressive strain in the $BaTiO_3$ films was measured by x-ray reciprocal space mapping (X-RSM)around the asymmetric $(\bar{1}03)$ Bragg reflection. Ferroelectric capacitors were then fabricated by depositing $SrRuO_3$/Pt top electrodes, and the polarization-voltage hysteresis loops were recorded at the frequency 1 KHz. The observed thickness effect on the lattice parameters and polarization in $BaTiO_3$ films was analyzed in the light of strain and depolarizing-field effects using the nonlinear thermodynamic theory. The theoretical predictions are in reasonable agreement with the measured thickness dependencies, although the maximum experimental values of the spontaneous polarization and the out-of-plane lattice parameter exceed the theoretical estimates markedly (43 μC/cm^2 vs. 35 μC/cm^2 and 4.166 Åvs. 4.143 Å). Possible origins of the revealed discrepancy between theory and

experiment are discussed.

DF 8: Dielectric and Ferroelectric Thin Films and Nanostructures II

Time: Wednesday 14:30–17:10 Location: H11

Invited Talk DF 8.1 Wed 14:30 H11

Piezoelectricity and pyroelectricity in amorphous perovskite thin films — •Alexander K. Tagantsev[1], Vera Lyahovitsky[2], David Ehre[2], Ellen Wachtel[2], Sidney R. Cohen[2], Konstantin Gartsman[2], and Igor Lubomirsky[2] — [1]Swiss Federal Institute of Technology (EPFL), Lausanne 1015, Switzerland — [2]Weizmann Institute of Science, Rehovot 76100, Israel

One customarily considers the crystallinity as a prerequisite for pyro- and piezoelectricity in a material. Though the theory does not impose such limitation, the long-standing experience in the field tells us that ionic structures exhibiting pyro- and piezoelectricity should be at least polycrystalline. In this paper, we demonstrate that the "common" behavior of perovskite dielectrics can be revolutionary influenced when thin films of these materials are treated with a specially tailored temperature gradient. Such treatment enables the transformation of non-polar amorphous films of $BaTiO_3$, $SrTiO_3$, and $BaZnO_3$ into a polar state that exhibits appreciable values of pyro- and piezoelectric coefficients. One should stress that, in the case of $SrTiO_3$ and $BaZnO_3$, the polar amorphous films are prepared from originally non-polar materials. This unusual phenomenon raises a body of intriguing questions concerning the physics behind it. In this paper we address two of these issues in detail: (i) the mechanism of temperature-gradient driven amorphous-to-amorphous-state transformation and (ii) the mechanism of polar-state formation in the amorphous materials.

DF 8.2 Wed 15:10 H11

Permittivity of sputtered thin films of TiO(2) — •Dieter Mergel, Janika Bolz, and Fred Fürtges — WG Thin Film Technology, Fb Physik, University Duisburg-Essen, 45117 Essen

Thin film capacitors have been prepared on Si substrates with bottom and top electrodes of RuO(2) or In(2)O(3):Sn. The deposition method was rf-diode sputtering. Depending on the details of the process (heating, grounded or floating substrate, sputter pressure, oxygen partial pressure) the TiO(2) films contained mainly anatase or mainly rutile grains or both.

Impedance spectroscopy delivered one semicircle in all cases. The dielectric permittivity at room temperature ranges between 80 and 300. The film stacks with RuO(2) disintegrated during the measurements at higher temperatures but were stable without electric field up to 300°C.

DF 8.3 Wed 15:30 H11

Electrostriction vs polarisation reversal in ferroelectric nanoislands — •Serge Röhrig and Andreas Rüdiger — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Piezoresponse Force Microscopy plays an important role in the investigation of ferroelectric nanostructures. The contrast mechanism for vertical PFM comprises piezoelectric and electrostatic contributions nurturing the discussions which one is dominating. Scanning over c-axis oriented nanoislands leads to a pronounced lateral signal at the slops of the islands. This signal is virtually free of electrostatic contributions. Detecting the second harmonic response, we observe a clear transition from quadratic (electrostriction) to linear (polarisation reversal) behaviour as we exceed the coercive field. The microscopic interpretation suggests a new type of non-volatile ferroelectric memory.

DF 8.4 Wed 15:50 H11

NMR Spectroscopy for Study of Size Effects in BaTiO3 fine particles and of Materials Embedded in Mesoporous Materials — P. Sedykh[1], E. V. Charnaya[2], G. Klotzsche[1], and •D. Michel[1] — [1]University of Leipzig, Institute for Experimental Physics II, Linnéstrasse 5, 04103 Leipzig — [2]Institute of Physics, St.Petersburg State University, St.Petersburg, 198904, Russia

Studies of size effects on ferroelectric properties have obtained a great impetus in recent years. Ultrafine BaTiO3 powders are prepared from a monomeric metallo-organic precursor through combined-solid state polymerization and pyrolysis (CPP) [1-3] with particle size (dm) in the range between 15 nm and 250 nm. The properties of BaTiO3 powders were characterized by various methods (FT-Raman, XRD, SEM and 137Ba NMR). Critical particle diameters for the disappearance of ferroelectricity are estimated. A structural model for a nanograin is derived. Moreover, we study the behavior of BaTiO3 and other ferroelectrics embedded into mesoporous MCM 41 materials and in porous glasses. An overview about our recent work will be given.

[1] H. J. Gläsel, E. Hartmann, R. Böttcher, C. Klimm, B. Milsch, D. Michel, H.-C. Semmel-hack, J. Hormes, J. Materials Science 34(1999)1-5 [2] E. Erdem, R. Böttcher, H.-C. Semmelhack, H.-J. Gläsel, E. Hartmann, D. Hirsch, J. Mater. Sci. 38 (2003) 3211-3217 [3] E. Erdem, PhD Thesis, University of Leipzig, 2006

DF 8.5 Wed 16:10 H11

Ultrafast Structure and Polarization Dynamics in Nanolayered Perovskites Studied by Femtosecond X-Ray Diffraction — •Clemens von Korff Schmising[1], Matias Bargheer[1], Mareike Kiel[1], Nicolai Zhavoronkov[1], Michael Woerner[1], Thomas Elsaesser[1], Ionela Vrejoiu[2], Dietrich Hesse[2], and Marin Alexe[2] — [1]Max Born Institut, Berlin — [2]Max Planck Institut, Halle

We apply ultrafast x-ray diffraction with 100 femtosecond temporal and 100 femtometer spatial resolution to study optically induced polarization dynamics in a nanolayered $PbZr_{0.2}Ti_{0.8}O_3/SrTiO_3$ (PZT/SRO) superlattice. Displacive ferroelectricity of crystals with a perovskite structure is essentially determined by two lattice coordinates, the tetragonal distortion η (i.e. the ratio of the out- and in-of-plane lattice constant) and the ion displacement ξ within the unit cell, which directly causes the macroscopic polarization P. Optical excitation of the metallic SRO layers generates ultrafast giant stress at the 1 GPa level, which compresses the ferroelectric PZT layers by up to 2%, thus directly modulating the tetragonal distortion η. The measured time-dependent x-ray intensity changes of two Bragg reflections provide complementary information on the coupled dynamics of the tetragonal distortion η and the ion displacement ξ. The evaluation of these transient Bragg reflections yield a maximal change of η after 1.5 ps. As a result, the ferroelectric polarization P is reduced by up to 100 percent with a slight delay that is due to the pronounced anharmonic coupling of the two modes. The resulting change of ξ reaches a maximum after 2 ps.

DF 8.6 Wed 16:30 H11

Computer simulation of ultralow-k dielectric materials based on C_{60}: Structural, mechanical and dielectric properties — •Kostyantyn Zagorodniy, Helmut Hermann, and Manfred Taut — IFW-Dresden, PF 270116, D-01171 Dresden, Germany

The International Technology Roadmap for Semiconductors (ITRS) predicts that continued scaling of devices will require materials with ultralow dielectric constant. In the present work we propose novel interlayer dielectric materials with ultralow dielectric constants and reasonable mechanical properties for future microelectronic applications. The model structure of the material for investigation consists of fullerene molecule C_{60} connected by bridge molecules. Classical and quantum-chemical methods are used to optimize the structures and to calculate dielectric and mechanical properties. The dependencies of structural, mechanical and dielectric properties on the bridge length and its realization have been investigated. The (static) dielectric constants, k, and elastic bulk moduli, B, of the proposed materials are in the range of $k = 1.7$ to 2.2 and $B = 5$ to 23 GPa, respectively. These values meet the demands of future microelectronic devices.

DF 8.7 Wed 16:50 H11

Optimization of porous low-k dielectrics by simulated sphere packings — •Antje Elsner and Helmut Hermann — Institute for Solid State and Materials Research, IFW Dresden, PF 260116, D-01171 Dresden, Germany

Computer generated dense random packings were used as model for porous low-k dielectrics. In this case the pores are represented by

spheres whereas the space around spheres stands for the base dielectric material. Main task was to find an optimum parameter set for pore size distributions to get a low dielectric constant. The dielectric constant decreases with increasing porosity but mechanical properties may get worse therefore. The main challenge is to optimize the porous structure so that mechanical properties are acceptable at preferably highest possible porosity. The model of dense packed spheres was then extended to simulate open pore systems with controllable parameters. Properties of open pore systems differ from closed pore systems. Simulations of models with different degree of open porosity and size distributions were analyzed in terms of specific surface, particle penetrability and other properties.

DF 9: Electric, Electromechanical and Optical Properties I

Time: Thursday 10:00–13:00 Location: H48

Invited Talk DF 9.1 Thu 10:00 H48

Electric Field Induced Critical Points and Electromechanical Response in Relaxor Ferroelectrics — •Zdravko Kutnjak[1], Robert Blinc[1], Jan Petzelt[2], and Stanislav Kamba[2] — [1]Jozef Stefan Iinstitute, Ljubljana, Slovenia — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

The giant electromechanical response in ferroelectric relaxors such as $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) is of great importance for a number of ultrasonic and medical applications as well as in telecommunications. Despite intensive research the origin of this effect is however still not fully understood.

