DF 3: Dielectric and ferroelectric thin films 2

Time: Monday 14:45–17:30 Location: MÜL Elch

Invited Talk DF 3.1 Mon 14:45 MÜL Elch

Advances of and by phase-field modelling in condensed matter physics — •Heike Emmerich — Lehrstuhl Matrial- und Prozesssimulation Universität Bayreuth

Phase-field modelling as it is understood today is still a young discipline in condensed matter physics, which established itself for that class of systems in condensed matter physics, which can be characterised by domains of different phases separated by a distinct interface. Driven out of equilibrium their dynamics results into the evolution of those interfaces, during which those might develop into well defined structures with characteristic length-scales at the nano-, micro- or mesoscale. Since the material properties of such systems are to a large extend determined by those small scale structures, acquiring a precise understanding of the mechanisms that drive the interfacial dynamics is a great challenge for scientists in this field. Phase-field modelling is an approach that allows to tackle this challenge simulation-based. This contribution provides a critical overview over the conceptual background of the phase-field method, the most relevant fields of condensed matter physics, approached by phase-field modelling until now, as well as the respective model formulations and the insight gained via their simulation and analysis so far. Moreover, it discusses directions of further development and the quality of the scientific contributions to be expected from those, highlightening them via examples from advances in nucleation theory and austenite-martensite type transitions.

5 min. break

DF 3.2 Mon 15:30 MÜL Elch

Orbital ordering in head-to-head domain walls — •Kourosh Rahmanizadeh, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, oxide polar interfaces have attracted considerable attention due to the emerging novel behaviors. E.g. the $LaAlO_3$ / $SrTiO_3$ interface can induce new properties since the electric potential diverges due to the polar discontinuity at the interface. Electronic localization or defects can help to avoid the divergence of the electric potential and keep an insulating interface.

Also at a ferroelectric head-to-head domain wall there is an uncompensated charge, which could form a two-dimensional electron gas in the insulator. However, the uncompensated charges can be accommodated by partial occupation of the Ti 3*d* band. We carried out density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as implemented in the FLEUR code (www.flapw.de) to study the $PbTiO_3$ and $BaTiO_3$ head-to-head domain wall. The structures have been optimized with GGA and GGA+U. The optimized structure and electronic structure depend on the choice of the Coulomb U. For vanishing U a broad, conducting domain wall is obtained, while increasing U leads to an insulating and sharp domain wall. Also in GGA+U calculations an orbital ordering and a $GdFeO_3$-like rotation of the TiO_6 octahedra have been found at domain wall.
This work was partly supported by IFOX project of EU-FP7

DF 3.3 Mon 15:50 MÜL Elch

Tunneling through ferroelectrics: the role of the electronic structure of the barrier — •Daniel Wortmann and Stefan Blügel — Peter Grünberg Institut and Institute for Advanded Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich

Some of the proposed novel functionalities of future oxide-based electronics will drive their physical origin in the use of ferroelectric materials for tunneling barriers. With different directions of the ferroelectric polarization the tunneling conductance is modified, thereby allowing to utilize the polarization state for data storage. In direct analogy to the tunneling-magneto-resistance (TMR) a tunneling-electro-resistance (TER) can be defined. One of the most basic microscopical sources of the TER is the change of the electronic transmission though the ferroelectric insulator because of the modified barrier potential.

We will discuss the basic theory of TER and we will demonstrate how a realistic description of the electronic structure as provided by density functional theory and the Green function formalism implemented in our FLEUR code [1,2] can be used to estimate the significance of the electronic structure of the barrier to the TER. We show that the change of the barrier potential in the simple prototype ferroelectric insulators $BaTiO_3$ and $PbTiO_3$ will lead to a very weak TER effect and thus the TER in junctions based on these materials will be dominated by interface effects.

[1] http://www.flapw.de

[2] D.Wortmann, H. Ishida and S. Blügel, PRB **66**,075113 (02)

DF 3.4 Mon 16:10 MÜL Elch

Electroresistance effects in ultrathin ferroelectric barriers — •Daniel Pantel, Silvana Goetze, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle (Saale)

Electron transport through ultrathin, fully depleted ferroelectric barriers sandwiched between two metal electrodes and its dependence on ferroelectric polarization direction are investigated by simulation and experiment.

In our calculations, we assume a polarization direction dependent ferroelectric barrier and include various transport mechanisms, namely direct tunneling, Fowler-Nordheim tunneling and thermionic injection. Electroresistance is found for all three transport mechanisms. Large electroresistance is favored in thicker films (on the expense of current density) or by switching between two transport mechanisms, e.g. direct tunneling and Fowler-Nordheim tunneling, by polarization switching.

