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.

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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 par-

ticle 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.

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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.

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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).