DF 9: Poster Session DF

Time: Tuesday 18:30–20:00 Location: P1

DF 9.1 Tue 18:30 P1

A comprehensive surface photovoltage investigation of the $SrTiO_3$ surface — •Elke Beyreuther, Andreas Thiessen, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

In the past, surface photovoltage (SPV) analysis has been successfully applied to derive the electronic defect status of a number of wide-bandgap semiconductor surfaces. Here, the method is applied to the model perovskite strontium titanate, whose SPV phenomena are comprehensively studied over seven decades of excitation-light intensity. The SPV was recorded by a Kelvin probe setup as a function of wavelength in order to extract the energetic positions of electronic surface states within the bandgap. At selected wavelengths addressing distinct surface states, SPV transients were measured as a function of light intensity and temperature. Several models known from the literature were used to estimate and cross check surface state parameters such as surface state densities, capture cross sections for photons and electrons, and the surface band bending in the dark and under illumination. In contrast to other wide-bandgap materials, SPV transients of SrTiO3 exhibit highly complex shapes, i.e. they (i) show signatures of multiple carrier transitions, (ii) mixtures of surface and bulk contributions, as well as (iii) both ex- and intrinsic SPV processes.

[E. Beyreuther et al., Surf. Sci. 612, 1–9 (2013)]

DF 9.2 Tue 18:30 P1

Lithium Niobate (0001) Surfaces in Thermodynamic Equilibrium with Ambient Conditions — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — University of Paderborn

$LiNbO_3$ (LN) is a frequently used material for optical and acoustic applications due to its strong piezoelectric, pyroelectric, and photorefractive properties. As for other ferroelectric materials, the (0001) surface reactivity can be manipulated by polarization reversal. This opens the possibility for the realization of devices such as molecular detectors[1].

In contrast to the popularity of the material, few is known about the microscopic structure of the (0001) surfaces. Recently the surface structure in liquid solution has been demonstrated by a joint AFM and DFT investigation[2]. At relatively dry conditions only the value for the surface charge is available[3].

As a further step towards the simulation of realistic surfaces, the adsorption of the most important components of dry air (N_2, O_2, CO_2, CH_4, H_2, N_2O, CO) is simulated and the adsorption energies and geometries are determined. We present phase diagrams in dependence of temperature and pressure for every component and in presence of different amounts of water. From these phase diagrams we can extract the desorption temperatures. Additionally the influence of the adsorbed molecules on the surface charge is estimated.

[1] D. Li, M. H. Zhao, et al., *Nat. Mat.* **7**, 473 (2008)
[2] S. Rode, R. Hölscher, et al., *Phys. Rev. B* **86**, 075568 (2012)
[3] F. Johann and E. Soergel, *Apl. Phys. Let.* **95**, 232906 (2009)

DF 9.3 Tue 18:30 P1

Studying interaction between mineral particles by atomic force spectroscopy — •Stefan Klima[1,2], Monika Mirkowska[1,2], Markus Kratzer[2], Helmut Flachberger[1], and Christian Teichert[2] — [1]Chair of Mineral Processing, Department Mineral Resources and Petroleum Engineering, Montanuniversität Leoben, Austria — [2]Institute of Physics, Montanuniversität Leoben, Austria

The processes taking place when two mineral particles come into contact are most important for the industrial applied triboelectrostatic separation (TS). During TS, charge is transferred between touching particles yielding positive/negative net charges on the particles. Subsequently, the particles are separated in an electric field. However, the mechanism of charge transfer is not yet completely understood. As a model system, we investigated the charging behaviour of a single micrometer-size mineral particle touching an insulator single crystal surface. For this purpose, atomic force microscopy (AFM) was employed and force-to-distance (F-x) curves with a mineral particle attached to the free end of an AFM cantilever have been recorded. An attempt was made to evaluate changes in the F-x-curves induced by the electrostatic particle-surface interaction. As a reference, we used the interactions between the single crystal surface and the commercial, unmodified AFM cantilever. Experiments were carried out under various conditions.