On the basis of dielectric, heat capacity, and piezoelectric investigations on PMN-PT crystals of various PT compositions we show the existence of a line of critical points for paraelectric to ferroelectric transformation in the composition–temperature–electric field (x-T-E) phase diagram [1]. This line effectively terminates a surface of first order transitions. Above this line supercritical evolution has been observed.

On approaching the critical point both the enthalpy cost to induce the intermediate monoclinic states decrease significantly. It is shown that the critical fluctuations in the proximity of the critical points are directly responsible of the observed enhancement of the electromechanical response in PMN-PT system [1]. Preliminary results of critical phenomena observed in other relaxor systems will be presented [2].

[1] Z. Kutnjak, R. Blinc, J. Petzelt, Nature vol. 441, 956 (2006)
[2] W. Kleemann et al., Phys. Rev. Lett. vol. 97, 065702 (2006)

DF 9.2 Thu 10:40 H48

Modifikation der Materialeigenschaften von Lithiumniobat durch Bestrahlung mit hochenergetischen ^{3}He-Ionen * — •Hilke Hattermann[1], Konrad Peithmann[1], Karl Maier[1] und Michael Kösters[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität zu Bonn, Nußallee 14-16, 53115 Bonn — [2]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität zu Bonn, Wegelerstraße 10, 53115 Bonn

Lithiumniobat ist ein ferroelektrisches Material, welches u.a. in der integrierten Optik vielseitige Verwendung findet. Durch die Bestrahlung mit hochenergetischen, leichten Ionen wie z. B. 40 MeV ^{3}He können die Eigenschaften von $LiNbO_3$ gezielt verändert werden. Zwei Beispiele werden in diesem Vortrag vorgestellt:

1.) Ein kongruent schmelzender $LiNbO_3$-Kristall wird periodisch bestrahlt, wobei sich im bestrahlten Bereich der Brechungsindex n verändert. Daher wird so eine periodische Modulation von n erzeugt, die bei einer Periode von einigen Mikrometern als Beugungsgitter für sichtbares Licht dienen kann.

2.) Wird ein mit Magnesium dotierter $LiNbO_3$- Kristall teilweise bestrahlt, so verändert sich sein Polungsverhalten und die Koerzitivfeldstärke im bestrahlten Bereich sinkt.

(*Gefördert durch DFG-FOR 557.)

DF 9.3 Thu 11:00 H48

Polaronic charge transport in reduced $LiNbO_3$ investigated by means of time-resolved ESA spectroscopy — •Christoph Merschjann, Bettina Schoke, Daniela Conradi, Mirco Imlau, and Manfred Wöhlecke — Department of Physics, University of Osnabrück, D-49069 Osnabrück

Charge-transport processes are investigated in differently reduced $LiNbO_3$ single crystals by means of time-resolved excited-state-absorption (ESA) spectroscopy. The detected transient light-induced absorption (α_{li}) upon intense pulsed laser illumination ($\lambda = 532\,\mathrm{nm}, \tau = 8\,\mathrm{ns}$) originates from four distinct types of metastable small polarons. From the temporal and spectral characteristics of α_{li} one is able to distinguish between bound Nb_{Li}^{4+} and free Nb_{Nb}^{4+} polarons, Nb_{Li}^{4+}:Nb_{Nb}^{4+} bipolarons, and bound O^- hole polarons. Among other results we find competing photochromic effects in the blue spectral range in reduced $LiNbO_3$. Furthermore, non-exponential relaxations of α_{li} are observed, whose time constants strongly depend on the state of reduction and purity of the samples. The excitation and recombination phenomena of photo-induced small polarons can be described by a charge transport model, based on a random-walk of excited charge carriers. The presented experimental method is an ideal complement to EPR and electrical measurements, yielding time-resolved spectra at room temperature.

Supported by the Deutsche Forschungsgemeinschaft (projects IM 37/2-2 and TFB 13-04).

DF 9.4 Thu 11:20 H48

Extrinsic defects in high quality CaF_2 crystals for optical applications — •Stephan Hausfeld, Janis Sils, and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Oxygen defects and other impurities were detected in CaF_2 single crystals by a highly sensitive method of photoluminescence under excitation by ultrashort UV laser pulses. To identify oxygen defects the luminescence was measured before and after annealing the crystal at 650°C and quenching it to room temperature. Only after this treatment luminescence of oxygen-vacancy dipoles in CaF_2 is visible. This observation can be explained by the dissociation of dipole dimers which do not contribute to the observed luminescence into simple oxygen-vacancy dipoles due to annealing and quenching. As major other impurities we identified Terbium, Cerium and Europium. Almost no luminescence of any impurity can be found in our crystals of highest quality. Only the oxygen defects remain as trace impurities in these samples.

DF 9.5 Thu 11:40 H48

Comparison of the light-induced absorption in single-domain $LiNbO_3$ and PPLN:Y after thermal reduction in vacuum — •Bettina Schoke[1], Christoph Merschjann[1], Mirco Imlau[1], and Inna Naumova[2] — [1]Department of Physics, University of Osnabrück, Germany — [2]Physics Department, Moscow State University, Russia

We study excitation and recombination processes of small polarons in nominally pure single-domain and yttrium doped periodically poled $LiNbO_3$ (PPLN:Y) after the samples were thermally reduced in vacuum. This treatment creates bipolarons (Nb_{Li}^{4+}:Nb_{Nb}^{4+}) which are stable at room temperature. They may be dissociated into small bound (Nb_{Li}^{4+}) and free (Nb_{Nb}^{4+}) polarons via light illumination ("optical gating"). The resulting light-induced absorption is measured time–resolved via excited–state–absorption (ESA) spectroscopy in the blue, red and infrared spectral range after optical excitation with intense ns laser pulses ($\lambda = 532\,\mathrm{nm}$). In thermally reduced PPLN:Y, as in single-domain $LiNbO_3$, we observe both dissociation and recombination of bipolarons. The investigations also indicate the existence of photo-induced hole polarons (O^-) at room temperature. From the direct comparison of both samples we can deduce the influence of the periodic poling on the charge transport of the small polarons and can clarify the role of the yttrium in $LiNbO_3$ with regard to the polaronic properties. Financial support by the DFG (projects TFB 13-04, IM 37/2-2 and GRK695).

DF 9.6 Thu 12:00 H48

Comprehensive study of surface damage induced by SFG in Lithiumtriborate (LBO) — •Stefan Möller, Änne Andresen, Christoph Merschjann, Manfred Neumann, and Mirco Imlau — Department of Physics, University of Osnabrück, D-49069 Osnabrück

We have investigated the build-up of surface damages of LiB_3O_5 single crystals generated during sum-frequency generation (SFG) of UV-light

(λ = 355 nm) by a focused Q-switched Nd:YAG laser (f = 20 kHz, τ_{1064} = 10 ns, $\overline{P}_{1064}$ = 1.5 W) on timescales > 100 h and intensities below the damage threshold. The comprehensive study was performed with low coherence microscopy, X-ray spectroscopy (XPS), excited-state absorption (ESA) and atomic force microscopy for optical, electrical and microscopic characterization of the damages. The aim of our work is to avoid the build-up of this damage in order to extend the lifetime of LBO in UV-laser systems. As a result we found two kinds of damages: The first is a deposition of foreign material on the surface. Here, XPS uncovers several foreign elements as Na, S, Si, Ca, C depending on the composition of the ambient atmosphere during SFG. The second kind of damage is characterized by an ablation of the surface of the crystal. Only this second kind of damage disturbs the beam quality noticeably, as a strong increase of the beam propagation factor M^2 was monitored simultaneously. With the results of the ESA studies we are able to discuss the role of polarons for the surface damage formation process as well as the cross-correlation of these two kinds of damages. Financial support by the DFG (TFB 13, project A5/13-04).

DF 9.7 Thu 12:20 H48

High-temperature-recorded index gratings in periodically-poled lithium niobate* — •Michael Kösters, Ulrich Hartwig, Theo Woike, and Karsten Buse — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany

Holographic index gratings based on a zero-electric-field photorefractive effect are recorded at high temperatures in copper-doped periodically-poled lithium niobate crystals. High-temperature recording causes strong absorption modulations which are linked to index gratings via the Kramers-Kronig relations as it is described in Ref. (1). The gratings do not originate from the electro-optic effect and can be read out regardless of their orientation in the crystal. Subsequently, the interplay between the periodic domain structure (grating vector **G**) and the index grating (grating vector **K**) is studied: The fundamental **K**-grating is strongly suppressed. Pronounced sideband gratings with $\mathbf{K}_s = \mathbf{K} \pm s\mathbf{G}$ appear, where s is an integer number. The findings are of great importance for applications, where both, index gratings and ferroelectric domain gratings, are needed, e.g. for a DFB-OPO (Distributed-Feedback Optical Parametrical Oscillator).

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

(1) U. Hartwig, K. Peithmann, B. Sturman, and K. Buse, Appl. Phys. B **80**, 227 (2005).

DF 9.8 Thu 12:40 H48

Reduction of optical damage in lithium niobate crystals by thermo-electric oxidization* — •Matthias Falk, Theo Woike, and Karsten Buse — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany

Lithium niobate crystals are a promising material for nonlinear-optical applications, e.g., second harmonic generation. But the conversion efficiency is limited because of unwanted light-induced refractive index changes, the so-called "optical damage". This effect is mainly caused by iron impurities that occur in the valence states Fe^{2+} and Fe^{3+}. Electrons from Fe^{2+} are excited by light, redistributed and finally trapped, preferentially in the darker areas of the crystal. Space-charge fields build up and change the refractive index via the electro-optic effect. A method to suppress such index changes, the thermo-electic oxidization treatment, is presented: The crystals are annealed in the presence of an externally applied electrical field. By this the iron impurities are nearly completely oxidized to the Fe^{3+} state, thus there are less photoexcitable electrons in the crystal. Consequently, the optical damage is suppressed by one order of magnitude. Furthermore, it is shown, that for charge compensation of the removed electrons, lithium and hydrogen ions leave the crystal during the treatment.