Furthermore, we show some experimental results on $PbZr_{0.2}Ti_{0.8}O_3$ / $La_{0.7}Sr_{0.3}MnO_3$ heterostructures grown on $SrTiO_3$ substrates with nanoscale elemental metal top-electrodes. We find that the polarization direction influences the transport at room temperature.

DF 3.5 Mon 16:30 MÜL Elch

Growth of epitaxial multiferroic tunnelling heterostructures by pulsed laser deposition — •Silvana Goetze, Daniel Pantel, Marin Alexe, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

A multiferroic tunnelling heterostructure is a system of a thin ferroelectric film sandwiched between ferromagnetic electrodes, which could be applied in next generation of storage devices. Furthermore, they can be used to investigate electroresistance and magnetoelectric effects at interfaces. Here, we report on the growth of such structures by pulsed laser deposition. We have chosen $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) as the ferroelectric layer and $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) as the ferromagnetic bottom and top electrode grown on $SrTiO_3$ (100) (STO) substrate. For tunnelling junctions a low resistivity and a low surface roughness of the LSMO bottom electrode is crucial. Therefore, we optimized the growth conditions (temperature, oxygen pressure, laser energy, laser frequency) accordingly. Transmission electron microscopy images demonstrate the epitaxial growth of LSMO and PZT. Both are fully strained to the STO substrate as can be seen by x-ray diffraction. Hence, thicker PZT films show good ferroelectric hysteresis loops with high remnant polarization. Piezo-response force microscopy proves the ferroelectric behaviour for thinner PZT films.

DF 3.6 Mon 16:50 MÜL Elch

Electrical properties of ultrathin $CaTiO_3$ layers in MIM capacitor stacks — Andreas Krause[1], •Walter M. Weber[1], Uwe Schroeder[1], Johannes Heitmann[1,2], and Thomas Mikolajick[1,3] — [1]NaMLab gGmbH, Noethnitzer Strasse 64, D-01187 Dresden — [2]Institut fuer Angewandte Physik, TU Bergakademie Freiberg — [3]Institut fuer Halbleiter- und Mikroelektronik IHM, TU Dresden, Noethnitzer Strasse 64, D-01187 Dresden

$CaTiO_3$ is a promising material for high-k dielectric applications in metal-insulator-metal capacitors, combining a high dielectric constant (k) with low leakage current values. $CaTiO_3$ was deposited by rf-sputtering at different deposition temperatures. The dielectric constants and leakage current properties were optimized by improvement of the bottom electrode material and roughness. k-values between 51 and 180 were reached depending on the degree of crystallinity of the $CaTiO_3$ layer. The electrical results correlate well with the structural properties. The reduced leakage current values for the lower k samples are associated with the passivation of the grain boundaries in an amorphous matrix, while the leakage current for completely crystallized films is the result of conduction along the grain boundaries [1].

[1] A. Krause et al., Evaluation of the electrical and physical properties of thin calcium titanate high-k insulators for capacitor applications, JVST B accepted

DF 3.7 Mon 17:10 MÜL Elch

Piezoelectric properties of BNT-BT epitaxial thin films by electroacoustic measurement — •Mehrdad Baghaie Yazdi[1,2], Wook Jo[1], Philipp Komissinskiy[1], Pavel Klang[2], Joachim Hillenbrand[1], Jürgen Rödel[1], and Lambert Alff[1] — [1]Technische Universität Darmstadt — [2]Technische Universität Wien

The need for environmental friendly, non-hazardous materials have motivated the scientific community to increase their efforts in the development of lead free piezoceramics, as the electronic market faces an ever increasing need for such devices. Thin films of such a promising lead free piezoceramic, (1-x)$Bi_{0.5}Na_{0.5}TiO_3 \cdot xBaTiO_3$ for $x = 0.6$, have been deposited using pulsed laser deposition (PLD) on 5% niobium doped $SrTiO_3$(STO:Nb) substrates. The lattice constant of the films was determined using high resolution X-ray diffraction. Out of plane measurements, $c = 3.89\,Å$, suggest the growth of a highly epitaxial cubic phase ($a = 3.90\,Å$) on STO:Nb ($a = 3.905\,Å$). The piezoelectric properties have been studied using an unconventional approach, namely electroacoustics, allowing the determination of d_{33} in the frequency range from 1 mHz to 1 MHz.