DF 9.4 Tue 18:30 P1

Vibrational properties of lithium niobate from density-functional perturbation theory — •Michael Friedrich, Arthur Riefer, Simone Sanna, Wolf Gero Schmidt, and Arno Schindlmayr — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

Lithium niobate ($LiNbO_3$) is a dielectric crystal with outstanding electro-optical properties. It is characterized by a ferroelectric-paraelectric structural phase transition at 1480 K, which has been studied both theoretically and experimentally. Despite these investigations, the mechanisms of the phase transition are far from being understood. Although the phonon modes in relation to the ferroelectric instability are believed to play a crucial role, our actual knowledge of the phonon spectrum is limited to the center of the Brillouin zone. In order to shed light on the lattice dynamics leading to the ferroelectric transition, we have modeled the vibrational properties of $LiNbO_3$ within the density-functional perturbation theory. In this work we present the full phonon dispersion of both the ferroelectric and the paraelectric phases.

DF 9.5 Tue 18:30 P1

Quantum dots and lanthanides as cw-emitters in polymeric microresonators — •Carolin Klusmann[1], Sarah Wiegele[1], Tobias Siegele[1], Tobias Wienhold[2], Sebastian Köber[2,3], and Christian Koos[2,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Institute of Photonics and Quantum Electronics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Polymeric whispering gallery mode (WGM) microresonators are considered to be very auspicious candidates for the label-free detection and characterization of individual nanoscale objects due to their high quality factor and small modal volume. So far, we utilized laser dyes embedded in a polymeric host matrix as active medium for the resonators. However, resonators doped with dyes should be operated with pulsed excitation sources to reduce bleaching effects. Thus, we are looking into emitters which allow the use of a continuous pump source. Quantum dots are considered to be promising candidates for this approach due to their high quantum yield, narrow and tunable emission in combination with broad absorption spectra, higher stability and lower photobleaching rates compared to organic fluorophores. Furthermore, lanthanides with fluorescence stemming from atomic transitions are appropriate emitters for our application because of their high photostability, sharp emission profile and large Stokes Shift. Using cw-emitters as active medium opens the possibility to observe mode-splitting by using a heterodyne detection system.

DF 9.6 Tue 18:30 P1

Monte Carlo Simulations of the Electrocaloric Effect in Relaxor Ferroelectrics — •Constanze Kalcher, Alexander Stukowski, and Karsten Albe — Institut für Materialwissenschaft, TU Darmstadt, Germany

Relaxor ferroelectrics (RFEs) are a promising material class for cooling devices based on the electrocaloric effect.

It is widely accepted, that polar nanoregions and quenched random fields arising from disorder in the atomic structure are inherent features of RFEs. However, their interplay is not yet fully understood.

Here we present the results of lattice based Monte Carlo simulations. We model a relaxor ferroelectric with a Random-Bond-Random-Field Ising model and study its behavior in an electric field using Wang-Landau sampling and a demon algorithm after Creutz. This allows us to predict the electrocaloric effect in the model material. Finally the results of the direct methods are compared with the indirect approach via the Maxwell equation.

DF 9.7 Tue 18:30 P1

Kerr gating efficiency of tellurite glasses as a function of their composition — •Christian Karras, Kay Schuster, Stephan Grimm, Wolfgang Paa, and Herbert Stafast — Institut für Photonische Technologien, Albert - Einstein - Straße 9, 07745 Jena

