DF 3: Poster I: Nano- and microstructured dielectrics, surfaces and interfaces, dielectric composites

Time: Monday 15:00–17:30 Location: Poster D1

DF 3.1 Mon 15:00 Poster D1

Lithium niobate nanoparticles: Orientation in externally applied electric fields* — •Bastian Knabe, Daniel Schütze, and Karsten Buse — Universität Bonn, Wegelerstr. 8, 53115 Bonn

The spontaneous polarization in lithium niobate leads to charged c-faces. It turns out that these surface charges of lithium niobate nanoparticles are not fully compensated. This leads to a remaining electrical dipole moment. We synthesize lithium niobate nanoparticles with a sol-gel method and measure their orientation in externally applied electric fields using this effect. By introducing dopants of different concentration and changing ambient conditions such as temperature, we investigate the various dependences of the dipole moment, which is generally about 10^{-3} of the dipole moment present for the uncompensated spontaneous polarization.

* Financial support by the Deutsche Forschungsgemeinschaft and the Deutsche Telekom AG is gratefully acknowledged.

DF 3.2 Mon 15:00 Poster D1

Formation and modification of Schottky barriers at the PZT/Pt interface — •Andreas Klein[1], Wenbin Wu[2], Feng Chen[1], and Robert Schafranek[1] — [1]Technische Universität Darmstadt, Institute of Material Science, Petersenstraße 32, D-64287 Darmstadt, Germany — [2]Hefei National Laboratory for Physical Science at the Microscale, University of Science and Technology of China, Hefei 230026, People's republic of China

A determination of the Schottky barrier height at the interface between ferroelectric Pb(Zr,Ti)O3 thin films and Pt using in-situ photoelectron spectroscopy is presented. The barrier height for holes, given by the energy difference of the valence band maximum and the Fermi energy, varies reversibly between 1.1 and 2.2 eV for oxidizing and reducing treatments. The changes in barrier are accompanied by a varying amount of metallic Pb at the interface. The most severe reduction is observed after storage in vacuum, which is attributed to the strongly reducing environment because of the presence of hydrogen and water in the residual gas of the vacuum system and the catalytically active Pt surface.

DF 3.3 Mon 15:00 Poster D1

DFT modelling of $SrO(SrTiO_3)_n$ Ruddlesden-Popper surfaces — •Matthias Zschornak[1,2], Emanuel Gutmann[1], Torsten Weissbach[1,2], Tilmann Leisegang[1], Dirk C. Meyer[1,3], and Sibylle Gemming[2] — [1]Nachwuchsgruppe Nanostrukturphysik, Institute of Structural Physics, TU Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, Germany — [3]Institute of Experimental Physics, TU Bergakademie Freiberg, Germany

Strontium titanate ($SrTiO_3$) is an oxide crystallizing with cubic perovskite-type of structure that exhibits a high tunability of dielectric, electric, mechanical and optical properties by means of defects. Apart from dopants, also intrinsic oxygen vacancies or ordered stacking faults, e.g. Ruddlesden-Popper (RP) phases $SrO(SrTiO_3)_n$, may influence these properties.

We have investigated the surface energy, relaxation and electronic properties of such RP surfaces up to $n = 3$ in comparison to 'pure' $SrTiO_3$ by means of density-functional theory for $\langle 001 \rangle$ and $\langle 100 \rangle$ directions and with all possible perfect crystal terminations. We find a significant influence of the surface-near SrO-OSr stacking fault on surface energies and rumpling. Migrating surface states decrease the band gap of TiO_2 terminations but all terminations show insulating character. A detailed discussion of surface-near relaxations will be presented.

DF 3.4 Mon 15:00 Poster D1

Ferroelectric lithography: The promising route for assembling metallic and molecular nanostructures — •Alexander Haussmann, Mathias Schröder, 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 assembling various functional nanostructures. This technique is claimed ferroelectric lithography [1], bearing the power for the controlled bottom-up assembly and integration of dissimilar species over large sample areas.

Here, we report on both the assembly and characterization of noble-metallic and molecular nanowires that were deposited photochemically at 180° domain walls on 5 mol% Mg-doped congruent $LiNbO_3$ single crystal templates [2]. By using different AFM techniques, the domain wall decoration was analyzed in detail with respect to the underlying domain structure (imaged by piezoresponse force microscopy, PFM). Furthermore, a promising explanation of this effect due to UV-induced domain wall conductivity will be discussed.

