# DF 1 Internal Symposium "Integrated Electroceramic Functional Structures"

Time: Monday 09:30–13:10 Room: MÜL Elch

## Invited Talk DF 1.1 Mon 09:30 MÜL Elch

**Barium Strontium Titanate Thin Film for RF Applications** — •Ulrich Böttger — RWTH Aachen, Insititut für Werkstoffe der Elektrotechnik II, Sommerfeldstr. 24, 52074 Aachen

Ferroelectric thin films are being intensively studied for wireless communication applications in voltage tunable RF and microwave devices. Tunable circuits like phase shifters, filters or matching networks offer the flexibility to adapt to changes in operating conditions, such as frequency, impedance environment or RF drive level. Key issues for the use of ferroelectric materials in such devices are high tunability, low dielectric losses, temperature stability and reliability, even with respect to alternative technologies based on semiconductor varactor diodes or MEMS (micro electro-mechanical systems). Much emphasis has been placed on thin film ferroelectric material barium strontium titanate, $Ba_{1-x}Sr_xTiO_3$ because of its promising high-frequency dielectric properties and its ability to device integration.

This talk reviews the properties of thin film $Ba_{1-x}Sr_xTiO_3$ and discuss the potential physical models of the origin of the tunability and of the correlated losses. Further, basic tunable devices are presented. Simulation results and measurements from such circuits are also given.

DF 1.2 Mon 10:10 MÜL Elch

**Electronic structures and mechanical stabilities of coherent and semi-coherent perovskite interfaces from first-principles** — •Christian Elsässer[1], Jan-Michael Albina[1], Matous Mrovec[1], and Bernd Meyer[2] — [1]Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany — [2]Ruhr-Universität Bochum, Bochum, Germany

Electroceramic thin-film heterostructures made of perovskite-type metal oxides are promising as alternatives to silicon-based components in microelectronics. The function and stability of such thin-film components are determined by the structure and chemistry of the few nm thin films and their contacts to substrates or electrodes. For the predictive development of electroceramic devices with desired functions, e.g., for dielectric or ferroelectric data storage, useful microscopic information about interfacial electronic structures and mechanical stabilities can be obtained from first-principles density functional theory. Calculations using the mixed-basis pseudopotential method were carried out for electronic energy barriers and mechanical separation energies of (001)-oriented interface models with $SrTiO_3$ in contact to three different perovskites: coherent $SrTiO_3/LaAlO_3$ with $LaAlO_3$ as an insulating substrate, coherent $SrTiO_3/SrRuO_3$ with $SrRuO_3$ as a conducting electrode, and semi-coherent $SrTiO_3/SrZrO_3$. For the latter system, with interfacial mismatch of 6%, a semi-coherent interface model with localized misfit dislocations separated by coherent regions was employed to estimate the influence of dislocation cores on electronic energy barriers and on mechanical separation energies.

DF 1.3 Mon 10:30 MÜL Elch

**Multifunctional materials on the basis of oxidic thin films** — •Matthias Opel[1], Karl-Wilhelm Nielsen[1], Stephan Geprägs[1], Sebastian T.B. Goennenwein[1], Rudolf Gross[1], Wentao Yu[2], Jürgen Simon[2], and Werner Mader[2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Str. 8, 85748 Garching — [2]Institut für Anorganische Chemie, Universität Bonn, Römerstr. 164, 53117 Bonn

Transition metal oxides can show very different properties, e.g. superconductivity, semiconductivity, ferromagnetism, and/or ferroelectricity. Due to the enormous progress in thin film deposition technology, these properties can be integrated in oxidic heterostructures, resulting in novel functionalities.

In this contribution, we discuss the state of the art in pulsed laser deposition for the growth of thin oxide films. Taking ferromagnetic materials such as $Zn_{1-x}Co_xO$, $Sr_2CrWO_6$, $Fe_3O_4$, and $BiMO_3$ (M = Fe, Cr) as an example, we report on the influence of strain and crystal orientation on the magnetic properties. We furthermore address multifunctional heterostructures consisting of ferromagnet/semiconductor multilayers, as well as the possibility to realize (multiferroic) ferromagnetic/ferroelectric multilayers. High-resolution transmission electron microscopy and electron energy loss spectroscopy give important insight into the role of defects and inhomogeneities in the layers and at the interfaces.

DF 1.4 Mon 10:50 MÜL Elch

**Inorganic and organic layers for high-k and organic memory applications** — •Karsten Henkel, Mohmaed Torche, Carola Schwiertz, Ioanna Paloumpa, Rakesh Sohal, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, 03013 Cottbus, P.O. Box 101344, Germany

We report about organic and inorganic MIS stacks for new possibilities for high frequency and high power applications as well as for non volatile memory cell. The organic stack contains a ferroelectric polymer as the functional layer.

