DF 11: Dielectric and ferroelectric thin films and nanostructures I

Time: Wednesday 14:00–17:00 Location: EB 107

DF 11.1 Wed 14:00 EB 107

The impact of strain on the properties of ferroelectric bilayers: A LGD approach — •Ludwig Geske, I.B. Misirlioglu, Ionela Vrejoiu, Marin Alexe, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120

Interfaces and defects may significantly alter the properties of ferroelectric thin films. Epitaxial bilayers consisting of $PbZr_{0.2}Ti_{0.8}O_3$ (*PZT20/80*) and $PbZr_{0.4}Ti_{0.6}O_3$ (*PZT40/60*) were grown by pulsed laser deposition with the scope to create defects in a controlled manner in order to investigate their influence. The films were deposited on vicinal $SrTiO_3$ (001) substrates using a perovskite $SrRuO_3$ bottom electrode which grows pseudomorphically to the subtrate. A large impact of the layer sequence on the defect generation and the formation of an a/c domain structure can be observed. These structural changes lead to a strong shifting of the remanent polarisation and the dielectric constant. In the attempt to understand this behaviour, the Landau-Ginzburg-Devonshire (LGD) theory is used, which is a versatile tool to describe the behaviour of ferroelectric materials. A short introduction into the LGD theory modified for the treatment of ferroelectric thin films will be given together with the results for single layered *PZT20/80* and *PZT40/60* films. Subsequently the influence of the electrostatic coupling at the interface between the *PZT* layers will be demonstrated. Finally the theory will be applied to the specific case of the *PZT* bilayers on $SrTiO_3$ to find an explanation for the behaviour of the ferroelectric properties by adapting the possible relaxation states and coupling terms.

DF 11.2 Wed 14:20 EB 107

Ferroelectricity in antiferroelectric epitaxial $PbZrO_3$ films with different orientations — •Ksenia Boldyreva[1], Lucian Pintilie[1,2], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany — [2]NIMP, P.O. Box MG-7, 077125 Bucharest-Magurele, Romania

$PbZrO_3$ (PZO) is a well known antiferroelectric (AFE) material with orthorhombic crystal structure. Due to antiparallel lead-ion shifts the remnant polarization is nominally zero. With a sufficiently large applied electric field, PZO undergoes a field-driven phase transition into a ferroelectric (FE), rhombohedral phase. However, the existence of a FE polarization along the c-axis of PZO (without applied field) was predicted by Jona *et al.* with an estimated value of 25 $\mu C/cm^2$ [1]. We have investigated the temperature dependence of hysteresis and capacitance in PLD-grown epitaxial PZO films with two different orientations in the 4.2-400K temperature range. It was observed that $(120)_o$-oriented films (index o-orthorhombic) show a mixed AFE and FE behaviour on the entire temperature range, the FE behaviour being more stable at low temperatures. In contrast, the $(001)_o$-oriented films show a FE hysteresis only at temperatures up to 60 K. Above 60 K the hysteresis splits into two loops, typical for antiferroelectrics. The results indicate the coexistence of FE and AFE properties in PZO films, particularly at low temperature.

[1] F. Jona, G. Shirane, F. Mazzi, and R. Pepinsky, Phys. Rev. **105**, 849 (1957)

DF 11.3 Wed 14:40 EB 107

Static and Dynamic Properties of Ferroelectric Nanostructures and Multiferroic Bulk Systems: A Multiscale Approach — •Thomas Michael[1], Julia Wesselinowa[2], and Steffen Trimper[1] — [1]Institute of Physics, Martin-Luther-University, D-06099 Halle, Germany — [2]University of Sofia, Department of Physics, Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria

Ferroelectric nanostructures and multiferroic bulk systems are studied in a multiscale approach. The excitation energy and the associated damping of ferroelectric modes as well as the polarization and the hysteresis are presented as a function of the temperature, the defect concentration, size and shape of the nanomaterials. The softening of the mode is strongly influenced by the kind of doping ions, the surface configuration and the defect composition. The analysis is based on a modified Ising model in a transverse field. A Green's function technique in real space provides the static and dynamic properties, which differ significantly from the bulk behavior. Additionally a mesoscopic approach is carried out similar to the Landau-Lifshitz equation with Gilbert damping for ferromagnets. The temperature dependence of the damping paramters is discussed. The analysis is extended to multiferroic bulk systems, where the magnetic moments interact via the Heisenberg model and the multiferroic coupling term differs for hexagonal and orthorhombic materials. We present the dielectric function and the dynamic properties of the coupled model. Both, the Green's function technique and the mesoscopic Landau-Lifshitz equation are applicable here. Theoretical results are compared with experiments.