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

DF 10: Dielectric and Ferroelectric Thin Films and Nanostructures III

Time: Thursday 14:30–17:50 Location: H48

DF 10.1 Thu 14:30 H48

Structure and charge modulations in the mixed oxides In2O3(ZnO)m: Electron holography and quantum chemical computations — •Falk Röder[1], Martin Linck[1], Hannes Lichte[1], Thomas Bredow[2], Oliver Köster-Scherger[3], and Werner Mader[3] — [1]Institute of Structure Physics, Triebenberg Lab, Technische Universitaet Dresden — [2]Institute for Physical and Theoretical Chemistry, University of Bonn — [3]Institute for Inorganic Chemistry, University of Bonn

Compounds of the type In2O3(ZnO)m, m = 2,3,4,..., are ideal model systems of wide-spaced electric field modulations, to study distribution and relaxation of charge in solids for the first time. They consist of ZnO domains separated by fully occupied layers of In3+ ions and layers of unoccupied metal sites. These layers are strictly alternating and periodically arranged at a spacing controllable by the quantity m. Formally, the layers carry a charge of one electron per site, which would produce huge electric fields of ca. 200 GV/m without accounting for structural and electronic relaxations. In a TEM, the respective intrinsic electric fields modulate the phase of the electron wave hence are measurable by means of electron holography; in fact, they are clearly revealed from the reconstructed phase images. Quantum chemical computations were performed for compounds with m = 3;5 using the crystalline orbital program package CRYSTAL06. It is found that half of the In3+ ions occupy sites close to the unoccupied layers. The calculated electric fields are used to interpret the results of the electron holographic measurements.

DF 10.2 Thu 14:50 H48

Characterisation of Ferroelectric Nanoparticles by HRTEM and Electron Holography — •Margarita Weiss[1,4], Hannes Lichte[1], Gil Markovich[2], Tcipi Fried[2], Sebastian Wohlrab[3], and Michael Lehmann[4] — [1]Institut für Strukturphysik, TU Dresden, 01062 Dresden — [2]School of Chemistry, Tel Aviv University, Tel Aviv 69978, Israel — [3]Institut für Anorganische Chemie, TU Dresden, 01069 Dresden — [4]Institut für Optik und Atomare Physik, TU Berlin, 10623 Berlin

As bulk materials, BaTiO3 and PbTiO3 are known to be ferroelectric below their Curie temperature of Tc=120°C and Tc=480°C, respectively. However, ferroelectric nanoparticles show different properties. For example, there is a critical size effect, in that the Curie temperature Tc is decreasing with decreasing particle size. Unfortunately, there are no reliable figures in literature for the critical size, below which ferroelectricity is not observed.

In this work, particles of the size of 10nm up to around 100 nm were investigated by means of electron holography, which allows directly measuring the atomic ferroelectric polarisation as well as electric stray fields around nano-sized specimens. There are no indications for electric dipole stray fields around the ferroelectric particles. But BaTiO3 particles of a diameter of about 40 nm show hints for interior ferroelectric polarisation, whereas smaller particles do not reveal any indication of ferroelectricity. By HRTEM investigations it was observed that lattice planes of these small particles are very inhomogeneous. This might prevent the ferroelectric polarisation.

DF 10.3 Thu 15:10 H48

Electric Fine Structure in Ferroelectrics by Electron Holography — •Hannes Lichte[1], Martin Linck[1], Marianne Reibold[1], and Koichiro Honda[2] — [1]Triebenberg Laboratory, Institute of Structure Physics, Technische Universität Dresden, 01062 Dresden — [2]Fujitsu Laboratories Ltd, Atsugi 243-0197, Japan

In many materials, the arrangement of atoms is mainly interesting in the sense that it produces certain intrinsic fields, such as functional magnetic or electric fields. This is true for example, for ferroelectrics and those materials with regular charge modulation [1]. Since, in a TEM, these fields modulate the phase of the electron waves, they can best be analyzed by electron holography [2]. By holography, we analyze the electric structure of ferroelectrics (BaTiO3, PZT, PTO,..) at medium resolution [3], but also the details on a nanometer scale. It

turns out that we can distinguish between stacked ferroelectric and non-ferroelectric layers, and determine ordering and orientation of the polarization in nanometer dimensions. Financial support by the German Research Society (DFG) through FOR 520 is gratefully acknowledged.

[1] Roeder et al., this conference.
[2] Lichte et al., Ultramicroscopy 93 (2002) 199.
[3] Matzeck et al., this conference.

DF 10.4 Thu 15:30 H48

Tip-enhannced Raman spectroscopy on nanoscale oxide electronics — •Andreas Rüdiger and Serge Röhrig — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Tip-enhanced Raman spectroscopy bypasses the diffraction limited lateral resolution of conventional microscopy and provides an aperture-less optical tool for true nanoscale characterization. Being sensitive to a very small volume and thus to surface conditions we investigate nanoscale oxide electronics under vacuum and ambient conditions and present recent results for hard- and soft-mode phonons.

DF 10.5 Thu 15:50 H48

Ferroelectric like hysteresis and piezoelectricity in open porous polymers: theoretical predictions and experimental observations — •Sergej Zhukov and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, 64287 Darmstadt

The open porous polymers form a new attractive class of piezoelectric materials. Up to now it has been demonstrated that the porous film after proper charging and polarizing is responsible for the high piezoelectric response if confined between two electrically blocking layers. Such sandwich-structures reveal outstandingly large quasi-static piezoelectric coefficients of up to 1000pC/N. Here a theoretical model is proposed for a 3-layer sandwich which quantitatively explains obtainable polarization and its hysteresis behaviour at different poling voltages. It is observed that such sandwich structures exhibit a certain poling limit above which the induced polarization becomes unstable due to back-switching. This phenomenon limits the obtainable remanent polarization and hence the piezoactivity of sandwich structures. The variation of the maximum remanent polarization for different polymer film thicknesses will also be reported.

The work is supported by Arbeitsgemeinschaft industrieller Forschungsvereinigungen (AiF) *Otto von Guericke* e.V.

DF 10.6 Thu 16:10 H48

Observation of modulational instability in the 1st and 2nd band of a self-defocusing one-dimensional nonlinear waveguide array — Jürgen Wisniewski, •Christian Rüter, and Detlef Kip — Institut für Physik und Physikalische Technologien, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld

Modulational instability (MI) is a universal phenomenon common to many nonlinear systems. Due to the interplay between nonlinearity and dispersion a propagating plane wave can become unstable to amplitude or phase modulations of certain frequencies which grow exponentially. MI has been investigated in various physical systems ranging from fluids to Bose-Einstein condensates, optical fibers, and electrical circuits, to mention a few. Here we explore this phenomenon in a discrete periodic nonlinear waveguide array consisting of parallel channel waveguides which are close enough to allow for tunneling of energy from one channel to its neighbours. The linear modes in such periodic lattices are extended Floquet-Bloch modes with a transmission spectrum consisting of allowed bands and forbidden gaps. In the nonlinear case, these modes experience instabilities, and break up into spatially modulated patterns of high regularity. As proposed by Kivshar it has already been observed at the edge of the first Brillouin zone of the first band of a waveguide array with a defocusing nonlinearity. We will present experimental results showing MI at the edge of the 1st band and the center of the 2nd band. The experimental results are confirmed by numerical simulations.

DF 10.7 Thu 16:30 H48

Crystal Phase Control of Luminescing alpha-NaGdF4:Eu3+ and beta-NaGdF4:Eu3+ Nanocrystals — •Pavel Ptacek, Helmut Schäfer, Karsten Kömpe, and Markus Haase — Institute of Chemistry, University of Osnabrück, Barbarastraße 7, D-49076 Osnabrück

NaGdF4:Eu3+, NaEuF4, and NaGdF4 nanocrystals with mean particle sizes between 11 and 15 nm were synthesized in the high-boiling coordinating solvent 2-Hydroxyethyl ethylenediamine (HEEDA) under very similar reaction conditions. Phase pure nanomaterials, crystallizing either in the cubic alpha-phase or the hexagonal beta-phase, were obtained by adjusting one reaction parameter only, i.e. the molar ratio between metal and fluoride ions in the synthesis. The hexagonal beta-phase is formed, if this molar ratio is close to stoichiometric, whereas the cubic alpha-phase is obtained in the presence of excess metal ions. The optical properties of the Eu3+ doped samples are different for the two crystal phases. The results indicate an increased number of oxygen impurities close to Eu3+ ions, if excess metal ions are used in the synthesis.

Supported by the Deutsche Forschungsgemeinschaft

DF 10.8 Thu 16:50 H48

$PrO_x/AlON$ stacks as a high-k candidate on SiC — •Karsten Henkel, Rakesh Sohal, Mohamed Torche, Carola Schwiertz, Yevgen Burkov, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

We study the chemical stability and electrical properties of Pr-oxides-SiC MIS stacks. In MISFET devices for high power applications the electric field scaling at the interface between semiconductor and insulator is determined by the ratio of their permittivity values. A high-k material can be used to optimize the performance of such devices. In previous studies we had to understand that the chemical reactivity of the PrO_x/SiC interface causes a destructive interaction yielding silicate and graphite formation as well as poor electrical performance after direct deposition of PrO_x onto SiC. Therefore we introduced an additional chemically inert layer and in this contribution we focus on $PrO_x/AlON$ as a suitable insulator stack.

In our spectroscopic investigations we recognized a stable AlON/3C-SiC interface even for annealing steps up to 900°C. First electrical characterizations are performed on Si substrates and we find a strong improvement in the leakage current by several orders of magnitude down to values of $10^{-7} A/cm^2$ at an EOT of 4nm and interface state densities of mean values of $5 * 10^{11}/eVcm^2$. We also report on our ongoing electrical characterization of such stacks on SiC substrates.

