DF 18: Dielectric and ferroelectric thin films

Time: Wednesday 16:00–18:20 Location: GER 37

DF 18.1 Wed 16:00 GER 37

An unexpected depolarization current peak in polyethylene oxide — •Bjoern Martin and Herbert Kliem — Saarland University, Germany

Thin films of polyethylene oxide (PEO) are investigated as model systems for a solid electrolyte. Metal-PEO-metal capacitance structures show a pronounced relaxational behaviour with a thickness dependent effective dielectric permittivity caused by a space charge polarization of mobile ions.

In the experiment it is found that the transient polarization and depolarization currents after application of small field steps follow a power law in the long time range. By using higher fields charge injection during the polarization sets in resulting in nearly constant currents in the long time range. The depolarization currents now show an unexpected maximum in time. The time to the maximum depends on the height of the voltage applied before, the polarization time, the sample thickness, the temperature, and the Li doping.

A discrete three-dimensional model is developed to describe the charge motion. Single charges are regarded. Negative ions can fluctuate thermally activated over energy barriers in a multiwell potential. Positive immobile ions provide charge neutrality. Additionally, electrons can be injected into the system and also be extracted from the dielectric. Interactions of the charges with the electrodes using the method of images and all other electrostatic interactions are considered.

From these simulations it is shown that the appearance of the transient depolarization current maximum is caused by injected electrons.

DF 18.2 Wed 16:20 GER 37

Correlation between structural and ferroelectric properties of epitaxial PMN-PT films — •Michael Mietschke[1,2], Sebastian Fähler[1,3], Ludwig Schultz[1,2], and Ruben Hühne[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden — [2]Technische Universität Dresden — [3]Technische Universität Chemnitz

Ferroelectric materials like lead magnesium niobate-lead titanate (PMN-PT) show an electrocaloric effect induced by an electrical field during a diffusionless phase transition, which might be used for novel solid state cooling devices. However, the interplay between the microstructure and the ferroelectric properties is not completely understood so far. To study this in detail, epitaxial 0.68 $Pb(Mg_{1/3}Nb_{2/3})O_3$-0.32 $PbTiO_3$ films were grown by pulsed laser deposition on (001) single crystalline $SrTiO_3$ (STO) substrates with a miscut angle between 0 and 15 degrees towards the [100] direction. The influences of the deposition parameters and the miscut angle on the PMN-PT structure was studied by x-ray diffraction, atomic force microscopy and scanning electron microscopy. A capacitor like structure was realized by growing the PMN-PT film on a conducting buffer layer with additional Pt-top electrodes on the surface. A nearly pure perovskite phase was found using $La_{0.7}Sr_{0.3}Co_3$ buffer layers on (001) STO substrates and low deposition temperatures. An increasing miscut angle improves the purity of the PMN-PT perovskite phase further. Finally, a correlation of the ferroelectric properties with the phase purity of the PMN-PT film was found.

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DF 18.3 Wed 16:40 GER 37

First principles study of the electrocaloric effect in strained $BaTiO_3$ — •Madhura Marathe and Claude Ederer — Materials Theory, ETH-Zurich, Switzerland

The electrocaloric (EC) effect – a reversible change in temperature of a material by applying an external electric field – has been known for a very long time [1]. Recently however, the discovery of a "giant electrocaloric effect" [2] has stimulated extensive work on the EC effect, due to its huge potential to increase the efficiency of cooling devices. We have studied how misfit strain affects the EC temperature change in bulk $BaTiO_3$.

We have performed molecular dynamics simulations for an effective Hamiltonian based on first-principles density functional theory [3]. The calculated EC temperature change ΔT reduces when $BaTiO_3$ is only clamped but not strained, but increases again with increasing misfit strain. Further with increasing misfit strain, there is a shift in the ΔT peak towards higher temperatures. Therefore the misfit strain can be utilized in two ways – (i) to enhance the EC temperature change and (ii) to achieve a maximal effect in the temperature range of interest for a given application.

[1] J. F. Scott, Annu. Rev. Mater. Sci. **41**, 229 (2011).
[2] A. S. Mischenko, *et al.*, Science **311**, 1270 (2006).
[3] T. Nishimatsu, *et al.*, Phys. Rev. B **82**, 134106 (2010).

DF 18.4 Wed 17:00 GER 37

Multilayer Thin Films of Ferroelectric VDF-TrFE Copolymer Characterized by Dielectric Nonlinearities — •Danny von Nordheim[1], Andreas Austin[1], K.H. Chew[2], and Bernd Ploss[1] — [1]Department of SciTec, University of Applied Sciences Jena, Carl-Zeiss-Promenade 2, 07745 Jena, Germany — [2]Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia

Multilayer ferroelectric structures consist of two or more layers, usually thin films, with at least one of them exhibiting ferroelectric properties. Ceramic multilayers and superlatticess have attracted immense attention during the last years due to their unique behaviour and potential applications namely data and energy storage. Organic materials provide a nontoxic, easily processable alternative. As a model system a stack of two ferroelectric P(VDF-TrFE) thin films with a composition of 56/44 mol% and 70/30 mol% and a thicknesses of approx. 200 nm each has been deposited on a glass substrate covered with aluminium electrodes. The single layers and the multilayer have been characterized regarding their nonlinear dielectric properties at different temperatures. The results have been evaluated with reference to phase transitions and remanent polarisation.

