DF 6: Poster Session DF

Time: Monday 19:00–21:00 Location: Poster C

DF 6.1 Mon 19:00 Poster C

Analysis of immittance spectra: unambiguous electrical equivalent circuits representing the underlying physics — •Julian Alexander Amani, Tristan Koppe, Hans Hofsäss, and Ulrich Vetter — II. Physikalisches Institut der Georg-August-Universität Göttingen, Deutschland

We propose an approach of analysing immittance spectra with electrical equivalent circuits, which not only eliminates circuit ambiguity but also directly extracts the parameters of the selected physical models.

Analysis of immitance spectra is usually performed by optimising the values of idealised, lumped components in an electrical equivalent circuit to fit the measured data. Those circuits consisting only of idealised components are known to be ambiguous, i. e. different arrangements of components fit the measured data equally well. Hence, definite association of circuit components with physical parts of the system is not possible.

To find the arrangement representing the underlying physics correctly, we derived a fundamental electrical equivalent circuit from Maxwell's equations, describing a homogeneous piece of material, that allows non-linear components dependent on external parameters. In the resulting Voigt circuit, actual physical models are used as resistive and a complex capacitive components. Using measurements of a heterostructure as example we show how, with variation of external parameters (e. g. bias voltage), the unambiguous circuit can be used to extract parameters of the model (e. g. Schottky barrier height) instead of single values of resistance and capacitance.

DF 6.2 Mon 19:00 Poster C

Water-Lithiumniobate Interface from Ab initio Molecular Dynamics — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — Universität Paderborn

$LiNbO_3$ (LN) has been intensively used since decades for various optical and acoustic applications due to its pronounced piezoelectric, pyroelectric, and photorefractive properties and optical nonlinearities. More recently, the possibility to manipulate locally the surface reactivity and surfaces properties by means of polarization reversal of ferroelectric domains has stimulated interest in novel applications from the areas of e.g. nanochemistry or molecular detectors[1].

In order to effectively exploit the phenomena related to the strong and switchable electric fields at ferroelectric surfaces, a detailed microscopic understanding is indispensable. Previous studies [2,3] indicate a highly specific adsorption behaviour of water molecules depending on the surface polarization for water thin films of monolayer thickness. Here we extend the study to the interface between bulk water and LN and perform ab initio molecular dynamics at a wide temperature range. The result show a layered water structure below and slightly above the freezing temperature.

At higher temperatures the molecular water clusters dissolve and the water double layer cannot be recognized anymore.

[1] D. Li, M. H. Zhao, et al., Nat. Mat. 7, 473 (2008)
[2] S. Sanna, R. Hölscher, W.G. Schmidt, PRB 86, 205407 (2012)
[3] S. Rode, R. Hölscher, et al., PRB 86, 075568 (2012)

DF 6.3 Mon 19:00 Poster C

Dielectric, ferroelectric, and energy density properties of barium titanate based ceramics — •Tino Band and Martin Diestelhorst — Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany

Barium titanate ($BaTiO_3$) has been investigated extensively as a dielectric for energy storage due to its high dielectric constant. To achieve higher energy densities a large dielectric breakdown strength (BDS) should be reached by adding a glass or polymer. As is generally known the matrix influences also the dielectric response of the final capacitor. We performed impedance spectroscopy, hysteresis and DC measurements on the ceramics to characterize them. As a result we present the influence of sample properties, like thickness, fraction of the additive or sintering temperature, and external factors, such as frequency or amplitude. Additional we discuss possible effects e.g. interfacial polarization or porosity.

DF 6.4 Mon 19:00 Poster C

AC eletrical measurement on amorphous phase change materials — •Chao Chen[1], Volker Hanno[1], Peter Jost[1], and Wuttig Matthias[1,2] — [1]I. Institute of Physics (IA) of the RWTH Aachen, Germany — [2]JARA-FIT, RWTH Aachen, Germany

Phase-change materials (PCMs) have already been employed in rewritable optical data storage (eg. Blue-ray disc). In the near future, PCM-based electrical memories, phase-change random access memories (PCRAM), could become a competitor for both Flash and DRAM [1,2]. Therefore it is necessary to understand the electronic transport properties of phase change materials for electrical storage.

There is a tremendous difference between crystalline and amorphous PCMs in terms of optical and electrical properties, which is attributed to the presence of resonant bonding in crystalline PCMs [3]. The crystal structure and electrical properties of crystalline PCMs have already been intensively studied. However, the phenomena of resistance drift and threshold switching in amorphous PCMs are not yet well understood. Here we present AC conductivity and impedance spectroscopy data which have been measured in order to investigate the electrical and dielectric properties of the amorphous phase. We expect these data to provide valuable insight into the structural and bonding properties which are supposed to be responsible for the aforementioned phenomena.