This work is supported by Deutsche Forschungsgemeinschaft within priority program 1157 (DSCH 745/9-2).

DF 10.9 Thu 17:10 H48

Thin-film piezodevices based on expanded PTFE with improved thermal stability — •Torsten Finnberg[1], Sergej Zhukov[2], Bernd-Joachim Jungnickel[1], and Heinz von Seggern[2] — [1]Deutsches Kunststoffinstitut, Schlossgartenstrasse 6, Darmstadt, Deutschland — [2]Fachbereich Material- und Geowissenschaften, TU Darmstadt, Petersenstrasse 23, Darmstadt, Deutschland

Piezoelectric sensors and actors are important devices in a large number of applications ranging from the entertainment to the automotive industry. Present research is focused on a new class of piezoelectric materials based on cellular polymer films. The inherent flexibility and easy processability of these materials opens new fields of applications. High quasistatic piezocoefficients of up to 300 pC/N have already been demonstrated in the usually used polypropylene. A lasting challenge concerns the thermal stability of the piezocoefficient in that material. The use of expanded polytetrafluorethylene (PTFE) could solve that problem. However, this material exhibits open pores, necessitating multilayer systems by sandwiching it between solid PTFE films. It is shown by measurements of the dynamic inverse piezocoefficient in the acoustic frequency range, that such multilayer systems have a similar performance as commercially available cellular piezoelectric polypropylene. It is shown by measurements of thermally stimulated currents, that the poling temperature strongly influences the thermal stability of the polarisation. By poling at elevated temperatures, a significant increase of the thermal stability of the piezocoefficent can be achieved, as demonstrated by forced cyclic ageing at 80 °C.

DF 10.10 Thu 17:30 H48

Ab initio study of the critical thickness for ferroelectricity in ultrathin lead titanate films between conducting electrodes — •Christian Elsässer[1,4], Yoshitaka Umeno[2], Bernd Meyer[3], and Peter Gumbsch[4,1] — [1]Fraunhofer-Institut für Werkstoffmechanik, Freiburg — [2]Graduate School of Engineering, Kyoto University, Japan — [3]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum — [4]Institut für Zuverlässigkeit von Bauteilen und Systemen, Universität Karlsruhe

The ferroelectricity of single-domain ultrathin PbTiO3 films sandwiched between metallic Pt electrodes has been studied using ab-initio density-functional theory (DFT) calculations within the local-density approximation [1]. For stress-free PbTiO3 films with an in-plane lattice constant of the tetragonal bulk phase we find that the films lose ferroelectricity below a critical thickness of about 4 and 6 unit cells (1.6 nm and 2.4 nm) for PbO- and TiO2-terminated films, respectively. This result is in contradiction to a recent DFT study by Sai, Kolpak and Rappe [2], in which the persistence of ferroelectricity for Pt/PbTiO3/Pt films down to one unit cell (0.4 nm) has been reported. Careful tests with different types of pseudopotentials and density-functionals reveal that this discrepancy is due to insufficiencies of the widely used generalized-gradient approximations PW91 and PBE, which have been employed by Sai et al. for describing perovskite compounds. [1] Y. Umeno, B. Meyer, C. Elsässer, P. Gumbsch, Phys. Rev. B 74, 060101(R) (2006). [2] N. Sai, A. M. Kolpak, A. M. Rappe, Phys. Rev. B 72, 020101(R) (2005).

DF 11: Poster Session

Time: Thursday 14:30–18:00 Location: Poster C

DF 11.1 Thu 14:30 Poster C

Buffer layer investigation of MFIS stacks with an organic ferroelectric layer — •Bernd Seime, Karsten Henkel, Ioanna Paloumpa, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

Ferroelectric field effect transistors are considered as future non volatile and non destructive readout memory cells. Conventional Perowskite-type ferroelectric materials are shown to work but they need expensive high temperature and high partial pressure processing steps inducing also unintentional and undefined interfacial layers. A possible low cost solution is the use of poly[vinylidene fluoride trifluoroethylene] (P[VDF/TrFE]). This is a ferroelectric polymer which can be spin coated at room temperature onto silicon suited with well defined buffer layers.

Using P[VDF/TrFE] we focus on metal ferroelectric insulator semiconductor (MFIS) structures. In MFIS structure a part of the programming voltage drops over the buffering insulator. We report on attempts to minimize this fraction by optimizing the voltage divider over the buffer and the ferroelectric layers. CV measurements for different thickness of the buffer (10-235nm) and the ferroelectric layer (100nm-1μm) and for different permittivity values of the buffer layer (SiO_2, Al_2O_3, HfO_2) will be presented.

This work is supported by Deutsche Forschungsgemeinschaft within priority program 1157 (DSCH 745/11-1).

DF 11.2 Thu 14:30 Poster C

X-Ray Diffraction Studies of PrO_2/Si(111) — •Lars Boewer[1], Joachim Wollschläger[1], Thomas Weisemoeller[1], Carsten Deiter[1], Peter Zaumseil[2], and Thomas Schroeder[2] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück Germany — [2]IHP-Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Due to the progressive miniaturization of electronic devices and the problem of leakage current, the search for oxides with high dielectric constants has become very important.

PrO_2 is a good candidate for Si(111) based technology due to its small lattice mismatch of 0.7% with respect to the Si substrate. However, PrO_2 is not stable under UHV conditions, but it is known that Pr_2O_3 films can be transformed to PrO_2 films by annealing in oxygen. Here we investigate Pr_2O_3 films of 5nm thickness deposited at 625°C on Si(111) and annealed in oxygen at 300°C and 700°C, respectively. XRD and GIXRD studies were performed at beamlines W1 and BW2 at HASYLAB (DESY).

Comparing the obtained data with the lattice spacing of Pr_2O_3 and PrO_2 shows that the entire film is apparently converted to PrO_2, although the vertical lattice constant is increased with respect to bulk PrO_2 is caused by lateral compression of the pseudomorphic PrO_2 film. In addition analyzing the thickness of the crystalline part of the PrO_2 films shows that the crystalline film annealed at 300°C is thicker than the film annealed at 700°C. This loss of crystalline PrO_2 can probably be attributed to the formation of Pr silicate at the interface.

DF 11.3 Thu 14:30 Poster C

Size and Doping Effects of Ferroelectric Nanoparticles: A Microscopic Model — Thomas Michael[1], •Julia Wesselinowa[2], and Steffen Trimper[1] — [1]Institute of Physics, Martin-Luther-University Halle, D-06099 Halle Germany — [2]University of Sofia, Department of Physics, Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria

A microscopic model for describing ferroelectric nanoparticles is proposed. It enables the calculation of the macroscopic polarization as a function of an external electric field, the temperature, the defect concentration and the particle size. Furthermore the excitation energy of the soft mode and its damping can be computed. The constituents of the material are arranged in layers. Their interaction depends on both the coupling strength at the surface and that of defect shells in addition to the bulk values. The analysis is based on an Ising model in a transverse field. It is modified in such a manner to study the influence of size and doping effects on the hysteresis loop of spherical nanoparticles. Using a Green's function technique in real space we find the coercive field, the remanent polarization and the critical temperature which differ significantly from the bulk behavior. Depending on the kind of doping ions and the surface configuration the coupling strength varies. Hence the coercive field and the remanent polarization can either increase or decrease in comparison to the bulk behavior. Theoretical results are compared with experimental data.

DF 11.4 Thu 14:30 Poster C

Breakdown-induced light emission and poling dynamics of porous fluoropolymers — •Sergej Zhukov and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, 64287 Darmstadt

Until today the charging mechanisms of novel porous electrets materials are not completely understood. The present study is focused on the investigation of light emission during corona poling of films of expanded polytetrafluoroethylene (ePTFE) and sandwiched structures with the ePTFE film between two solid FEP films. One observes that as soon as the applied electric field exceeds a certain threshold value the individual film as well as the sandwich structure starts to emit light due to electrical breakdown in the pores. It will be demonstrated that a polarization hysteresis loop can be derived from the emitted light intensity in a polarization switching experiment. In the case of free-standing ePTFE films a continuous light emission indicates that breakdown generated charges are not trapped permanently at the fibers in the open pore media. The present results explain the drastic difference in piezoactivity between individual porous films and sandwiched structures.

The work is supported by Arbeitsgemeinschaft industrieller Forschungsvereinigungen (AiF) *Otto von Guericke* e.V

DF 11.5 Thu 14:30 Poster C

Electron Holography on Ferroelectric 180°-Domains coupled "head-to-head" — •Christopher Matzeck, Hannes Lichte, and Marianne Reibold — TU Dresden, Triebenberg-Labor

Ferroelectric polarization modulates both amplitude and phase of the electron wave in an electron microscope, which can be measured by electron holography. In [1] is described that the gradient, respective the increase of the phase of the modulated object wave, is proportional to the projected ferroelectric polarization. Hence, the analysis of the gradient of the phase gives information about the domain coupling.

Ferroelectric domains are assumed to be not capable of arranging a stable configuration in head-to-head or tail-to-tail coupling, because, in that case, a charge would be found within the domain wall. This is not possible in an energetically stable state. However, several reconstructed phase images show a-domains that seem to be coupled head-to-head.

But a closer look discovers several hints that there could be a c-domain in between the others. Comparisons with simulations of a possible configuration match very well to the experimental data.

References:
[1] H. Lichte, M. Reibold, K. Vogel, M. Lehmann, Ultramicroscopy 93 (2002) 1999
[2] The financial support from the Deutsche Forschungsgemeinschaft for the Research Group on Ferroic Functional Components FOR520 is gratefully acknowledged

DF 11.6 Thu 14:30 Poster C

In-situ Electron Holography of Ferroelectric Polarization Switching — •Christopher Matzeck, Hannes Lichte, and Bernd Einenkel — TU Dresden, Triebenberg-Labor

For many applications of ferroelectrics, e.g. nonvolatile memories, their behavior under external electric fields is extremely important. Since ferroelectric polarization modulates the phase of the electron wave in a TEM and electron holography is capable of measuring this, it is possible to determine the projected polarization in principle. Mathematically, the projected polarization is directly related to the gradient of the phase shift [1]. This makes electron holography a powerful tool for investigation of ferroelectric domains.