DF 11.4 Wed 15:00 EB 107

Ferroelectric lithography on doped $LiNbO_3$ single crystals — •Alexander Haussmann and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

The presence of different surface charges and thus different surface reactivities offers the possibility of exploiting domain-structured ferroelectrics as templates for nanostructure assembling. Recent work has reported on the photochemical adsorption of noble-metal nanoparticles to such surfaces serving as pin-points for attaching desired organic molecules [1].

Here, we report on the formation of domain structures of μm-sizes in 5 mol% Mg-doped congruent $LiNbO_3$ single crystals by (a) UV-induced poling using a HeCd laser beam ($\lambda = 325$ nm) focused through liquid electrodes, as well as (b) the application of high voltage between a contact mode AFM tip and a back electrode. Subsequently, the deposition of wire-like metal structures at the domain wall positions was stimulated by illuminating the sample dipped into aqueous solutions of $AgNO_3$ or $Pt(NO_3)_2$ by super bad-gap illumination ($\lambda < 310$ nm) using a Hg spectral lamp. Structural properties of the resulting nano- and mesowires were examined using non-contact AFM and Kelvin probe force microscopy [2]. Electrical conductivity of 300 μm long Pt wires between macroscopic electrodes could be demonstrated by performing I-V-scans.

[1] S.V. Kalinin, D.A. Bonnell et al., Nano Letters **2**, 589 (2002)

[2] U. Zerweck, Ch. Loppacher et al., Phys. Rev. B **71**, 125424 (2005)

DF 11.5 Wed 15:20 EB 107

Electron emission from ferroelectric thin films induced by polarization switching — •Oliver Mieth[1], Hannes Klumbies[1], Günter Milde[2], Gerald Gerlach[2], and Lukas Eng[1] — [1]Institut für Angewandte Physik, Technische Universität Dresden — [2]Institut für Festkörperelektronik, Technische Universität Dresden

Ferroic materials are promising candidates for high-efficient electron emission in various applications. However, most work in this research field so far did focus on electron emission from bulk ferroelectric materials.

Here we present studies on electron emission under ultra-high vacuum conditions (base pressure $< 10^{-9}$ mbar) using PZT and other thin ferroelectric films as the emitter source that measure some hundred nanometer in thickness. Electron emission is collected through 10 - 20 μm-sized apertures lithographically manufactured into the top electrode. We show that current densities of up to 10^{-11} A/cm^2 are measurable by simply switching the thin film in the 10 Volt regime. The count rates measured as a function of applied switching voltage showed an almost linear behavior, in contrast to bulk PMN-PT single crystals which exhibited an exponential relationship. For correlating these results to known ferroelectric properties, e.g., coercive field and local imprint effects, local hysteresis loops were recorded simultaneously using Piezoresponse Force Microscopy. We are able to demonstrate that polarization switching induces the onset of electron emission. These experimental findings were consistently interpreted using Finite Element Method (FEM) modeling of the investigated structure.

DF 11.6 Wed 15:40 EB 107

Field effect transistor of graphitized polyimide with P(VDF-TrFE) as gate insulator — •I. Lazareva[1], Y. Koval[1], P. Müller[1], I. Paloumpa[2], K. Müller[2], and D. Schmeisser[2] — [1]Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg, Erwin-Rommel Str. 1, 91058 Erlangen, Germany — [2]Lehrstuhl Angewandte Physik/Sensorik, Brandenburgische Technische Universität Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus,

Germany

Surfaces of polyimide films were graphitized by low-energy ion irradiation. The conductivity was between 10^{-5} to 200 S/cm [1]. We prepared field effect transistors using this material. Ferroelectric P(VDF-TrFE) was used as gate insulator. The thickness of P(VDF-TrFE) varied from 120 nm to 1200 nm. Properties of P(VDF-TrFE) were investigated by current-voltage measurements of metal/ P(VDF-TrFE)/metal capacitors. We have found that at room temperature, the coercive field of P(VDF-TrFE) does not depend on the film thickness. At lower temperatures the coercive field increases proportionally to the reciprocal temperature. Remnant polarization is 9.5 μC/cm^2. It slightly rises with decreasing temperature. Our recent results of field effect mobility, carrier concentration and threshold voltage are presented.