[1] S.V. Kalinin et al., *Nano Letters* **2**, 589 (2002).
[2] A. Haussmann et al., *Nano Letters* **9**, 763 (2009).

DF 3.5 Mon 15:00 Poster D1

Kohärente Phononen in oxidischen Materialien — •Peter Gaal, Daniel Schick und Matias Bargheer — Universität Potsdam, Karl-Liebknecht Str. 24-25, 14476 Potsdam-Golm

Kohärente Phononen in Perovskit-Materialien lassen sich durch Impulsive Stimulierte Ramanstreuung (ISRS) erzeugen. In unserem Experiment werden zwei Replika eines ultrakurzen Lichtimpulses in verschiedene Kristalle (Strontium-Titanat, Barium-Titanat, etc.) und Multischichtstrukturen fokussiert. Durch Interferenz der beiden Lichtpulse wird ein transientes Gitter geschrieben, an dem ein dritter, zeitversetzter Lichtpuls gebeugt wird. Die beim Schreiben des transienten Gitters erzeugte kohärente Überlagerung unterschiedlicher Phonon-Polaritonen hängt in ihrer Energie und in ihrem Wellenvektor vom relativen Winkel sowie von der zeitlichen Dauer der interferierenden Lichtimpulse ab. Damit lassen sich prinzipiell selektiv bestimmte Phononenbänder anregen. Mit dieser Methode können z.B. Phasenübergänge in oxidischen Materialien untersucht werden.

DF 3.6 Mon 15:00 Poster D1

Growth of TiO_x Thin Films by Liquid Delivery Atomic Layer Deposition for future RRAM Applications — •Marcel Reiners, Seong Keun Kim, Susanne Hoffmann-Eifert, Jiahua Zhang, Carsten Kuegeler, and Rainer Waser — Forschungszentrum Juelich, IFF-6 and JARA-FIT, 52425 Juelich, Germany

Titanium-dioxide ($TiO_{2-\delta}$) is widely studied as material for redox based resistive switching memories. The Atomic Layer Deposition (ALD) enables dense and 3D conformal films down to a thickness of a few nanometer. Here we report on liquid delivery ALD of TiOx from Titanium-tetramethylheptanedoinato-di-isopropoxide ($Ti(TMHD)_2(O\text{-}i\text{-}Pr)_2$) and Titanium-tetrapropoxide ($Ti(O\text{-}i\text{-}Pr)_4$) as precursors with water as oxygen source. The film growth was characterized by XRR and XRF and the morphology was analyzed by means of AFM and HRTEM. TiO_2 films prepared from $Ti(TMHD)_2(O\text{-}i\text{-}Pr)_2$ deposited on Pt|ZrO2|SiO2|Si in a temperature range from 340°C-390°C show a nanocrystalline anatase-type structure with a smooth morphology and a rms roughness about 0.1 nm. TiO_2 films deposited from $Ti(O\text{-}i\text{-}Pr)_4$ at a temperature of 250°C undergo a structural change from an amorphous to a polycrystalline phase above a critical film thickness of about 10 nm. Low current bipolar resistance switching was confirmed in 100x100 nm^2 small Pt|TiO_2|Ti|Pt structures with integrated 8 nm TiO_x films.

This work was supported by the Deutsche Forschungs Gemeinschaft (DFG, DE790/5-1 & HO2480/2-1).

DF 3.7 Mon 15:00 Poster D1

Investigation of the optical phonon modes of $BaTiO_3$ thin films using Raman scattering spectroscopy and IR spectroscopic ellipsometry — •Christian Kranert, Chris Sturm, Stefan Schöche, Rüdiger Schmidt-Grund, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The coupling of the switchable and non-switchable polarization of ferroelectric and pyroelectric materials in heterostructures results in new physical effects which can be used for modulators, sensors and, memories.[1] The properties of the ferroelectric polarization are strongly re-

lated to the phonon spectrum. In this work we present the investigation of the optical phonon modes of ZnO and $BaTiO_3$ and ZnO-$BaTiO_3$ heterostructures by Raman spectroscopy and infrared spectroscopic ellipsometry. A comparison of the phonon modes in heterostructures with those of single films provides access to the properties of the polarization interaction in these heterostructures.