Experiments under field switching are done with a special TEM-holder with an electrical feedthrough and individual prepared specimens to apply an external electric field perpendicular to the electron beam. This is important because only these so-called in-plane components of the polarization modulate the electron wave.

References:
[1] H. Lichte, M. Reibold, K. Vogel, M. Lehmann, Ultramicroscopy 93 (2002) 1999
[2] The financial support from the Deutsche Forschungsgemeinschaft for the Research Group on Ferroic Functional Components FOR520 is gratefully acknowledged

DF 11.7 Thu 14:30 Poster C

Amorphous lanthanum lutetium oxide thin films as an alternative high-k gate dielectric — •Joao Marcelo Jordao Lopes[1], Martin Roeckerath[1], Tassilo Heeg[1], Jürgen Schubert[1], Uffe Littmark[1], Siegfried Mantl[1], Valeri Afanasiev[2], Sheron Shamuilia[2], Andre Stesmans[2], Yunfa Jia[3], and Darrell Schlom[3] — [1]Institute for Bio- and Nanosystems (IBN1-IT), Research Center Jülich, Jülich, Germany — [2]Department of Physics, University of Leuven, Leuven, Belgium — [3]Department of Materials Science and Engineering, Pennsylvania State University, Pennsylvania, USA

A large number of alternative materials is in discussion to replace SiO_2-based films as the gate dielectric in future MOSFET nanodevices. In this contribution we report results on $LaLuO_3$ thin films deposited on (100) Si substrates. The films were grown by pulsed laser deposition using a stoichiometric ceramic target. Rutherford backscattering spectrometry, transmission electron microscopy, atomic force microscopy, X-ray diffraction and X-ray reflectometry were employed to structurally investigate the samples. The results indicate the growth of stoichiometric, amorphous, and smooth $LaLuO_3$ films showing thermal stability up to 1000 °C. Internal photoemission and photoconductivity measurements show a band gap width of 5.2 +/- 0.1 eV and symmetrical conduction and valence band offsets of 2.1 eV at the Si/high-k interface. The electrical characterization also reveal promising results. C-V curves with small hysteresis and free of irregularities were achieved, while I-V measurements indicate low leakage current density levels. Additionally, a k value of 32 was derived from a EOT plot.

DF 11.8 Thu 14:30 Poster C

Interdiffusion at the interface of high-k Pr_2O_3 layers grown on Si — •Christian Borschel[1], Martin Schnell[1], Hans Hofsäss[1], Christian Wenger[2], and Carsten Ronning[1] — [1]II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen — [2]IHP microelectronics, Im Technologiepark 25, D-15236 Frankfurt (Oder)

When scaling down semiconductor devices, the thickness of the gate oxide layer must be reduced to maintain a certain value of gate capacitance. The reduced thickness poses a problem as the leakage tunnelling current increases and with that the power consumption and heat dissipation of the device. As an alternative to SiO_2 as the gate dielectric, rare earth oxides such as Pr_2O_3 have been proposed. To evaluate the feasibility to use these materials, their processability has to be studied, for example their thermal stability is of particular interest. For this purpose high resolution Rutherford backscattering spectrometry experiments with a depth resolution of about 1 nm have been conducted on Pr_2O_3 thin layers grown on Si as a function of annealing temperature. The experiments revealed that significant interdiffusion of both Pr and Si atoms occurs only at annealing temperatures above 800° C.

DF 11.9 Thu 14:30 Poster C

Time Dependence of Electric Field-Induced Structural Phase Transitions in the Near-Surface Region of Strontium Titanate at Room Temperature — •Hartmut Stöcker, Stephan Ritter, Alexandr A. Levin, and Dirk C. Meyer — Institut für Strukturphysik, 01062 Dresden

Time dependence of electric current and an almost completely reversible structural change of near-electrode regions of an (001) SrTiO3 (STO) single-crystal plate in an external electrical field [1] have been investigated. Changes of the crystal structure remaining after cyclic processing are discussed in terms of a memory effect. The time dependence of the current is compared with temporal change of the structure of STO at near-surface regions as observed by means of X-ray diffraction. The interplay of charge carrier transport and structural evolution allows to interpret the structural transition as solid-state electrolysis and also to characterize the transformed crystal from the point of view of its electrical properties.

[1] D. C. Meyer, A. A. Levin, T. Leisegang, E. Gutmann, P. Paufler, M. Reibold, W. Pompe, Appl. Phys. A 84 (1-2), 31-35 (2006)

DF 11.10 Thu 14:30 Poster C

Simulation and Electron Holographic Investigation of the Polarization Field in Ferroelectric (BaTiO3) / Antiferroelectric (WO3) Structures — •Dorin Geiger, Axel Rother, Christopher Matzeck, and Hannes Lichte — Triebenberg Laboratory, Institute of Structure Physics, Technische Universitaet Dresden, D-01062 Dresden, Germany

Electron holography is an adequate instrument to study electric field distributions on an atomic scale by quantitative determination of both amplitude and phase in the object exit wave. In particular the phase is directly proportional to the projected Coulomb potential of the specimen in the case of slowly varying or weak potentials. Ferroelectrics intrinsically comprise a permanent electric polarization field that can be directly extracted from the phase. The unit cell structure, the geometry of the electrically polarized area (domain) and depolarization fields produce the shape of the potential wedge. For both ferroelectric (BaTiO3) and antiferroelectric (WO3) materials the macroscopic fields are calculated for differently shaped domains on different length scales using homogeneously polarized unit cells, whereas the polarization density and the local Coulomb potential is calculated from ab-initio principles, i.e. Density Functional Theory. For comparison with the simulations, electron holograms are recorded. The observed phase wedge is used for determination of the permanent polarization of the structure. [1] Support from DFG in the Framework of FOR 520 is gratefully acknowledged.

DF 11.11 Thu 14:30 Poster C

Grenzflächeneigenschaften von PZT auf LSMO- und Pt-terminierten Substraten — •Salah Habouti[1], Claus-Henning Solterbeck[1], Mohammed Es-Souni[1], Vladimir Zaporojtchenko[2] und Franz Faupel[2] — [1]Institut für Werkstoff- und Oberflächentechnologie, Fachhochschule Kiel — [2]Lehrstuhl für Materialverbunde, Christian-Albrechts-Universtät zu Kiel

Dünne Schichten aus $Pb(Zr_{0.52}Ti_{0.48})O_3$(PZT), die mit dem Sol-Gel-Verfahren hergestellt wurden, zeigen in ihren Eigenschaften deutliche Hinweise auf Einflüsse von der Grenzfläche zum Substrat. Wir untersuchen die Grenzfläche zu $La_{0.8}Sr_{0.2}MnO_3$ (LSMO) im Vergleich zu Platin. XPS-Tiefenprofile zeigen Veränderungen in der Stöchiometrie durch Diffusion sowie auch die Entstehung von Grenzflächenschichten, die beide deutlich von den Präparationsbedingungen abhängen. Die Diffusion von La und Mn in die PZT-Schicht hinein verbessert deren elektrische Eigenschaften und führt zu einer geringeren Dickenabhängigkeit der elektrischen Eigenschaften.

DF 11.12 Thu 14:30 Poster C

Einfluss von Substitutionen auf die elektrischen und magnetischen Eigenschaften von $BiFeO_3$ — •Salah Habouti, Claus-Henning Solterbeck und Mohammed Es-Souni — Institut für Werkstoff- und Oberflächentechnologie, Fachhochschule Kiel

Dünne Schichten aus $BiFeO_3$ (BFO) und mit La und Mn substituiertem BFO wurden mit dem Sol-Gel-Verfahren auf Pt- und $La_{0.8}Sr_{0.2}MnO_3$-terminierten Substraten hergestellt. Die Substitutio-

nen haben einen positiven Einfluss auf die elektrischen Eigenschaften. Der gemessenen Leckstrom ist wesentlich niedriger als beim reinen BFO, und entsprechend ist die ferroelektrische Polarisaton höher. Die Substitution dominiert die magnetischen Eigenschaften. Diffusion aus dem Substrat in die dünne Schicht erklärt die verbesserten Eigenschaften von BFO auf LSMO.

DF 11.13 Thu 14:30 Poster C

Local distribution of resistive switching channels in Nb-doped SrTiO3 — •Ruth Münstermann, Regina Dittmann, Krzysztof Szot, Chun-Lin Jia, Shaobo Mi, Paul Meuffels, and Rainer Waser — Institut für Festkörperforschung and Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

We have investigated the local current distribution in Nb-doped SrTiO3 (STO) single crystals and thin films by conductive AFM. STO films with 1 wtWe will discuss the influence of the Nb-rich nanoclusters on the current distribution and the switching phenomena and compare the data to self-doped, oxygen deficient STO [1]. [1] K. Szot, W. Speier, G. Bihlmayer and R. Waser, *Switching the electrical resistance of individual dislocations in single-crystalline SrTiO3*, Nature Materials 5 (4), 312-320, April 2006

DF 11.14 Thu 14:30 Poster C

X-Ray Studies of Structure Changes of Ferroelectric Thin $PbTiO_3$ Films under DC Voltage — •Valentin Iov[1], Ulrich Gebhardt[1], Chang Kim[1], Peter Wochner[1], and Helmut Dosch[1,2] — [1]Max-Planck-Institute for Metals Research, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Institute for Theoretical and Applied Physics, Pfaffenwaldring 57, 70569 Stuttgart, Germany

This contribution investigates the structural changes of ferroelectric films of $PbTiO_3$ of various thicknesses under a static DC voltage. The samples consist of a $PbTiO_3$ film grown on (001) oriented $SrTiO_3$ using $SrRuO_3$ as a buffer layer and as bottom electrode, the top electrode consists of Au patches of various sizes. After a short DC voltage was applied to the heterostructure, we measured the intensity changes around the $(00L)$ Bragg reflections. The influence of the growth parameters, the choice of the material and the size of the top electrode on these effects will be discussed.

