DF 7 Dielectric and Ferroelectric Thin Films and Nanostructures II

Time: Wednesday 14:30–16:50 Room: KÖN Farb

DF 7.1 Wed 14:30 KÖN Farb

Temperature dependence of elastic electron tunnel currents through thin tantalum oxide films — •Yanka Jeliazova and Detlef Diesing — Institut für Physikalische Chemie, Universität Duisburg Essen

The tunnel process through thin tantalum oxide layers is investigated in tantalum–tantalumoxide–gold thin film tunnel devices. They consist of metal layers (30 nm tantalum, 15 nm gold) separated by a 3.5 nm thick oxide layer. Field strengths up to 1 GV / m were applied to the device and the tunnel current was measured from the 10 $pA \cdot cm^{-2}$ to 10 $mA \cdot cm^{-2}$. At tunnel voltages exceeding the barrier height ($e \cdot U_T > \varphi_B$) a clear fingerprint of the Fowler-Nordheim tunnel process should be expected in the current voltage plot. This can be barely seen in the experiment with a single current voltage plot at one dedicated temperature. Thereby the band structure of the devices has to be determined by another method. We recorded current voltage plots from 60 K to 500 K and evaluated the temperature dependence of the tunnel current for dedicated tunnel voltages. For tunnel voltages ($U_T < 1$ V) only a weak increase of the tunnel current of 30 % could be observed while heating the sample from 60 K to 500 K . For tunnel voltages ($U_T > 1.3$ V) a strong current increase about 4 orders of magnitude was detected. These experimental findings can be rationalized by a thermally induced increase of Fowler Nordheim tunneling processes through a tunnel barrier with 1.8 eV height.

DF 7.2 Wed 14:50 KÖN Farb

Charge states of native point defects in Pr-based high-k dielectrics — •Jarek Dabrowski[1], Andrzej Fleszar[2], Grzegorz Lupina[1], Gunther Lippert[1], Anil Mane[1], and Christian Wenger[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt(Oder), Germany — [2]Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

High-k dielectric films can trap electric charge, which aggravates their application in silicon technology as dielectrics in MOS transistors and MIM capacitors. On the basis of ab initio calculations for band offsets and defect formation energies we discuss the charge states of native point defects in Pr oxides and silicates. In particular, we find that oxygen vacancies in Pr_2O_3 introduce electron transition states at Fermi energies falling within the range of the Si substrate band gap. In thin films grown on Si, oxygen intersitials are always negatively charged in Pr_2O_3 (i.e., they act as negative fixed charges there) and always electrically neutral in PrO_2. In Pr silicates, a valence alternation defect consisting of a Si atom with a dangling bond interacting with an O atom from the silicate network is expected to be the source of a positive fixed charge.

DF 7.3 Wed 15:10 KÖN Farb

Impedance spectroscopy study of thin film capacitors with SrTiO(3) as dielectric — •Kesav Reddy[1], Dieter Mergel[1], and Werner Osswald[2] — [1]Thin film working group, Physics Department, University Duisburg-Essen, 45117 Essen — [2]Institute for Solid-State Chemistry, Chemistry Department, University Duisburg-Essen, 45117 Essen

Planar thin films capacitors with RuO(2) electrodes and SrTiO(3) as dielectric layer have been prepared by rf-magnetron sputtering. Substrate temperature (up to 700°C), oxygen content of the sputter gas and thickness of the dielectric layer have been varied.

The capacitors were investigated by x-ray diffraction and impedance spectroscopy in the range 10 Hz to 10 MHz and for temperatures from 20°C to 200°C. Contributions from the electrode-dielectric interface, grain boundaries and bulk grains could be distinguished by modelling the spectra with RC-elements. The conductivity and the dielectric permittivity of the bulk SrTiO(3) grains were extracted. The dielectric permittivity ranges from 150 to 350. Its temperature dependence shows Curie-Weiss behaviour with characteristic temperatures between 30 and 50 K.

DF 7.4 Wed 15:30 KÖN Farb

Optical Characterization of Suspensions of Lithium Niobate Nanoparticles* — •Judith Schwesyg, Helge A. Eggert, and Karsten Buse — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn

Using suspensions of ferroelectric nanoparticles in liquids one can combine the outstanding properties of the nanoparticles with the characteristics of fluids. Stable suspensions of lithium niobate nanocrystals in liquids are produced in a high-energy ball-milling process. The size of the particles is of the order of 20–50 nm. We present the details of the methods for producing such stable suspensions and for investigating the characteristic parameters of these liquids. Furthermore, we present data of absorption and scattering experiments. In addition one can apply external electric fields to measure the field-induced birefringence of the suspensions. Alignment of the nanocrystals breaks the inversion symmetry and should enable frequency conversion processes in suspensions of ferroelectric nanoparticles.

