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 Substitutionen 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 nanoscale 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.

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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 pro-

duced 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.