

## DF 5 Dielektrische und ferroelektrische dünne Schichten und Nanostrukturen I

Zeit: Montag 10:00–13:00

Raum: TU TC6

**Hauptvortrag**

DF 5.1 Mo 10:00 TU TC6

**Physics of Ultra-Thin Dielectrics** — ●JAMES F. SCOTT — Symetrix Centre for Ferroics, Department of Earth Science, University of Cambridge, Cambridge CB2 3EQ, UK

A combined Cambridge-Belfast collaboration has prepared and characterized high-dielectric single crystals, emphasizing barium titanate, down to 35 nm thickness. Rather surprisingly these materials exhibit perfectly bulk characteristics, with sharp first-order phase transitions at the known bulk Curie temperatures and dielectric constants peaking over 25 000. This shows that previously reported effects of broadening or conversion to second-order thermodynamics in ceramic films are due to extrinsic causes, such as oxygen vacancy gradients. With these data as a clue, we have studied the broad phase transitions in equally thin fine-grained (40 nm) ceramic films of barium strontium titanate (BST) and find that if the samples are cooled to  $T = 50$  K, the sharp bulk transitions are observed as reentrant upon warming; this shows clearly that transitions in such thin films are limited by sluggish kinetics and not by thermal equilibrium. Finally, we measure leakage currents up to  $E = 1.4$  GV/m (5 x the highest previous values) and show that at high fields these are space charge limited and not variable range hopping.

DF 5.2 Mo 10:40 TU TC6

**Structure of nanocrystalline BaTiO(3)-films prepared at different temperatures.** — ●KESAV REDDY<sup>1</sup>, DIETER MERGEL<sup>1</sup>, STEFAN REUTER<sup>1</sup>, VOLKER BUCK<sup>1</sup> und MARTIN SULKOWSKI<sup>2</sup> — <sup>1</sup>AG Dünnschicht-Technologie, Universität Duisburg-Essen, 45117 Essen — <sup>2</sup>Institut für Umwelt-Analytik, Universität Duisburg-Essen

BaTiO(3) films were prepared by rf magnetron sputtering at substrate temperatures between 450°C and 750°C and analyzed by means of XRD, optical transmittance and Raman spectroscopy.

The films prepared at 450°C exhibit a distinct close-range order but no higher-order XRD reflexes. The films prepared below or above 650°C grow preferentially in (100)- or (110)-direction, respectively. The position of the XRD-reflexes is closest to those of the hexagonal phase. Raman spectra exhibit peaks of both the hexagonal and cubic structure.

These results are discussed on the basis of a structural model of nanocrystallites comprising the stacking of close-packed planes (111 in the cubic structure) with a high degree of twinning.

DF 5.3 Mo 11:00 TU TC6

**Flache und tiefe Störstellen in Perowskiten mit hoher Dielektrizitätskonstante: Ihr Einfluss auf das Leckstromverhalten** — ●HERBERT SCHROEDER — IFF (IEM) und CNI, FZ Jülich, 52425 Jülich

Mischoxide mit Perowskit-Struktur (z.B. (Ba,Sr)TiO<sub>3</sub>) mit hohen Dielektrizitätskonstanten sind Kandidaten als Ersatz für die immer dünner werdenden SiO<sub>2</sub>- und SiN<sub>x</sub>-Dielektrika in Speicherkondensatoren von DRAMs und als Gateoxide in MOSFETs, unter anderem wegen zu hoher Leckströme, die zu unerwünschten Ladungsverlusten führen. Leckströme, die auch in den Ersatzmaterialien zu Problemen führen können, sind in den Perowskiten noch wenig verstanden. Ein kürzlich vorgestelltes Modell, dass die sich sonst ausschließenden Mechanismen der Ladungsinjektion an den Elektroden (Interface limitiert) und des Ladungstransportes im Film (Bulk limitiert) miteinander verbindet, konnte experimentelle Daten in BST in Abhängigkeit vom angelegtem Feld, Temperatur und Filmdicke beschreiben. In diesem Beitrag werden Simulationsrechnungen für dieses Modell in Abhängigkeit von experimentell schwer zugänglichen Parametern wie der Defektkonzentration von Donatoren und Akzeptoren und ihrer Defektenergie in Bezug auf die Fermienergie des Systems (flache und tiefe Störstellen) präsentiert und die neuen Erkenntnisse mit experimentellen Daten verglichen.

DF 5.4 Mo 11:20 TU TC6

**Characterization of laterally confined ferroelectric nanostructures** — ANDREAS RÜDIGER<sup>1</sup>, FRANK PETER<sup>1</sup>, SVEN CLEMENS<sup>2</sup>, KRISTOF SZOT<sup>1</sup>, THEO SCHNELLER<sup>2</sup>, STEPHAN TIEDKE<sup>3</sup>, RAINER WASER<sup>1</sup>, ●ANDREAS RÜDIGER<sup>1</sup>, FRANK PETER<sup>1</sup>, SVEN CLEMENS<sup>2</sup>, KRISTOF SZOT<sup>1</sup>, THEO SCHNELLER<sup>2</sup>, and STEPHAN TIEDKE<sup>3</sup> — <sup>1</sup>Center of nanoelectronic systems for information technology, FZ Jülich, 52425 Jülich — <sup>2</sup>Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen, 52074 Aachen — <sup>3</sup>Aixact-Systems GmbH, Dennewartstr. 25-27, 52068 Aachen

Ferroelectricity is a cooperative phenomenon of coupled electric dipoles in a crystal lattice. For only a few nanometers lateral extension, Landau theory predicts the disappearance of macroscopic polarization. As we now experimentally approach this regime, quantitative measurements become imperative to determine the phase change behavior at this critical size. As it turns out, the ultimate limit of ferroelectricity is to a large extent governed by extrinsic effects such as lattice mismatch with the substrate, local stoichiometry, and surface contaminations. We discuss a new fabrication method, recent measurements and ways to make use of some side-effects. Direct electrical characterization and piezoelectric force microscopy of individual structures as well as a careful integration over numerous structures are presented.