DF 11.15 Thu 14:30 Poster C

The influence of elliptical polarization on self-organized nanostructures upon femtosecond laser ablation — •Olga Varlamova[1,2], Guobin Jia[2], and Juergen Reif[1,2] — [1]LS Experimentalphysik II, BTU Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus — [2]IHP/BTU Joint-Lab, Konrad-Wachsmann-Allee 1, 03046 Cottbus

The orientation of self-organized periodical structures on solid surfaces upon multishot femtosecond laser irradiation is known to depend crucially on the polarization of the incident light. In this contribution, we present a systematic study of this phenomenon, varying the polarization from linear over elliptical to circular. We find that not only the direction but also the coordination length of the structures is strongly influenced by the degree of the ellipticity and the direction of the principal axis. An analysis of the generated structures with Scanning Electron and Atomic Force Microscopy reveals new morphological dependencies, also on the angle of incidence of circularly polarized pulses.

DF 11.16 Thu 14:30 Poster C

Topographic investigation of IR-, VIS- and UV-induced damages on LiB_3O_5 surfaces by low coherence microscopy — •Anne Andresen, Stefan Möller, and Mirco Imlau — Department of Physics, University of Osnabrück, D-49069 Osnabrück

The topographic development of IR-, VIS- and UV-induced damages on the output surfaces of LiB_3O_5 (LBO) crystals has been investigated by low coherence microscopy (LCM) as a function of exposure. The surface damages were caused during long-term exposure with a focussed beam of a Q-switched Nd:YAG laser at wavelengths of 1064, 532 and 355 nm, a repetition rate of 20 kHz, pulse lengths of 10 ns, an average power of $\bar{P}_{1064\,\mathrm{nm}} = 1.5\,\mathrm{W}$ and a beam waist of $20\,\mu\mathrm{m}$. The LCM-method enabled us to distinguish between deposition and ablation processes on the LBO surface with an accuracy of up to 1 nm in z-direction. Additionally, the influence of the single wavelengths as well as the mixing of two and three wavelengths on the damage formation can be estimated. The results are interpreted in the frame of surface damage formation during sum-frequency generation in LBO crystals. The particular role of ambient atoms and surface polishing procedures for the damage formation is discussed. Financial support of the Deutsche Forschungsgemeinschaft (TFB 13-04, GRK 695) is gratefully acknowledged.

DF 11.17 Thu 14:30 Poster C

Amplification behavior of photo-induced near-surface scattering — •Volker Dieckmann, Andreas Selinger, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

The influence of the crystal thickness on photo-induced surface, near-surface and bulk scattering phenomena is investigated in iron-doped lithium niobate (0.1 wt. % Fe). Crystals of thickness d between 0.1 mm and 4 mm are illuminated perpendicular to their c-axis by extraordinary polarized light of wavelength 532 nm and intensities up to $10\,\mathrm{kW/m^2}$. Four scattering patterns develop: i) polarization-isotropic lobes in ±c-direction of the sample (Ashkin et al., Phys. Lett. **9**, 72, 1966), ii) a polarization-anisotropic ring (Temple et. al., J. Opt. Soc. Am. B **3**, 337 (1986)), iii) a polarization-isotropic line perpendicular to the c-axis (Morozovska et. al., Sem. Phys. Quant. Elec. Optoelec. **6**, 324 (2003)) and iv) a polarization-anisotropic elliptical-shaped pattern (A. Selinger et. al., TOPS **99**, 61 (2005)). The first two pattern result from parametric processes and their thickness dependence of the steady-state scattered intensity I_s follows the well known amplification law $I_s \propto \exp(\Gamma d)$, with the gain factor Γ. Pattern iii) is known to result from a photo-induced formation of ferroelectric domains. Hence its amplification is thickness independent. The elliptical-shaped pattern shows an unusual amplification behavior. Its steady-state intensity of the scattered light decreases with increasing sample thickness.

Financial support by the DFG (projects IM 37/2-2, GRK 695).

DF 11.18 Thu 14:30 Poster C

Comparison of light-induced absorption in nominally pure $LiNbO_3$ and $LiNbO_3$ doped with different concentrations of Mg or Zn — •Daniela Conradi, Christoph Merschjann, Bettina Schoke, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück

Nominally pure $LiNbO_3$ has a tendency of non-stoichiometry ([Li]/[Nb]<1), leading to the incorporation of Nb_{Li}-antisite-defects and Li-vacancies. Bound Nb_{Li}^{4+} small polarons, Nb_{Li}^{4+}:Nb_{Nb}^{4+} bipolarons and bound O^- hole polarons, all yielding broad absorption bands in the VIS and NIR spectrum, are related to these intrinsic defects. Intense light illumination leads to a metastable population of the polaronic states, which is observed as a transient light induced absorption. Mg- and Zn-doping suppresses the intrinsic defects. The behavior of the small polarons thus depends on the doping concentration. We investigate the photochromic effect in nominally pure $LiNbO_3$ and Mg- and Zn- doped $LiNbO_3$ by means of excited-state-absorption spectroscopy using ns laser pulses of $\lambda = 532\,\mathrm{nm}$ and probe light in the VIS and NIR region. The temporal and spectral behavior of the photo-induced small polarons is studied and the influence of doping on the concentration and the lifetime of metastable polarons is discussed. Supported by the Deutsche Forschungsgemeinschaft (IM 37/2-2, TFB 13-04 and GRK 695).

DF 11.19 Thu 14:30 Poster C

Parametric hybrid scattering on photorefractive gratings and light-induced ferroelectric structures — •Andreas Selinger, Volker Dieckmann, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

We report on a special type of photo-induced parametric light scattering in iron-doped lithium niobate which manifests itself as a polarization-anisotropic elliptical light pattern. It appears as a part of the entire photo-induced scattering pattern which can be induced by a single pump beam. The geometry and intensity of the kinetics of the elliptical pattern are analyzed in respect to beam fanning, the polarization-anisotropic scattering cone, and light scattering from photo-induced microdomains appearing simultaneously. We show that both photorefractive gratings and light-induced ferroelectric structures contribute to the elliptical scattering. Moreover, it is shown experimentally that the light of the participating scattering processes shows intensity oscillations in the steady state with particularly defined frequencies. This allows us to assign the amplification processes yielding the respective scattering pattern to frequency detunings. An Ewald construction is presented to define the corresponding phase-matching

conditions. Financial support by the DFG (projects IM 37/2-2, GRK 695).

DF 11.20 Thu 14:30 Poster C

Conical light scattering in strontium barium niobate crystals related to an intrinsic composition inhomogeneity — Kathrin Bastwöste, Uwe Sander, and •Mirco Imlau — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück

Conical light scattering is uncovered in poly- and mono-domain, nominally pure and Eu-doped strontium barium niobate (SBN) crystals over a wide temperature regime. The appearance of two scattering cones, a scattering line and a corona is observed and can be explained comprehensively within the Ewald sphere concept. Photorefraction, scattering from domain boundaries or from growth striations can be well excluded to explain the origin of the scattering. It is shown that the temperature-resistant scattering process is related to a growth-induced seeding rod, i. e., a composition inhomogeneity primarily localized in the center of the SBN sample. The rod is directed parallel to the polar axis and yields a refractive-index modulation with spatial frequencies on the micro-scale. The significant impact in the frame of material analysis is reflected by the possibility of phase-transition studies of the relaxor-ferroelectric SBN up to temperatures as high as 750 K.
Financial support by the DFG (GRK 695) is gratefully acknowledged.

DF 11.21 Thu 14:30 Poster C

First-principles study of point defects in barium titanate: thermodynamics and electrical conductivity — Paul Erhart and •Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstraße 23, 64287 Darmstadt

The thermodynamic and kinetic properties of mono and di-vacancy defects in cubic (para-electric) barium titanate are studied by means of density-functional theory calculations. Depending on the thermodynamic boundary conditions either metal or oxygen vacancies prevail. The assumption that the vacancies occur in their nominal charge states throughout the band gap, which underlies the most widely employed defect models, is confirmed. Only within about 0.1 eV of the band edges transition levels are found. For the dominating range of the band gap the di-vacancy binding energies are constant and negative. The system, therefore, strives to achieve a state in which under metal-rich (oxygen-rich) conditions metal (oxygen) vacancies are bound in di-vacancy clusters. Since oxygen vacancies readily migrate at typical growth temperatures, di-vacancies can be formed at ease. The formation and migration energies are employed to derive the dependence of the equilibrium Fermi level and the charge carrier concentrations on the chemical conditions and the temperature. Thereby, it is also possible to deduce the relation between the conductivity and the oxygen partial pressure which compares very well with experiments. Furthermore, we are able to demonstrate the correspondence between the Kröger-Vink analysis, widely applied in defect chemistry, and the equations of semiconductor physics.

DF 11.22 Thu 14:30 Poster C

Optical properties of bulk CaF_2 and its F center — •Yuchen Ma and Michael Rohlfing — Fachbereich Physik, Universität Osnabrück, D-49069 Osnabrück, Germany

We present the quasiparticle band structures and optical excitation spectra of bulk CaF_2 and of the F center in CaF_2 using first-principle methods. The quasiparticle band structures are evaluated in Hedin's GW approximation. Thereafter, the electron-hole interaction is calculated and the Bethe-Salpeter equation is solved, yielding the optical absorption spectra. The calculated quasiparticle band gap of bulk CaF_2 is 11.5 eV, which is in agreement with experiment (11.8 eV). The calculated optical absorption spectrum and reflectivity spectrum of bulk CaF_2, which consist of an exciton peak at 10.7 eV and several resonant-exciton peaks between 12 eV and 16 eV, are in good agreement with experiment. The first exciton peak corresponds to the excitation from the occupied F 2p orbitals to the s orbitals at the Γ-point of the lowest unoccupied conduction band.

