DF 10: Dielectric surfaces and interfaces

Time: Wednesday 14:00–17:30 Location: H11

Invited Talk DF 10.1 Wed 14:00 H11

Molecular self-assembly on calcite — •Angelika Kühnle, Philipp Rahe, Jens Schütte, and Sebastian Rode — Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, 55099 Mainz

Calcite, the most stable polymorph of $CaCO_3$, is one of the most abundant minerals on earth that plays a crucial role in a variety of different fields such as biomineralization and environmental geochemistry. Moreover, calcite precipitates upon scaling, a process that is deliberately prevented by polyelectrolyte addition in many daily life as well as industrial applications such as laundry and water desalination.

Consequently, the $(10\bar{1}4)$ calcite cleavage plane as well as molecule adsorption onto calcite $(10\bar{1}4)$ has attracted great attention. Despite this, a controversy exists as to whether the $(10\bar{1}4)$ cleavage plane of calcite reconstructs or not. Atomically resolved scanning force microscopy images taken in liquids will be presented, revealing a bulk-truncated (1x1) surface. When imaged under ultra-high vacuum conditions, however, clear experimental evidence is provided for a (2x1) reconstruction.

Self-assembly of different functionalized organic molecules on calcite will be reported, demonstrating the formation of both, two-dimensional ordered molecular layers as well as uni-directional wire-like structures.

5 min. break

DF 10.2 Wed 14:45 H11

Room temperature domain wall conductivity in Mg-doped lithium niobate — •Mathias Schröder, Alexander Haussmann, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Deposition routes for metallic and molecular nanowires on the 180° domain walls of lithium niobate through ferroelectric lithography are well established [1,2]. However, a detailed understanding of the underlying processes is still missing, which implies the necessity of further systematic studies of specific domain wall properties.

Here, we report on conductive-AFM (c-AFM) measurements on 5 mol% Mg-doped congruent $LiNbO_3$ single crystals. We compare the c-AFM results with the domain distribution recorded by piezoresponse force microscopy (PFM). Surprisingly, we find an enhanced current density at room temperature and in air along the 180° domain walls under UV-illumination above the band gap of 4 eV. This domain wall conductivity was then studied as a function of wavelength and light intensity. Implications for ferroelectric lithography on $LiNbO_3$ templates 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 10.3 Wed 15:05 H11

Theoretical atomic-scale study of the interaction of grain boundaries with domain walls in ferroelectric $PbTiO_3$ — •Pavel Marton and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Perovskite-type ferroelectric ceramics for actuators and sensors like $PbTiO_3$ or $Pb(Zr,Ti)O_3$ have dense polycrystalline microstructures. Within micrometer-sized grains, even smaller ferroelectric domain structures are found. Both domain walls (DW) and grain boundaries (GB) play an important role in the macroscopic material performance.

An objective of this work is an investigation of fundamental properties of interactions of DW with GB in tetragonal $PbTiO_3$. Atomic-scale experimental observations of GB in perovskites are rare and difficult to obtain. Therefore, the interfaces studied theoretically in this work were motivated by experimental observations of Sigma=3 [1] and Sigma=5 [2] symmetrical tilt GB in $SrTiO_3$. We focus on interfaces, which are both GB and ferroelectric DW. Atomic structures were obtained using atomistic shell-model simulations and ab-initio density functional theory (DFT) calculations. For the chosen GB, DFT calculations provide detailed insight into atomic arrangements, energetic stabilities and electronic states of the interfaces. We discuss properties of GB with DW in dependence on their type, and we compare them with properties of interfaces in cubic $SrTiO_3$ [3].

[1] S. Hutt et al., J. Phys.: Condens. Matter 13 3949 (2001).
[2] M. Imaeda et al., Phys. Rev. B 78 245320 (2008).
[3] N. Benedek et al., Phys. Rev. B 78, 064110 (2008).

DF 10.4 Wed 15:25 H11

An electronic defect state analysis in perovskite heterostructures by surface photovoltage spectroscopy — •Jana Becherer, Elke Beyreuther, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Surface photovoltage (SPV) spectroscopy provides a nondestructive, contact-free method to characterize and quantify electronic trap states within the bandgap of a semiconducting material. In the present study we apply the method to determine electronic defect states of wide-bandgap perovskite oxides.

For different perovskites ($SrTiO_3$ and $BaTiO_3$ single crystals, lead zirconate titanate and lanthanum manganite thin films on $SrTiO_3$ substrates) wavelength-, intensity-, temperature-, and time-resolved surface photovoltage spectroscopy was performed using a Kelvin probe setup in air. Analysis of these measurements provides surface, interface, and bulk state properties, i.e., their energy position and distribution, density, and transition probabilities such as the thermal and optical cross sections. We discuss the results and their impacts in detail.

DF 10.5 Wed 15:45 H11

In situ high pressure synchrotron photoemission study of the $SrTiO_3$/Pt interface — •Robert Schafranek[1], Christoph Körber[1], Andre Wachau[1], Andreas Klein[1], Michael Haväcker[2], Axel Knop-Gericke[2], and Robert Schlögl[2] — [1]Darmstadt University of Technology, Institute of Materials Science, Surface Science Division, Petersenstrasse 23, D-64287 Darmstadt, Germany — [2]Fritz-Haber Institute, Department of Inorganic Chemistry, Faradayweg 4-6, 14195 Berlin, Germany

The (Ba,Sr)TiO_3/Pt interface present e.g. in tunable capacitors for microwave applications plays a crucial role for device properties, which can be explained by a variation of the Schottky barrier height with preparation conditions. It has been shown by photoemission experiments that the barrier height can be reversibly switched between a reduced state with a low barrier height (0.5 eV) and an oxidized state with a high barrier height (>1.2 eV) by annealing at 400°C in vacuum and oxygen, respectively. An in situ high pressure synchrotron photoemission study of the $SrTiO_3$/Pt interface was carried out for further understanding of the dependence of the Schottky barrier height on the O_2 pressure. The experiments were performed at the ISISS dipole beamline at the BESSY II synchrotron in Berlin at different temperatures using a $SrTiO_3$:Nb single crystal covered with a 3 nm thick Pt layer. A modification of the barrier height of 1eV could be observed even for the lowest used sample temperature of 100 °C. Furthermore the variation of the barrier height with O2 pressure could be verified by O2 pressure-dependent I-V measurements.