Poly[vinylidene fluoride trifluoroethylene] (P[VDF/TrFE]) is spin coated from a solution onto oxidised silicon substrates. We report on the polarisation induced flatband voltage shifts.

For the inorganic stack our attempt is to combine higk-k dielectrics with high band gap semiconductors (SiC). Praseodymium oxide layers are prepared by electron beam evaporation from $Pr_6O_{11}$ powder and in situ controlling of interface and volume composition (XPS). Praseodymium silicate layers were prepared either by metal evaporation onto a thin oxide on top of the semiconductor and following annealing steps or by a wet chemical process out of aqueous $Pr(NO_3)_3$ solutions. Using spectroscopic characterisation we investigate the stability of the various interfaces within the stacks as well as the reactivity of the metal electrodes on thin $Pr_2O_3$. We report the results of electrical characterisation consisting of permittivity values, leakage current and density of interface states.

DF 1.5 Mon 11:10 MÜL Elch

**Resistive Switching in Pt/TiO2/Pt Thin Film Capacitors for Non-volatile Memory Applications.** — •Doo Seok Jeong and Herbert Schroeder — IEM / IFF and CNI, Forschungszentrum Jülich GmbH, Germany.

Non-volatile memory (NVM) devices such as switchable resistors (ReRAM) are discussed for future ultra-large scale-integrated memory chips in cross-bar architecture because of their simple geometry. Among the large variety of candidates under discussion are ferroelectric and paraelectric oxides. We have produced metal/insulator/metal (MIM) capacitor structure with sputtered TiO2 thin films between platinum electrodes showing resistive memory switching. The DC electrical properties were measured in dependence of applied voltage or current, temperature and sample geometry. The main results are: a) All produced titanium oxide films are insulating and amorphous with stoichiometry close to TiO2. b) The films had to be electroformed at 5 to 8 V to show resistive switching. A current compliance between 1 and 10 mA had to be applied to induce the electroforming successfully, but not to degrade the film completely (permanent dielectric breakdown). c) The *Reset* voltage to the higher resistance state (*Off*-state) was 0.7 +/- 0.1 V. The resistance ratio between *On*- and *Off*-state was of the order of 1000. The set voltage for inducing the *On*-state again showed larger variations, 1.5 +/- 0.25 V, with a similar current compliance. The results will be discussed in the light of common mechanisms for resistive switching.

DF 1.6 Mon 11:30 MÜL Elch

**Correlations between Microstructural Changes and Resistive Switching: An Approach by In-situ TEM Investigations** — •Herbert Schroeder and Doo Seok Jeong — IEM / IFF and CNI, Forschungszentrum Jülich GmbH, Germany.

Among the material candidates for resistive non-volatile memories are functional oxides, e.g. ferroelectric and paraelectric oxide thin films. There are numerous experimental (leakage) current data published for each material class demonstrating the switchable memory effect but there is no agreement on the working mechanism. To a large extent this is due to the lack of microstructural information on the changes during formation and switching of the devices. If these effects are connected with microstructural changes these may be observable in a transmission electron microscope (TEM). Therefore, in this contribution we present a rather seldom used approach for a TEM experiment to observe the microstructure of a metal/insulator/metal (MIM) capacitor structure before and after (ex-situ) as well as during (in-situ) resistive switching due to an applied external voltage or current. We use a special TEM sample holder allowing controlled application of temperature (RT to 300°C) with a heating stage and of voltage (current) as a part of a 4-point resistance measurement set-up for ex- and in-situ experiments. This is combined with a special TEM sample preparation method, the so-called window-technique. Special electrode configurations have been designed to allow nearly undisturbed TEM observation of the switching insulator. Examples for first observations in a (Pt/amorphous TiO2 thin film/Pt) stack on the resistive switching will be presented.

DF 1.7 Mon 11:50 MÜL Elch

**Domain structure of ferroelectric nanograins by piezoelectric force microscopy** — •Serge Röhrig[1], Frank Peter[1], Andreas Rüdiger[1], Sven Clemens[2], Theo Schneller[2], and Rainer Waser[1,2] — [1]Center of Nanoelectronic Systems for Information Technology, Research Center Jülich, 52425 Jülich, Germany — [2]Institut für Werkstoffe der Elektrontechnik 2, RWTH Aachen, Sommerfeld Str. 24, 52074

Piezoelectric force microscopy in vertical and lateral operation has made tremendous progress in the characterization of ferroelectric nanostructures. We discuss some of our latest findings in laterally confined ferroelectrics of $BaTiO_3$ on $SrRuO_3$ and $PbTiO_3$ on Pt. Special attention is devoted to the sample-tip interaction as lateral PFM picks up signals that are prohibited by symmetry in an otherwise ideal c-axis oriented system. Lead titanate nanograins are fabricated by chemical solution deposition and post-treated by chemical mechanical polishing to modify their size distribution. Their ferroelectric functionality is proven by inversion of the piezoelectric tensor. We give an outlook to an upcoming new technique of tip-enhanced Raman spectroscopy on ferroelectric nanoislands and discuss some key issues like heat dissipation and the detection of soft-modes.