One of the most prominent point defects of CaF_2 is given by the F center. The F center is characterized by a hole level which we find 6.6 eV above the top of the valence band. An exciton peak is observed at 3.5 eV for F center, which corresponds to the F center optical absorption peak (3.3 eV) observed in experiments. The excited electron is localized at the Ca atoms and F atoms surrounding the vacancy, exhibiting d-orbital character and p-orbital character, respectively. The hole occupies the s orbital centered at the vacancy and the p orbitals centered at the surrounding Ca atoms and F atoms.

DF 11.23 Thu 14:30 Poster C

Local structural phenomena in Ba-containing $PbSc_{0.5}B"_{0.5}O_3$ (B"=Ta, Nb) — •Anna-Maria Welsch[1], Boriana Mihailova[1], Thomas Malcherek[1], Bernd Guettler[2], Carsten Paulmann[1], Marin Gospodinov[3], and Ulrich Bismayer[1] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany — [2]PTB, Bundesallee 100, D-38116 Braunschweig, Germany — [3]ISSP-BAS, Blvd. Tsarigradsko Chausse 72, 1784 Sofia, Bulgaria

Relaxor-ferroelectric state is characterized by the existence of nano-scale polar clusters of different size and shape distributed inside a paraelectric matrix. Best known materials with relaxor-ferroelectric properties are Pb-based perovskite-type complex oxides of the general formula ABO_3. The perovskite structure enables ion substitutions on both A- and B-sites. Variations in the chemical composition influence the nano-domain structure and thus allow enhancement of the desired relaxor properties. Here we present our results on the structure of Ba-containing $PbSc_{0.5}(Ta,Nb)_{0.5}O_3$. The structural changes caused by the A-site doping were studied by complementary application of single-crystal X-ray diffraction and polarized Raman spectroscopy. The loading of stereochemically non-active ions causes lattice distortions and changes in the local symmetry. Our results indicate fragmentation of the ferroic clusters in the host matrix by breaking the pattern of Pb^{2+} off-centre shifts and generation of new ferroic species.

DF 11.24 Thu 14:30 Poster C

Investigation of domain structuring in the relaxor system strontium-barium-niobate by k-space spectroscopy — •Uwe Voelker, Urs Heine, Christoph Gödeker, Rainer Pankrath, and Klaus Betzler — Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, 49069 Osnabrück

We present results of second-harmonic-generation (SHG) investigations of the relaxor system strontium-barium-niobate $Sr_{0.61}Ba_{0.39}Nb_2O_6$ (SBN). Since the small birefringence in SBN prevents phase-matched SHG, we use a quasi-phase-matched arrangement in which the spatial distribution of the second harmonic intensity reflects the density distribution of domain sizes. This technique allows for conclusions on the k-space representation of the correlation lengths (*k-space spectroscopy*). We present information on the domain structuring forced by external electric fields. Repoling effects of particular size-classes of domains are studied and compared to pyroelectric measurements. The evolution of the domain morphology whilst passing the ferroelectric to paraelectric phase transition is reported. Supported by DFG (project GRK 695).

DF 11.25 Thu 14:30 Poster C

Second harmonic generation studies of $Sr_{1-x}Ba_xNb_2O_6$ single crystals — •Markus Heckhoff, Theo Kleinefeld, Vladimir Shvartsman, and Wolfgang Kleemann — Angewandte Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

$Sr_{1-x}Ba_xNb_2O_6$ (SBN) are polar oxides with the unfilled tungsten bronze structure and a single component order parameter. Upon increasing the Sr^{2+} concentration x a gradual transformation from ferroelectric to relaxor behavior is observed. The mechanism of this transformation is still under discussion and targeted investigations are urgently demanded. We present results of second harmonic generation (SHG) studies of SBN single crystals with different Sr/Ba ratios (x = 0.4, 0.5, 0.61, 0.75). Since the intensity of the SHG signal in polar materials is proportional to the polarization squared, this method is useful for investigating the phase transition. From the temperature dependence of the SHG signal, $I_{2\omega}(T)$, we obtained information on the evolution of the order parameter in the vicinity of the Curie temperature. The SHG data for compositions from ferroelectric (x=0.4) to extreme relaxor-like (x=0.75) SBN are compared. In order to obtain information on the domain structure, $I_{2\omega}(T)$ was analyzed as a function of the light incidence angle.

DF 11.26 Thu 14:30 Poster C

Magnetic properties of Mn-doped Strontium Titanate — Subhankar Bedanta[1], •Vladimir V. Shvartsman[1], Wolfgang Kleemann[1], Alexander Tkach[2], and Paula M. Vilarinho[2] — [1]Angewandte Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal

Over the last decades there has been a growing interest in studies of incipient ferroelectrics doped with different impurities. In particular, relaxor-type behaviour was found recently in $Sr_{1-x}Mn_xTiO_3$ (SMnT) ceramics with a moderate Mn content ($x \leq 0.03$) [1, 2]. Furthermore, the Mn-doping may induce distinct magnetic properties. We studied them on SMnT with $x = 0.02$ by SQUID magnetometry and *ac*-susceptometry. Both the temperature dependencies of the magnetization, $M(T)$, and of the magnetic susceptibility, $\chi(T)$, show an anomaly around 35 K. Below this temperature magnetic hysteresis is found. On the other hand, the dielectric permittivity shows a maximum in the same temperature range [2] indicating a correlation between polar and magnetic order. Efforts are put into understanding, if the observed magnetic behaviour at low temperatures might be due to superparamagnetic cluster formation or to a magnetically ordered state. A possible coupling between dielectric and magnetic properties is discussed.

[1] A. Tkach *et al.*, Appl. Phys. Lett. **86**, 172902 (2005).
[2] A. Tkach *et al.*, Phys. Rev. B **73**, 104113 (2006).

DF 11.27 Thu 14:30 Poster C

^{181}Hf(^{181}Ta) and ^{77}Br(^{77}Se) PAC measurements in calcium fluoride — •Thomas Geruschke and Reiner Vianden — HISKP, Universität Bonn, Nußallee 14-16, 53115 Bonn

Calcium fluoride is nowadays not only used in optical applications like lenses or windows for UV-laser. Nanostructures on silicon are produced with calcium fluoride masks and even as dielectric gate material in organic thin films transistors (OTFTs) it get more and more important.

To achieve more information about defects and the material itself we use the perturbed angular correlation method (PAC). First results of the annealing behaviour of the implanted probe ions ^{181}Hf(^{181}Ta) and ^{77}Br(^{77}Se) are presented and discussed.

DF 11.28 Thu 14:30 Poster C

Pulsed x-ray scattering on laser excited barium titanate — •Anton Plech[1], Konstantin Istomin[1], Vassilios Kotaidis[1], and Qingyu Kong[2] — [1]Fachbereich Physik, Uni Konstanz, Universitätsstr. 10, D-78457 Konstanz — [2]ESRF, BP 220, F-38043 Grenoble

Pulsed x-ray scattering is used to resolve the structural dynamics of laser excited barium titanate powder. The sample is excited by intense near-IR femtosecond laser pulses close to the ferroelectric to paraelectric phase transition. By using the synchronized pulses of the Synchrotron Radiation source ESRF it was possible to resolve the lattice transformation and order parameter change at a 100ps time resolution. It is shown, that the polarization of the unit cell decouples from the thermal lattice change in the picosecond regime.

K. Istomin, V. Kotaidis, A. Plech and Q. Kong, Appl. Phys. Lett. (2007) in press.

DF 11.29 Thu 14:30 Poster C

3D-Laue diffraction of thin micrometer scaled crystals with visible light — •Marcel Roth and Ullrich Pietsch — Institute of solid state physics, University of Siegen, 57072 Siegen, Germany

The interaction of crystals with lattice constants in the micrometer range - such as photonic crystals or colloidal crystals - with visible light shows a plenty of faszinating effects and useful applications. For example light can be strongly manipulated when using quantum optical effects that occur for photonic crystals.

On the other hand the 3D-Laue diffraction of visible light on photonic and colloidal crystals is promising for a selection of various optical wavelengths out of a white beam. This effect is a part of the basic functionality of the human vision.

There is a similarity to the Laue diffraction know for x-rays, but essential differences exit as well. The latter one is due the fact that the refraction index for optical light is far from unity. Therefore simple 1.Born approximation is not valid and one has to consider multiple scattering effects. In this presentation we show first light diffraction experiments from artificial crystals with lattice parameters of about 1 μm. The 3D structure of the crystal is analysed by ω scans and results are interpreted in terms of an extended scattering theory.

DF 11.30 Thu 14:30 Poster C

High-pressure infrared study of the multiferroic $BiFeO_3$ — •A. Pashkin[1], C. A. Kuntscher[1], R. Haumont[2], and J. Kreisel[3] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Laboratoire de Physico-Chimie de l'Etat Solide ICMMO - UMR CNRS, Université Paris Sud, 91405 Orsay Cedex, France — [3]Laboratoire des Matériaux et du Génie Physique (CNRS), INP Grenoble - MINATEC 38016 Grenoble, France

Magnetoelectric multiferroics currently attract much attention. $BiFeO_3$ is one example, which exhibits antiferromagnetic ($T_N \sim 370$ °C) and ferroelectric ($T_C \sim 830$ °C) orders up to very high temperatures. A recent attempt has been made to understand the role of phonons for the multiferroic character of $BiFeO_3$ by temperature-dependent Raman measurements [1]. Besides temperature or electric/magnetic field, pressure is a good parameter to find out more about the underlying mechanism of multiferroicity.

We report a high-pressure infrared spectroscopic study of $BiFeO_3$ in the far-infrared range up to 21 GPa. The eigenfrequencies of the phonons appreciably increase with increasing pressure. Moreover, several modes show a non-linear pressure dependence with kinks at around 5 and 12 GPa, supporting the results of recent pressure-dependent Raman studies.