DF 7.5 Wed 15:50 KÖN Farb

DFT investigation of PZT bulk and surface properties — •Igor Chaplygin, Sibylle Gemming, and Gotthard Seifert — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden.

Density-functional investigations on the structural, electronic and elastic properties of lead zirconate titanate (PZT) were carried out, employing both an all-electron and a pseudopotential technique. The lead/zirconium distribution was studied with a supercell approach and with the random mixing provided by the CPA and the alchemical mixing scheme. All approaches yield a nearly linear dependence of the structural and eleastic properties of the Zr:Ti ratio. Only the character of the conduction band changes from Pb-based 6p states to Ti-3d states if the Ti content exceeds 50 Thus, the (001) surfaces of PZT were investigated with the alchemical mixing technique. All surfaces exhibit an inward relaxation of the termination plane and a less pronounced outward relaxation of the next lower plane. The strongest relaxations of up to 20 constant occur at the less densely packed PbO termination. Similarly, the relaxations of the Zr-rich systems are larger than the ones in the Ti-rich models. Thus, the slab thickness required to obtain stable bulk-type PZT in the centre of the slab varies between 1.6 to 2.4 nm.

DF 7.6 Wed 16:10 KÖN Farb

Computational investigations on the Kohlrausch relaxation law for interacting dipole systems — •Markus Kühn and Herbert Kliem — Saarland University, Institute of Electrical Engineering Physics, P.O. Box 151150, 66041 Saarbrücken, Germany

For an interacting system of permanent dipoles calculations of transient polarization relaxations show a pronounced Kohlrausch behaviour. It can be described in the time domain by stretched exponential functions or power laws. The model which is employed here is based on permanent dipoles which fluctuate thermally activated in double-well potentials. The dipoles are statistically distributed with respect to their centres and the direction of their axes. The long-range electrostatic dipole-dipole interaction strongly influences the local fields at the dipoles. The iterative algorithm mainly consists of two steps. For each current configuration the local electric fields at the dipoles are deterministically calculated. Then the transition times of the dipoles which depend on the local electric fields are computed in a following weighted probabilistic Monte Carlo step. Simulation results yield a strong dependence of the Kohlrausch behaviour on the dipole charge, the dipole length and the dipole density. Further calculations show the influence of the geometrical dimensions, the temperature, the intrinsic activation energy for a dipole flip and the external electric field.

DF 7.7 Wed 16:30 KÖN Farb

COMBINING HALF-METALS AND MULTIFERROICS FOR SPINTRONICS — •Hélène Béa[1], Manuel Bibes[2], Gervasi Herranz[1], Martin Sirena[1], Karim Bouzehouane[1], Stephane Fusil[3], Eric Jacquet[1], Jean-Pierre Contour[1], Patrycja Paruch[4], Matt Dawber[4], and Agnès Barthélémy[1] — [1]Unité Mixte de Physique CNRS-Thales, RD 128, 91767 Palaiseau, France — [2]Institut d'Electronique Fondamentale, Université Paris-Sud, 91405 Orsay, France — [3]Université d'Evry, Bât. des Sciences, rue du Père Jarlan, 91025 Evry, France — [4]Condensed Matter Physics Department, University of Geneva, 24 quai Ernest Ansermet, CH-1211 Geneva 4, Switzerland

Multiferroic materials possess simultaneously ferroelectric and ferro-

or antiferromagnetic orders and a coupling between the two order parameters. A first step towards fabrication of magnetoelectric functional devices is to grow these materials as thin films. One of the best candidates is $BiFeO_3$ (BFO) which shows ordered states at high temperatures (it is antiferromagnetic below $T_N = 647$ K and ferroelectric below $T_C = 1043$ K). We have explored the influence of deposition pressure and temperature on the growth of BFO thin films by pulsed laser deposition onto (001)-oriented $SrTiO_3$ substrates. Single-phase BFO films are obtained in a narrow region close to 10^{-2} mbar and 580°C. We have characterized the structural and functional properties of BFO/$La_{2/3}Sr_{1/3}MnO_3$ (LSMO) bilayers. We show that the BFO layer has a ferroelectric tunnel barrier behavior. This would open a way to combine the half-metal properties of LSMO with the multiferroic properties of BFO in devices.