DF 18.5 Wed 17:20 GER 37

Photo-electronic processes in $BiFeO_3$ — •Akash Bhatnagar[1], Young Heon Kim[2], Dietrich Hesse[1], and Marin Alexe[1,3] — [1]Max Planck Institute of Microstructure Physics, D-06120 Halle, Germany — [2]Korea Research Institute of Standards and Science, Daejeon 305-304, Rep. of Korea — [3]University of Warwick, Department of Physics, Coventry CV8 2EN, United Kingdom

Recently, reports regarding the observation of above-band gap open-circuit voltages (V_{oc}) in $BiFeO_3$ (BFO) thin films under illumination, i.e. the photovoltaic effect (PV), has attracted much attention in the field of ferroelectric materials. Initial investigations primarily attributed this effect to charge separation at ferroelastic domain walls . Subsequent studies, via localized measurements, revealed the presence of shallow trap levels which might be contributing towards the effect . Thus till now, the origin of this effect has been under some clouds of speculations.

In the present work we have elaborated upon conclusive evidence to determine the actual role of domain walls in the PV effect. Moreover, an analytical model will be presented via which the generation of PV current in different directions can be calculated. By performing temperature dependent and angle resolved measurements we prove that the bulk photo effect, which has been at the origin of the PV effect in other ferroelectric materials, is also responsible in case of BFO. However, the presence of ferroelastic domains and domain walls largely influences its manifestation. Similar measurements performed on strained BFO provide an insight into different conduction mechanisms.

DF 18.6 Wed 17:40 GER 37

Epitaxial PLD growth of strained ferroelectric KxNax-1NbO3 thin films and superlattices — •Jan Sellmann, Jutta Schwarzkopf, Dorothee Braun, Andreas Duk, Albert Kwasniewski, and Martin Schmidbauer — Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin

(K,Na)NbO3 single crystals exhibit excellent ferro-/piezoelectric properties, however, they are less investigated in thin film form. We have deposited KxNa1-xNbO3 single layers and (NaNbO3)n/(KNbO3)m superlattices epitaxially by Pulsed Laser Deposition (PLD) on various lattice mismatched substrates providing compressive and tensile lattice strain. KxNa1-xNbO3 films have been realized by the use of KxNa1-xNbO3 ceramics (x = 0 - 0.75) as PLD targets. Increased K incorporation up to x = 0.5 into the films leads to a significant improvement of both the piezoresponse and to an increased lattice mismatch between film and substrate. In order to obtain higher critical thicknesses for

fully strained film growth superlattice structures were grown by the alternating deposition of NaNbO3 and KNbO3 films with individual film thicknesses between 1 to 20 monolayers. While alternating layers with nominal thicknesses of up to three monolayers result in single layers consisting of a KxNa1-xNbO3 solid solution, superlattice structures (NaNbO3)n/(KNbO3)m were successfully deposited with individual layer thicknesses of seven or more monolayers. In particular, high piezoresponse was obtained on films with 5x(NaNbO3)17/(KNbO3)9 superlattice structure. We present a detailed study of different m/n ratios on piezoresponse and local ferroelectric hysteresis curves.

DF 18.7 Wed 18:00 GER 37

Asymmetric oxygen vacancy distribution in $CaTiO_3$ capacitors — •Andreas Krause[1], Walter M. Weber[1], Uwe Schroeder[1], Johannes Heitmann[1,2], and Thomas Mikolajick[1,3] — [1]NaMLab gGmbh, D-01187 Dresden — [2]Institut fuer Angewandte Physik, TU Bergakademie Freiberg — [3]Institut fuer Halbleiter- und Mikroelektronik IHM, TU Dresden

$CaTiO_3$ is a promising material as a high-k dielectric in metal-insulator-metal capacitors, combining a high dielectric constant (k) and relatively low leakage currents. Using various electrodes, $CaTiO_3$ shows intrinsic differences for both top and bottom charge carrier injection in addition to electrode dependent injection. Therefore, the band offset between valence band of the dielectric and the work function of the electrode material is not the only parameter responsible for leakage currents. As previously stated in literature for $SrTiO_3$[1], electrodes induce differences in oxygen vacancy distribution in the dielectric. Here, $CaTiO_3$ exhibits a conduction behavior comparable to $SrTiO_3$ with different electrodes Pt, C, Ru and TiN. This indicates an universal behavior of high-k perovskites and may be crucial for future device integration.

[1]*Kim et al.* Understanding of Trap-Assisted Tunneling Current - Assisted by Oxygen Vacancies in $RuO_x/SrTiO_3$/TiN MIM capacitor for the DRAM application. *Memory Workshop, 2012 4th IEEE International*