The $BaTiO_3$ and ZnO thin films as well as the $BaTiO_3$-ZnO heterostructures were grown by pulsed laser deposition (PLD). The Raman measurements were carried out using two different lasers at a wavelength of 532 nm and 325 nm, respectively, in order to realize an excitation below as well as above the band gap of both the materials which allows to control the penetration depth of the probe-light in the films and heterostructures, respectively.

[1] O. Auciello and R. Ramesh, MRS Bull. Vol. **29**, No. 7 (1996)

DF 3.8 Mon 15:00 Poster D1

A theoretical description of constant phase element — •Mohammad Reza Shoar Abouzari[1], Frank Berkemeier[2], and Guido Schmitz[2] — [1]Department of Physics, Zabol University, Zabol, Iran — [2]Institut fuer Materialphysik, Wilhelm-Klemmstr. 10, 48149 Muenster

In most cases, the experimental results of impedance spectroscopy fit precisely to the parallel circuit of an Ohmic Resistance and a phenomenological Constant Phase Element (CPE) instead of a simple RC equivalent circuit. For this reason, this empirical model is widely used, but the physical meaning of the CPE is rarely discussed. We have introduced a physical interpretation of the CPE based on the Concept of Mismatch and Relaxation theory (CMR) of Funke et al. Complex impedance spectra of ion-conducting lithium borate network glasses are used to study the deformed shape of impedance semicircles which are usually described by a parallel circuit of R-CPE. Based on the CMR, we have introduced an equivalent circuit, named CMR-C model. It takes into account the contribution of the static glass network by introducing an additional capacitor. This model describes the experimental data accurately. Upon this model we found that the CPE can be considered to be equivalent to three basic elements, R(ω), C(ω), and C(inf) , which are defined by the parameters of the CMR.

DF 3.9 Mon 15:00 Poster D1

Fatigue in ferroelectric polymers: Polyvinylidene fluoride (PVDF) — •Jörg Schütrumpf, Sergej Zhukov, and Heinz von Seggern — Technische Universität Darmstadt, Darmstadt, Deutschland

A strong piezoelectricity, pyroelectricity and ferroelectricity in polyvinylidene fluoride (PVDF) made this polymer an object of detailed studies over the last 20 years. Ferroelectric polymers have an advantage over traditional ferroelectric materials due to their good mechanical properties. Although the stability of the ferroelectric polarization in PVDF is not satisfying for a wide range of applications, it still remains a model material for numerous studies on polarization and hysteresis phenomena in ferroelectric polymers. In order to gain a more systematic understanding of the polarization properties we performed fatigue experiments on 9 μm thin uniaxial stretched PVDF films. After bipolar stressing of the samples above the coercitive field strength E_c at frequencies from 50 Hz up to 10 kHz, switching curves and hysteresis loops were investigated. By comparing fatigued with unstressed samples the underlying effects of aging and fatigue are determined. We also report on the back-switched fraction of the polarization after an applied electric field is switched off with and without fatigue. Therefore the poling times are varied over nine decades for each electric field and the back-switched part during short-circuiting is measured at the end of each poling pulse.

DF 3.10 Mon 15:00 Poster D1

Experimental studies of dielectric constants in multi-layer systems — Axel Hommes[1], Christian Krebs[1], •Gört Luedtke[2], Dirk Nüssler[1], and Klaus Wandelt[2] — [1]Fraunhofer Institute for High Frequency Physics and Radar Techniques (FHR), Dep. mm-wave radar and high frequency sensors (MHS), Neuenahrer Straße 20, 53343 Wachtberg, Germany — [2]University of Bonn, Institute for Physical and Theoretical Chemistry, Dep. Surfaces and Interfaces, Wegeler Str. 12, 53115 Bonn, Germany

The results of experimental studies of the dielectric properties of multilayer systems and relevant absorption spectra will be presented. The measurements have been performed in the terahertz frequency range for different materials with varying layer thickness. Based on multi reflections in a multi layer structure, thickness measurement of single layers is a critical task for every measurement system. Reflections and interferences are unwanted influences during the measurement, but under well known conditions they can be utilized to characterize the layer thickness in multilayer structures. Based on the material parameters for the single layers like permittivity, attenuation etc. changes in the thickness of the different layers can be detected. An exact model of the multilayer structure is necessary including different attenuation coefficients, permittivities, etc. Based on this model changes in the layer thickness of the multilayer structure can be predicted. The estimation of layer thickness can be realized through continuous wave systems of the mmW or THz frequency range. The poster describes and compares modeling and first measurements with artificial structures.