Tellurite glasses were announced to be a promising material for optical Kerr gating (OKG) [1]. We investigated the applicability of tellurite glasses as OKG switching material as function of its composition. Therefore we used a dual frequency Kerr gating setup where the material was pumped at 800 nm and the transient Kerr signal was observed at 530 nm. Four different composite tellurite glasses with varying ratios of TeO_2 and K_2O or ZnO were investigated with respect to the optimum gating efficiency, the optimum pump power, and the temporal resolution. Especially the gating efficiency strongly depended on the material composition. For materials with a high TeO_2 concentration gating efficiencies above 50% could be achieved at moderate pump intensities below 1 TW/cm^2. We compared the switching behavior of the tellurites glasses with other promising materials for OKG, such as fused silica, zinc sulfide and Schott SF56, a heavy flint glass. All tellurites showed superior behavior in terms of efficiency but had a significantly extended minimum gating time compared to fused silica. We considered dispersion to be a major reason for the latter effect. Therefore we applied an easy pulse propagation model in order to estimate the signal broadening due to dispersion.

[1] Z. Hang et al., Journal of Optics, 14(6), 065201 (2012).

DF 9.8 Tue 18:30 P1

Optical properties of Ti indiffused LiNbO3 from first principles — •Arthur Riefer, Simone Sanna, Arno Schindlmayr, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn, Germany

Lithium niobate (LN) is one of the most important ferroelectric materials and the most important nonlinear optical material. Recently, the linear and nonlinear optical properties of highly ordered stoichiometric as well as of congruent LN have been investigated theoretically[1,2,3]. However, many applications, such as waveguides for signal processing or sensor systems, are based on Ti indiffused LiNbO3, whereby the Ti doping modifies in particular the refractive index[4]. In the present work, we investigate the electronic and optical properties of Ti indiffused LN from first-principles. Different concentrations of Ti are simulated by substitutions of Li or Nb atoms with Ti atoms. Based on this approach the electronic properties are calculated within DFT-GGA. The optical response is determined at the level of independent particles.

[1] W. G. Schmidt *et al.*, Phys. Rev. B **77**, 035106 (2008)
[2] Riefer *et al.*, IEEE Trans. on Ultrasonics, Ferroelectrics and Frequency Control **59**, 1929 (2012).
[3] Riefer *et al.*, Phys. Rev. B **87**, 195208 (2013)
[4] G. Singh *et al.*, "Ti indiffused Lithium Niobate ..", in "New Advanced Technologies" (2010), ISBN: 978-953-307-067-4

DF 9.9 Tue 18:30 P1

Magnetization dynamics and chirality control in the Cu_2OSeO_3 skyrmion compound — •Rolf Versteeg, Matteo Montagnese, and Paul Van Loosdrecht — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77

Skyrmions are 2D-topologically protected magnetic structures which appear as screw-like nanostructures. The combination of different magnetic interactions gives rise to these intriguing structures with sizes generally between 20-90nm. Skyrmions promise to be of great technological value in the form of nano-sized, easily writeable and readable bits. Apart from the technological interest these magnetic structures also open new avenues in fundamental research in light-matter interaction, magnetization dynamics and chirality. Our ideas and recent efforts to study Skyrmion dynamics and their formation in the multiferroic insulator Cu_2OSeO_3 by means of different optical techniques will be presented.

DF 9.10 Tue 18:30 P1

Selective preparation and detection of phonon polariton wavepackets by stimulated Raman scattering — •Jan-Etienne Pudell[1], Jewgeni Goldshteyn[2], Andre Bojahr[1], Peter Gaal[2], Daniel Schick[1], and Matias Bargheer[1,2] — [1]Institut für Physik & Astronomie, Potsdam, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany

Wavevector-selective impulsive excitation of phonon-polaritons by a spectrally broad femtosecond transient gratings produces wavepackets propagating in opposite directions. The photons in spectrally narrow probe pulses are scattered from these elementary excitations in Lithium Niobate (LiNbO3). Both elastically and inelastically scattered photons are simultaneously detected in a spectrometer. The Stokes- and anti-Stokes shifted probe pulses uniquely determine the propagation direction of the detected polariton wavepacket component and correspond to creation and annihilation of phonon-polaritons, respectively. This experiment with spectrally broad pump and spectrally narrow probe pulses allows dissecting the four-wave-mixing process into two sequential stimulated Raman scattering events. Based on this analysis, we selectively prepare phonon-polariton wavepackets propagating only in one direction according to a spectrally assymmetric excitation by two light pulses.