5 min. break

DF 10.6 Wed 16:10 H11

(Ba,Sr)TiO_3 tunable capacitors with Al_2O_3 barrier layer — •Shunyi Li[1], Yuliang Zheng[2], Andre Wachau[1], Robert Schafranek[1], Rolf Jakoby[2], and Andreas Klein[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany — [2]Mikrowellentechnik, Technische Universität Darmstadt, Darmstadt, Germany

(Ba,Sr)TiO_3, due to its high non-linearity of dielectric constants under electric field, is considered as a promising material for tunable integrated components for microwave applications. However, the high dielectric loss and high leakage current still remain a main impediment, where the interface between electrodes and dielectrics plays an important role. BST varactors with Al_2O_3 barrier layers at the interfaces are prepared via RF magnetron sputtering. The interface formation has been studied by using x-ray photoelectron spectroscopy with in situ sample preparation. A high energy barrier for electrons is formed at the BST/Al_2O_3 contact. Leakage current measurements show that the injection of charge carriers into dielectrics can be effectively reduced by the barrier layer. Significant changes of dielectric properties are observed during dielectric characterizations. The capacitance and

the tunability are reduced due to the insertion of Al_2O_3, and the overall capacitance can be well simulated by serial capacitor model. The quality factor of the varactor is improved due to the better insulating interfaces. By introducing the Al_2O_3 layer, charged interfaces are observed in the dielectric measurements, which is considered as the result of accumulation of charge carriers at the BST/Al_2O_3 interfaces.

DF 10.7 Wed 16:30 H11

Energy level alignment and electric and dielectric properties of BST with ITO electrodes — Shunyi Li, •Cosmina Ghinea, André Wachau, Robert Schafranek, and Andreas Klein — Petersenstraße 23, 64287 Darmstadt, Germany

The interface formation of (Ba, Sr) TiO3 thin films and magnetron sputtering SrTiO3 single crystal with transparent conducting Sn-doped indium oxide (ITO) have been studied by photoelectron spectroscopy with in situ sample preparation via RF. The energy level alignment indicates a very small barrier height at the ITO / BST and STO / ITO interfaces. Current-voltage and dielectric measurements have been performed on BST thin films with parallel-plate structure using Pt and ITO for both top and bottom electrodes. A strong influence of electrode materials on electrical and dielectric properties of the BST films is observed. BST capacitors with Pt electrodes show a back-to-back diode behavior and a relatively low leakage current and high dielectric constant. In contrast, the BST films with ITO electrodes show high leakage currents and high dielectric losses.

DF 10.8 Wed 16:50 H11

Energy band alignment between Pb(Zr,Ti)O_3 and high and low work function conducting oxides - from hole to electron injection — •Robert Schafranek[1], Feng Chen[1], Shunyi Li[1], Wenbi Wu[2], and Andreas Klein[1] — [1]Darmstadt University of Technology, Institute of Materials Science, Surface Science Division, Petersenstrasse 23, D-64287 Darmstadt, Germany — [2]Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, People's Republic of China

Metal/oxide interfaces are important for a variety of applications. For example in ferroelectric random access memories based on Pb(Zr,Ti)O_3 (PZT) the fatigue (reduction of the of the polarization with switching cycles) depends substantially on the used electrode material. While for Pt electrodes a fast degradation of the polarization is reported, this effect is not observed for RuO_2 electrodes up to 1012 cycles. The contact properties between Pb(Zr,Ti)O_3 and the high work function conducting oxide RuO_2 respectively the low work function conducting oxide In_2O_3:Sn (ITO) were studied using in situ photoelectron spectroscopy (PES). In an ultra high vacuum system stepwise deposition of RuO_2 and ITO on PZT thin films by magnetron sputtering and interface characterization via PES were carried out without breaking vacuum. From the PES experiments a smaller barrier for the hole injection into PZT is found for RuO_2 while for ITO the injection of electrons is favored.

DF 10.9 Wed 17:10 H11

Preparation and dielectric investigation of organic metal insulator semiconductor (MIS) structures with a ferroelectric polymer — René Kalbitz[1], Peter Frübing[1], Reimund Gerhard[1], and •Martin Taylor[2] — [1]Department of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476, Potsdam, Germany — [2]School of Electronic Engineering, Bangor University, Dean Street, Bangor Gwynedd, LL57 1UT, UK

Ferroelectric field effect transistors (FeFETs) offer the prospect of an organic-based memory device. Since the charge transport in the semiconductor is confined to the interface region between the insulator and the semiconductor, the focus of the present study was on the investigation of this region in metal-insulator-semiconductor (MIS) capacitors using dielectric spectroscopy. Capacitance-Voltage (C-V) measurements at different frequencies as well as capacitance-frequency (C-f) measurements after applying different poling voltages were carried out. The C-V measurements yielded information about the frequency dependence of the depletion layer width as well as the number of charges stored at the semiconductor/ insulator interface. The results are compared to numerical calculations based on a model introduced by S. L. Miller (JAP, 72(12), 1992). The C-f measurements revealed three main relaxation processes. An equivalent circuit has been developed to model the frequency response of the MIS capacitor. With this model the origin of the three relaxations may be deduced.