DF 1.8 Mon 12:10 MÜL Elch

**Polarisation-induced Functionality at Ferroelectric Surfaces** — •Sibylle Gemming, Walter Alsheimer, Regina Ermrich, and Gotthard Seifert — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden.

Density-functional investigations on titanate-based ceramics have confirmed that the rich defect chemistry of these materials strongly influences the structural, electronic, and elastic properties of the bulk phases and at surfaces. Strong structural relaxations at stepped titanate (10n) surfaces were obtained, which can compete with the ferroelectric distortion. The electronic structure does not differ quantitatively from the bulk properties, and no edge-specific states inside the band gap of the bulk compound are induced. On the other hand, the electric field above a stepped surface differs from the one above a planar surface at distances, which are typical in adsorbate-substrate systems. Thus, the prereqisites for a polarisation-driven self-organisation of field-sensitive molecules on polar surfaces are given. A screening of several molecule classes revealed the thiophene series as promising candidates.

DF 1.9 Mon 12:30 MÜL Elch

**Optical waveguides in single-crystalline LiNbO3 films** — •Carsten Dubs[1,2], Andreas Lorenz[1,2], Matthias Will[2], Jens-Peter Ruske[2,3], and Andreas Tünnermann[2] — [1]INNOVENT e.V., Prüssingstr. 27B, D-07745 Jena — [2]Institut für Angewandte Physik, Friedrich-Schiller-Universität, Max-Wien Platz 1, D-07743 Jena — [3]Guided Color Technologies GmbH, Göschwitzer Str. 25, D-07745 Jena

Lithium Niobate (LiNbO3) is one of the most extensively used dielectric material for optical waveguides at telecommunication wavelengths around 1.5 mm. Commonly LiNbO3 integrated optical devices for optical switches, modulators, second harmonic generation devices were fabricated by a combination of microfabrication techniques and metal diffusion (e.g. Ti) or ion-exchange (H+-ions) processes. Because of the considerably light-induced refractive index changes in the visible as well as at high power densities in the near-infrared spectral range only (damage-resistant) substituted LiNbO3 materials of reproducible high quality are usable for optical components exhibiting a well-defined performance. We prepared planar waveguides based on epitaxially grown zinc-substituted LiNbO3 by liquid phase epitaxy technology. We will report about film properties like surface morphology, crystalline perfection, homogeneity as well as about optical properties of the so obtained planar waveguides. Beside investigation of the film microstructure and waveguide properties results of ridge waveguide fabrication for the visible wavelength range and for application at high power densities will be reported. *

DF 1.10 Mon 12:50 MÜL Elch

**Simulation of electronic transport in nanoscale ferroelectric tunnel junctions** — •Klaus Michael Indlekofer[1] and Hermann Kohlstedt[2] — [1]Institute of Thin Films and Interfaces (ISG-1) and Center of Nanoelectronic Systems for Information Technology (CNI), Research Centre Jülich GmbH, D-52425 Jülich, Germany — [2]Institute for Solid State Research (IFF) and Center of Nanoelectronic Systems for Information Technology (CNI), Research Centre Jülich GmbH, D-52425 Jülich, Germany

The usage of nanoscale ferroelectric films as tunnel barriers in electronic devices offers a unique possibility to study the physics of ultrathin ferroelectric materials by means of electronic transport. By use of a nonequilibrium Green's function approach in combination with a self-consistent Hartree potential we have simulated the current-voltage characteristics of a metal-ferroelectric-metal tunnel junction. Such an approach offers a consistent treatment of quantum interference und tunnel effects under the influence of ferroelectric polarization charges.

In this presentation, we discuss the role of quantum effects (such as Friedel oscillations) and depletion regions, which lead to deviations from the conventional semiclassical description of contacts in such a tunneling structure. In the simulated I-V characteristics we observe a well-pronounced bistable resistive switching effect, depending on the polarization state of the ferroelectric tunnel barrier. Ferroelectric tunnel junctions in general might be a first step into a new class of application-relevant tunnel systems. [1]

[1] K. M. Indlekofer and H. Kohlstedt, Europhys. Lett. 72, 282 (2005)