DF 6.5 Mon 19:00 Poster C

Dynamics of Oxygen Vacancies in TiO2 — •Michael Wehlau, Jan M. Knaup, and Thomas Frauenheim — BCCMS Universität Bremen, Germany

Resistive switching materials like titania (TiO2) are potentially capable for applications in next-generation semiconductor devices or as components of artificial neurons. Resistive switching effect of metal oxides is based on phase-change mechanisms induced by accumulation of oxygen vacancy defects (VO) and following transformation of insulating TiO2 into substoichiometric conductive phases. For this reason the VO migration is a crucial mechanism for resistive switching. In this work we investigate the dynamics of oxygen vacancies in two ways. We involve thermodynamics in calculations of the free energy surface by metadynamics and obtain accurate minimum energy paths (MEP) for rutile and anatase. We calculate free energy profiles for the VO diffusion using metadynamics, employing a modified version of the PLUMED code, coupled to DFTB+, which implements a permutation invariant vacancy tracking (PIVOT) collective variable. This method provides a technique for rare event sampling without specifying reaction paths. Furthermore, we also perform nudged elastic band calculations to find the MEP for essential VO transitions using the ab-initio DFT method provided by the vasp code. We find free energy barriers and MEP in good agreement. We also find a strong dependency of the activation energy on the crystallographic direction, the crystal structure and the material density.

DF 6.6 Mon 19:00 Poster C

Müller-Matrix-ellipsometry analysis of blazed gratings produced by reactive ion beam etching — Lennart Fricke[1], Carsten Bundesmann[2], Renate Fechner[2], Matthias Burkhardt[3], Michael Helgert[3], Alexandre Gatto[3], Frank Frost[2], •Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universität Leipzig, Inst. für Experimentelle Physik II, Halbleiterphysik, Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V, Leipzig, Germany — [3]Carl Zeiss Jena GmbH, Jena, Germany

We have modeled the optical response of balzed gratings in fused silica using the topography profiles measured by atomic force microscopy for the real space geometry. The obtained spectra are in reasonable agreement with spectra measured by Mueller-Matrix ellipsometry at angles of incidence greater 65° and different azimuthal orientations.

For the simulation of the Mueller-Matrix spectra we employed the rigorous coupled wave approach. The dielectric function of fused silica was taken from a database, thus our modelling procedure is free of any adjustable parameters.

The gratings were produced using interference lithography and reactive ion etching to transfer the pattern defined by lithography into the fused silica substrate. To characterize the sample geometry evolution during etching we investigated a series of samples with different etching times by this modelling technique.

DF 6.7 Mon 19:00 Poster C

Phonon modes in thin-film lithium niobate: A basic study — •Sebastian Krehs[1], Kai Spychala[1], Michael Rüsing[1], Hui Hu[3,4], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics (CeOPP), 33098 Paderborn, Germany — [3]School of Physics, Shandong University, Jinan 250100, China — [4]Nanoln Co. Ltd., Shunhua Road 750, Jinan 250100, China

In the recent years ferroelectric thin films have attracted much attention due to the large quantity of possible applications like infrared detectors and optical filters. For further advancement a better understanding of its physical properties will be inevitable. Therefore the vibrational fingerprints of thin-film lithium niobate ($LiNbO_3$) were studied via μ-Raman spectroscopy. The main focus of the work was concentrated on classification of the occurring vibrational modes in thin-film $LiNbO_3$ with respect to the crystallographic orientation. Here we found a congruent phonon-mode signature to bulk crystal which permits us to conclude that the realized thin-films are of good crystalline quality. Due to the specific fabrication process of thin-film layers, the realized thin-films were attached to different kinds of interface layers. In this context we studied in a further step the influence of different interface layers (e.g. Si- or Cr-layer) on the vibrational properties of thin-film $LiNbO_3$. Furthermore an angle-dispersive characterization was utilized for a defined classification of emerging vibrational modes and a verification of mode-coupling respectively. Here differences could be found which might be linked to surface related effects.

DF 6.8 Mon 19:00 Poster C

Influence of charging temperature on the hysteresis behavior of tubular-channel fluoroethylenepropylene (FEP) ferroelectrets — •Markus Steffen, Xunlin Qiu, Werner Wirges, and Reimund Gerhard — Applied Condensed-Matter Physics,University of Potsdam

Ferroelectrets are internally charged polymer foams or polymer systems with internal cavities which exhibit strong piezoelectricity after bipolar charging (poling) [1].The gas-filled cavities can be charged via a series of dielectric barrier discharges (DBDs). During the DBDs, charges of both polarities are separated, and then deposited onto the internal top and bottom surfaces of the cavities, respectively. The internally charged cavities can be regarded as macroscopic dipoles, whose direction can be switched by reversing the applied electric field. Thus, DBDs inside the cavities lead to a phenomenological hysteresis behavior similar to that of other ferroic materials [2]. In the present study, the influence of the charging temperature on the hysteresis loops of tubular-channel fluoroethylenepropylene (FEP) ferroelectrets is systematically studied over a wide temperature range from -100 to $150°C$. The coercive field and the remanent polarization of the ferroelectret samples are determined as functions of the charging temperature. The results are discussed in the light of Paschen's law for electric breakdown by taking into account the respective gas temperature.

[1] S. Bauer, R. Gerhard(-Multhaupt) and G. M. Sessler, Phys. Today 57(2), 37 (2004).
[2] X. Qiu, *et al.*, J. Appl. Phys. 113, 224106 (2013).