DF 9.11 Tue 18:30 P1

Modified differential scanning calorimeter setup for the measurement of the electrocaloric effect in relaxor ceramics — •Mehmet Sanlialp, Vladimir Shvartsman, and Doru C. Lupascu — Institute for Materials Science, University Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany

Demand for energy-efficient refrigeration technologies with a reduced environmental impact has stimulated interest to materials that exhibit the electrocaloric (EC) effect. The EC effect is a change of temperature or entropy of a dielectric material under an applied electric field at adiabatic or isothermal conditions, respectively. In spite of intensive studies of EC materials during the last 5 years, reliable direct measurements of the EC effect still remain a challenge. In this presentation we report on the development of an experimental setup based on a differential scanning calorimeter for EC measurements of bulk samples at quasi-isothermal conditions in the temperature range 150-500 K at applied electric fields up to 100 kV/cm. We performed EC measurements in several lead-containing and lead-free ceramics:

(1-x)$PbMg_{1/3}Nb_{2/3}O_3$-x$PbTiO_3$, $(Pb_xLa_{1-x})(Zr_yTi_{1-y})O_3$, and(1-x)$Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$.

Effects of temperature, electric field magnitude as well as a degree of relaxor behavior on the measured EC effect are discussed. Furthermore we compare the results of direct EC measurements with indirect EC estimations based on the Maxwell relations to judge the compatibility of these two measurement methods.

DF 9.12 Tue 18:30 P1

Influence of leakage current in $BaTiO_3$-capacitors on stored energy — •Tino Band[1], Martin Diestelhorst[1], Sebastian Lemm[1], Mandy Zenkner[2], and Albrecht Rost[3] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, D-06099 Halle, Germany — [2]Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, D-06099 Halle, Germany — [3]University of Applied Sciences Merseburg, 06217 Merseburg, Germany

The development of dielectric energy storage is of prime importance. Our investigations are motivated by the expectation to realize higher power densities and much more load/reload cycles compared to electrochemical energy storages. Up to now the high energy densities of electrochemical storage batteries could not be achieved by dielectric materials. Therefore the aim is to raise the energy density of capacitors by finding dielectrics with high permittivities ε. At first glance ferroelectrics fulfil these requirements, because of their relatively high values of ε. We use modified $BaTiO_3$ ceramic capacitors for our research. It is well known that ceramic capacitors show a non negligible leakage current. Based on the equivalent circuit of real capacitors we discuss the influence of leakage currents on hysteresis measurements and the stored energy. As a result we present comparisons of our calculation and compensated hysteresis measurements.

DF 9.13 Tue 18:30 P1

Electrical and optical defect spectroscopy on high-k materials — •Patrick Scharf, Alexander Schmid, and Johannes Heitmann — Institute of Applied Physics, TU Bergakademie Freiberg, 09599 Freiberg

Temperature dependent electrical and optical defect spectroscopy on high-k materials, especially on Al_2O_3 and ZrO_2 was performed. High-k layers of varying thickness were realized by atomic layer deposition (ALD). The samples were prepared as MIS (metal-insulator-semiconductor) or MIM (metal-insulator-metal) structures on a silicon substrate. The electric contact to the top electrode was established by ball bonding of a 25 μm thick gold wire on Ti/Al/Ti/Au contact pads. For the MIM samples a 12 nm thick TiN layer was used as bottom electrode.

The samples were characterized by current voltage measurements. Therefore investigations were carried out in the range of room temperature down to 25 K. The current voltage characteristics were found to be strongly temperature dependent. For further investigation of defects in the high-k material and at the high-k/silicon interface, a

laser-assisted current voltage method is presented. By optical excitation with an infrared laser and measurement of the resulting current with respect to the incident wavelength, defect states in the band gap of the dielectric can be characterized.