DF 5.5 Mo 11:40 TU TC6

**Leckströme in ferroelektrischen dünnen Filmen** — ●HERBERT SCHROEDER — IFF (IEM) und cni, FZ Jülich, 52425 Jülich

Ferroelektrische dünne Filme sind die wichtigsten Bestandteile für neuartige nicht-flüchtige, hochintegrierbare Speicherelemente wie z.B. FeRAM (ferro-electric random access memory), FeFET (ferroelektrischer Feldeffekttransistor) und ReRAM (Resistive RAM). Für die ersten beiden Bauelemente sollte der Leckstrom bestimmte Grenzwerte nicht überschreiten, für das ReRAM-Bauelement ist ein polarisationsabhängiger Leckstrom essentiell, der ein Schalten zwischen verschiedenen Strom-Spannungs-Kennlinien ermöglicht. Ein kürzlich für die Beschreibung von Leckströmen durch MIM-Dünnschicht-Kondensatoren entwickeltes Modell ist auf ferroelektrische dünne Filme zwischen Elektroden übertragen worden. Das Modell kombiniert die Injektion von elektronischen Ladungsträgern durch thermionische Emission an den Elektroden mit der Bandleitung der Ladungsträger im ferroelektrischen Film. Ergebnisse der numerische Simulationen des Leckstroms für dieses Modells werden präsentiert. Neben der Variation von extrinsischen Parametern wie angelegte Spannung, Temperatur, Filmdicke, etc. wurden vor allem die experimentell nur schwierig zu kontrollierenden Eigenschaften der Interface (Barrierenhöhe, Interfaceschichten mit reduzierter Polarisierbarkeit, d.h. dead layer, verschiedene Defektkonzentrationen und -energien) systematisch untersucht. Die Ergebnisse zeigen generell einen von der ferroelektrischen Polarisierung abhängigen Leckstrom und unter bestimmten Bedingungen das für ein ReRAM nutzbare Schalten.

DF 5.6 Mo 12:00 TU TC6

**Structure of Plain and Stepped BaTiO<sub>3</sub> Surfaces** — ●WALTER ALSHEIMER, SIBYLLE GEMMING und GOTTHARD SEIFERT — Institut für Elektrochemie und Physikalische Chemie, TU Dresden, D-01062 Dresden

In the framework of miniaturization of semiconductor devices ferroelectric compounds in the perovskite structure attract much interest. For example one of our aims is to deliver a density-functional based understanding of an organic field effect transistor on a ferroelectric template like BaTiO<sub>3</sub>.

Because of the low computational costs of the density-functional based tight binding (DFTB) method allows one to study complex and large structures. Therefore in a first step we choosed this technique to perform calculations on the relaxation of plain and stepped surfaces with a slab model geometry. Trends for the interplanar spacings and the local coordination at the step edge are discussed for vicinal (10n) surfaces.

DF 5.7 Mo 12:20 TU TC6

**Collecting the nanoscale optical hysteresis in ferroelectrics** — ●TOBIAS OTTO, FRANK SCHLAPHOF, HASSAN CHAIB, STEFAN GRAFSTRÖM, and LUKAS ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Ferroelectric switching is of clue interest for determining temporal and dynamic stability, but equally for the quantitative deduction of electronic and dielectric properties of ferroelectric domain structures. The methods reported so far, such as monitoring the switching current with macroscopic surface electrodes or collecting the nanoscale ferroelectric hysteresis by means of scanning probe techniques such as piezoresponse force microscopy (PFM), are all based on electrical or electro-mechanical effects.

In this paper we present for the first time nanoscale optical hysteresis measurements in barium titanate (BaTiO<sub>3</sub>) single crystals us-

ing the electro-optical response [1] to monitor the polarization reversal. Nanoscale optical hysteresis loops obtained for several tip-sample separations are compared with nanoscale electrical switching recorded by PFM at the same surface spot. Finally, our experiments are discussed with respect to the effective electric field distribution under the probing tip as calculated by finite-element modelling [2].

[1] T. Otto et al., Appl. Phys. Lett. 84, 1168 (2004)

[2] T. Otto et al., Ferroelectrics 303, 149 (2004)

DF 5.8 Mo 12:40 TU TC6

**TEM and HRTEM Study Perovskite Nanoparticles Prepared by High-Energy Ball Milling** — •LUU TIEN HUNG<sup>1,2</sup>, DO HUNG MANH<sup>3</sup>, STEFFEN SCHULZE<sup>1</sup>, VO VONG<sup>3</sup>, and MICHAEL HIETSCHOLD<sup>1</sup> — <sup>1</sup>Solid Surfaces Analysis Group, Institute of Physics, Chemnitz University of Technology, Germany — <sup>2</sup>Department of Physics, Vinh University, Vinh, Vietnam — <sup>3</sup>Institute of Materials Science, VAST, Hanoi, Vietnam

Nanocrystalline perovskite materials are of interest for applications like catalysis and magnetoelectronics. Using a milling technique perovskites of the type  $AA'BB'O_3$  ( $A = La, A' = Sr, B = Co, Mn, B' = Zn$ ) have been prepared from powder raw component oxides  $La_2O_3, Co_3O_4, \dots$

XRD as well as TEM are applied for sample characterization. The material is found to consist of crystallites till to 5..15 nm size which show a strong tendency to cluster. Thermomagnetization measurements suggest that these clusters are the magnetic subunits responsible for magnetization domain formation.