Supported by the DFG. Provision of beamtime at the ANKA Angströmquelle Karlsruhe is acknowledged.

[1] R. Haumont et al., Phys. Rev. B **73**, 132101 (2006).

DF 11.31 Thu 14:30 Poster C

Li diffusion in the intercalated anode material $Li_{4+x}Ti_5O_{12}$ with $x > 0$ — •Wojciech Iwaniak[1], Martin Wilkening[1], Jessica Heine[1], Viktor Epp[1], Paul Heitjans[1], Malte Behrens[2], and Wolfgang Bensch[2] — [1]Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover — [2]Institute of Inorganic Chemistry, Christian-Albrechts University Kiel

Currently there is considerable interest in spinel-type structured $Li_{4+x}Ti_5O_{12}$ ($0 \leq x \leq 3$, space group $Fd\bar{3}m$) as a future anode in secondary Li ion batteries. Whereas the host material with $x = 0$ is a poor Li conductor [1], the intercalated compounds with $0 < x < 3$ show enhanced Li diffusivity. Additional Li can be inserted into $Li_4Ti_5O_{12}$ either chemically by treatment with *n*-butyl lithium or electrochemically. Diffusion parameters were studied by ^{7}Li spin-alignment echo (SAE) NMR as well as by ^{7}Li rotating frame spin-lattice relaxation NMR. Activation energies E_A of Li diffusion in the intercalated materials prepared by both routes are similar. Compared to the non-intercalated host E_A is reduced by about a factor of two. In the host ($x = 0$) an activation energy of 0.86(1) eV was recently found by SAE-NMR, see Ref. [1]. NMR results will be compared with data obtained by dc-conductivity measurements.

[1] M. Wilkening, R. Amade, W. Iwaniak and P. Heitjans, Phys. Chem. Chem. Phys., 2007, DOI:10.1039/b616269j, in press.

DF 12: Electric, Electromechanical and Optical Properties II

Time: Friday 10:30–12:50 Location: H11

Invited Talk DF 12.1 Fri 10:30 H11

Piezoelektrische Gradientenkeramik – Herstellung und Charakterisierung — •Ralf Steinhausen — Martin-Luther-Universität Halle, Institut für Physik, Friedemann-Bach-Platz 6, 06108 Halle

Monolithische piezoelektrische Keramiken mit einer inhomogenen chemischen Zusammensetzung und den damit verbundenen inhomogenen Materialeigenschaften sind spätestens seit der Einführung des RAINBOW-Aktuators durch Haertling et al. für Anwendungen insbesondere als Biegeaktuatoren interessant geworden. Ausgehend von Schichtstrukturen mit unterschiedlichen Ausgangsmaterialien und Schichtdicken kann der chemische Gradient gezielt beeinflusst werden. Es wird eine Reihe von Kombinationen von stark und schwach sowie harten und weichen piezoelektrischen, leitfähigen und elektrostriktiven Keramiken diskutiert. Allen ist gemeinsam, dass der chemische Gradient erst durch einen Polungsvorgang in einen piezoelektrischen Gradienten umgewandelt werden muss. Auf Grund der ebenso veränderlichen ferroelektrischen Eigenschaften kommt es zu einer stark inhomogenen Feldverteilung und damit zur Bildung eines Po-

larisationsgradienten. Der Polungsprozess kann durch ein einfaches Schichtmodell beschrieben werden, wobei die Einzelschichten durch ein Preisach-Modell modelliert werden. Die Rolle der elektrischen Leitfähigkeit wird dabei diskutiert. Mit der LIMM-Methode wurde die Polarisationverteilung an Ba(Ti,Sn)O3-Keramiken untersucht. Das elektromechanische Verhalten von bleifreien Gradientenkeramiken auf der Basis von BaTiO3 wurde mit Hilfe von Biegeexperimenten untersucht.

DF 12.2 Fri 11:10 H11

Doped Polyurethane as Matrix Material for Pyroelectric Composites — •Markus Krause and Bernd Ploss — Fachbereich SciTec, Fachhochschule Jena, Carl-Zeiss-Promenade 2, 07745 Jena

Composites of pyroelectric ceramic particles in a polymer matrix appear attractive as materials for pyroelectric sensors, in particular because of their compatibility with the process technology for integrated circuits.

There is, however, a substantial dielectric mismatch between the high dielectric permittivity of the ferroelectric ceramic particles and the significantly lower dielectric permittivity of the polymer matrix. This mismatch limits the pyroelectric activity and it is the reason for a relative low performance of such pyroelectric composites.

In recent theoretical studies we had shown that the dielectric mismatch can be reduced substantially when a well specified electric conductivity is introduced into the matrix material. Therefore, we have investigated experimentally how the dielectric function of polyurethane can be modified by doping in solutions of alkali halides. Parameters for an optimization of polyurethane as matrix material have been identified.

By applying this optimized doping to 0-3 composites of lead zirconate-titante (PZT) particles in polyurethane an increase in the pyroelectric coefficient by a factor of twenty has been achieved.

DF 12.3 Fri 11:30 H11

The influence of particle agglomeration on the dielectric and magnetic properties of a nanocomposite — •Béatrice Hallouet[1], Bernd Wetzel[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2, Experimentalphysik, Universität des Saarlandes Postfach 151150, 66 041 Saarbrücken, Germany — [2]Institut für Verbundwerkstoffe (IVW GmbH), University of Kaiserslautern D-67663 Kaiserslautern, Erwin-Schrödinger Str. Geb. 58, Germany

We have investigated a composite consisting of magnetic nanoparticles (magnetite) in a polymer matrix. We study permittivity and permeability for different particle concentrations using dielectric measurements in the frequency range from 5 Hz to 1 GHz as well as magnetic measurements from 10 MHz to 6 GHz. The measured permittivity shows already a relaxation of the pure matrix which is enhanced by the addition of particles. We use the spectral representation of Bergman in order to show that this effect is partly due to a polarization of the conducting particles, and partly due to a change of molecular polarisability at the interfaces between particles and matrix. The high frequency permittivity reflects the existence of the agglomerates. Combining this structural information and the measured permeability, the spectral representation allows us to evaluate the intrinsic permeability of the nanoparticles. In addition the ferromagnetic resonance is analyzed and it is shown that the resonance frequency doesn't depend on the filling factor.

DF 12.4 Fri 11:50 H11

Temperaturabhängige Ladungstransportprozesse in Lithiumniobat-Kristallen* — •Katharina Brands, Matthias Falk, Daniel Haertle, Theo Woike und Karsten Buse — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Ladungstransportprozesse in eisendotierten Lithiumniobatkristallen wurden mit Hilfe der Leitfähigkeitsspektroskopie temperaturabhängig untersucht. Mit dem „free energy random barrier"-Modell lassen sich aus den Spektren die Gleichspannungsleitfähigkeit und die Zeitkonstante τ_e, die der Grenzfrequenz zwischen dem frequenzunabhängigen Teil und dem frequenzabhängigen Teil des Spektrums entspricht, bestimmen. Über die Temperaturabhängigkeit dieser Größen wird auf Aktivierungsenergien geschlossen.
Es wurden zwei Aktivierungsenergien beobachtet, von ca. 0.3 eV, die den Elektronen zugeordnet wird, und von ca. 1.2 eV, die von Li^+-Ionen herrührt. Durch diese Experimente lässt sich auch das Konzentrationsverhältnis $c_{Fe^{2+}}/c_{Fe}$ sehr genau bestimmen. Damit konnten wir zeigen, dass dieses Verhältnis für thermoelektrisch oxidierte Kristalle auf bis zu 4.6×10^{-6} absinkt.

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DF 12.5 Fri 12:10 H11

Brechungsindex- und Absorptionsänderungen in Lithiumniobat-Kristallen durch Strahlenschäden und ihr Temperaturverhalten* — •Mohammad-Reza Zamani-Meymian, Konrad Peithmann und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn

Durch Bestrahlung mit leichten, hochenergetischen Ionen wie ^{3}He mit 40 MeV werden Änderungen des Brechungsindex Δn (bis zu 3×10^{-3}) sowie der Absorption $\Delta\alpha$ in kongruent schmelzenden Lithiumnibat-Kristallen erzeugt, was z. B. fuer die Herstellung vergrabener Wellenleiter genutzt werden kann. Die thermische Stabilitaet der erreichten Änderungen wird systematisch untersucht, um Aussagen ueber die Haltbarkeit der Materialmodifikationen machen zu koennen.
* gefördert durch die Deutsche Forschungsgemeinschaft (FOR557)

DF 12.6 Fri 12:30 H11

Association of oxygen vacancies with impurity metal ions in lead titanate: first-principles calculations and kinetic modeling — Paul Erhart[1], R.-A. Eichel[2], Petra Träskelin[3], and •Karsten Albe[1] — [1]TU Darmstadt, Institut für Materialwissenschaft — [2]TU Darmstadt, Eduard-Zintl-Institut — [3]University of Helsinki, Finland

Oxygen vacancies (V_O) and their associates are widely believed to play an important role in the ageing and the fatigue of ferroelectrics. Knowledge of their energetics is therefore instrumental in order to understand these processes. We have used DFT calculations in order to study the energy landscape for the formation and migration of free and complexed V_O in Cu and Fe doped $PbTiO_3$. It is found that nearest neighbor configurations are preferred and the migration barriers for V_O in the vicinity of metal impurities are significantly higher than for uncomplexed V_O. These insights permit us to review the assumptions underlying the Arlt-Neumann model for ageing. On the basis of our calculations we present a kinetic model which allows to study the redistribution of free and complexed oxygen vacancies in a tetragonal perovskite. It is shown that the conversion between free and complexed vacancies readily occurs during growth. In the absence of an electric field, one specific impurity atom–vacancy configurations is dominating. Upon application of an oscillating electric field near room temperature, however, a dynamic equilibrium between different impurity atom–vacancy configurations is installed. We propose that the fatigue of ferroelectric material is closely related to this dynamic balance.