DF 9.14 Tue 18:30 P1

Frequency Dispersions of Accumulation Capacitances of Metal/n-VO2/SiO2/p-Si Capacitors — Varun John[1], •Lei Zhang[1], Danilo Bürger[1], Ilona Skorupa[2], Oliver Schmidt[3], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — [3]Institute for Integrative Nanosciences, IFW Dresden

Admittance measurements have been performed on Al/n-VO_2/SiO_2/p-Si capacitors with different VO_2 thicknesses and on Al/SiO_2/p-Si reference MOS capacitors. The MOS capacitor with an extra VO_2 layer shows an anomalous frequency dependent capacitance for -7V accumulation bias due to bulk traps introduced to the SiO_2 layer during the growth of VO_2 by PLD[1]. The accumulation capacitance varies from a large value at the low AC test bias frequency of 1kHz to a value of 0.05 μF at the frequency of 1MHz which corresponds to the capacitance of the 80nm thick SiO_2 layer. The accumulation capacitance has a direct relation to the VO_2 layer thickness. The capacitance vs frequency curves of the Al/n-VO_2/SiO_2/p-Si capacitors are modeled using a distributed circuit model taking into account the admittance arising from the change in occupancy of bulk traps in SiO_2[2]. The position dependent density and the time constant of the traps have been obtained from the best fit parameters in the simulations. [1] György J. Kovács, et al., Appl. Phys. 109, 063708 (2011). [2] Y. Yuan, et al., IEEE Trans. on Electron Devices, 59, 2100-06 (2012).

DF 9.15 Tue 18:30 P1

Thermoelectric oxides in glass-ceramic materials — •Julian Lingner[1,2], Gerhard Jakob[1], and Martin Letz[2] — [1]Johannes Gutenberg-Universität Mainz — [2]Schott AG Mainz

Energy demand worldwide is a central topic which motivates the research in the field of conversion materials. Within this area, thermoelectric materials have received wide attention in the last 20 years and some major improvements have been made in order to tune their efficiency. Material classes like silicides, half-heusler compunds or oxides are currently under investigation with individual advantages and disadvantages. Materials that withstand high temperatures above 500°C are especially in great demand since the thermoelectric conversion efficiency is proportional to the applied temperature difference so that the potential fields of application are extended. Due to the requirement paired with environmental regulations it is very important to find materials which operate in these temperature regions while at the same time being naturally abundant and non-toxic. This presentation shows two unconventional glass-ceramic systems which contain thermoelectric active crystalline regions. Starting from a base glass system, a thermoelectric crystal structure is embedded in the glass-matrix via a controlled thermal treatment. This leads to many new properties of the material. Especially the possibility to induce small crystallites, the pore-free surface combined with the high-temperature durability of this material class support this approach. The preparation and results of thermoelectric measurements on different glass-ceramic systems are presented.

DF 9.16 Tue 18:30 P1

Ferroelectric Domains at the Phase Transition in Bariumtitanate — •Thorsten Limböck and Elisabeth Soergel — Institute of Physics, University of Bonn, Nussallée 12, 53115 Bonn, Germany

The classical example of a perovskite crystal, Bariumtitanate, exhibits several phase transitions, namely from rhombohedral to orthorhombic (at -90°C)to tetragonal (at +7°C) to cubic (at +120°C). In order to investigate the behave of the ferroelectric domain patterns at the phase transition occurring at +7°C we upgraded our scanning force microscope with a Peltier cooler/heating stage allowing for operation in a temperature range between -80°C and +120°C. Piezoresponse force microscopy (PFM) images, directly mapping the ferroelectric domain configuration, can be acquired either at fixed temperature or, when using a custom-designed script, during temperature ramps linked to the scanning process. We can thereby record the emergence of the domains at high temperatures but also the change of the domain patterns across the orthorhombic to tetragonal phase transition.