[1] I. Lazareva, Y. Koval, M. Alam, S. Strömsdörfer, P. Müller, Appl. Phys. Lett. 90, 262108 (2007)

DF 11.7 Wed 16:00 EB 107

Investigations on ferroelectric properties of $P(VDF/TrFE)$ and $BaTiO_3$ by local field and Monte Carlo computations — •Markus Kühn and Herbert Kliem — Saarland University, Institute of Electrical Engineering Physics, P.O. Box 151150, 66041 Saarbrücken, Germany.

For interacting model systems of the $P(VDF/TrFE)$ copolymer and the $BaTiO_3$ crystal dynamic Monte Carlo simulations are performed. The systems consist of field-induced point dipoles and permanent dipoles / ions. Both ferroelectric systems are placed between two coplanar conducting electrodes. All electrostatic interactions are considered and the electrodes are described by the method of images. The permanent dipoles / ions fluctuate thermally activated in double well potentials according to the Boltzmann statistics. The long-range electrostatic interactions strongly influence the local fields at the dipoles / ions. The iterative algorithm consists of two steps. For each current configuration the local fields at the dipoles / ions are deterministically calculated. Then the transition times of the dipoles / ions which depend on the local electric fields are computed in a following weighted probabilistic Monte Carlo step. As the main result we find ferroelectric hysteresis loops and polarisation switching curves. Further results for $P(VDF/TrFE)$ have shown that dielectric layers adjacent to the electrodes have an impact on the hystereses. Simulations of the (2 0 0)-plane for $BaTiO_3$ show a pronounced domain growth starting at the electrode. Snapshots of the system at different times further revealed a pronounced pinning effect at a discontinuity modelled by a vacancy.

DF 11.8 Wed 16:20 EB 107

Probing ferroelectricity in ultrathin wedged epitaxial $BaTiO_3$ films — •Adrian Petraru[1], Hermann Kohlstedt[1], Axel Solbach[2], Nikolay Pertsev[3], Uwe Klemradt[2], Willi Zander[4], Jürgen Schubert[4], and Rainer Waser[1] — [1]Institut für Festkoerperforschung und CNI, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, 52074 Aachen, Germany — [3]A. F. Ioffe Physico-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [4]Institut für Bio - und Nanosysteme und CNI, Forschungszentrum Jülich GmbH, Jülich, Germany

High quality epitaxial wedged $BaTiO_3$ ultrathin films were grown epitaxially on $SrRuO_3$-covered (001) - oriented $SrTiO_3$ substrates by high-pressure sputtering. The composition along the wedge was checked by Rutherford Backscattering Spectrometry (RBS). The thickness slope and the in-plane and out-of plane lattice parameters of the wedge were studied by x-ray diffraction using a laboratory source and synchrotron radiation. The $BaTiO_3$ films were fully strained by the substrate. Ferroelectric capacitors were then fabricated from $SrTiO_3/SrRuO_3/BaTiO_3$(wedge)$/SrRuO_3/Pt$ heterostructures using optical lithography and ion beam etching. Direct evidence of ferroelectricity in these films down to the thickness of 4 nm was obtained by measurements of polarization-voltage hysteresis loops.

DF 11.9 Wed 16:40 EB 107

A combined first principles and electron-holographic aproach to domain boundaries in (multi)ferroic materials — •Axel Rother[1], Nicola Spaldin[2], and Hannes Lichte[1] — [1]Institute for Structural Physics, TU Dresden, 01062, Germany — [2]Materials Department, University of California, Santa Barbara, CA 93106

Domain boundaries in ferroic materials deviate from the bulk in both the structural and electronic properties. Their presence in the material influences the total energy of the system as well as the dynamic properties, for instance during polarization switching. We report on a combined Density Functional Theory and Electron Holographic approach on domain boundaries in multiferroic $BiFeO_3$, ferroelectric $BaTiO_3$ and other (multi-)ferroic materials. Our model systems extend over different domain walls with respect to material composition and angular change and encompass between 50-120 atoms. The calculations were performed within VASP, a package for DFT using pseudopotentials and a plane wave basis set, particularly suited for such big systems. The calculations reveal the details of charge and structure modulation on the boundary, including the formation of dipole layers and a change in the magnetic behaviour in case of $BiFeO_3$. Electron holographic measurements support the findings of the calculations by measuring dipole layers and charge modulations on the domain boundaries.