DF 16: Thin Films and Nanostructures III

Time: Thursday 14:30–16:30 Location: WIL B321

Invited Talk DF 16.1 Thu 14:30 WIL B321

Simulation of Defects and Domain Structures in Ferroelectrics — •Ralf Müller — Department of Civil Engineering and Geodesy, Solid Mechanics, TU Darmstadt, Hochschulstr. 1, 64289 Darmstadt, Germany

The macroscopic material properties of ferroelectric materials strongly depend on their complex microstructure, which includes length scales from the atomistic level up to the grain size level. Crucial for the understanding of fatigue, degradation and aging phenomena is the interaction of domain walls and domain structures with various defects in the material. In order to analyse these interactions a thermodynamically consistent continuum mechanical approach is taken. Domain walls are modelled as sharp interfaces or are simulated by a phase field approach. The phase field approach can be understood as a regularization of the sharp interface model. Both models are implemented into a special finite element method. Techniques to incorporate localized defects in the continuum are discussed, by a comparative study between atomistic and continuum mechanical simulations. Additionally, the interaction between defects can be studied using thermodynamic arguments.

Pinning phenomena of domain walls at electrode and point defects are shown. Macroscopic material properties are derived from simulations with evolving microstructures by homogenization procedures. The simulated material behavior is compared to some of the few multiaxial experiments available in the literature.

5 min. break

DF 16.2 Thu 15:10 WIL B321

Optische und strukturelle Untersuchung an Bariumtitanat-Dünnfilmen — •Stefan Schöche, Rüdiger Schmidt-Grund, Chris Sturm, Holger Hochmuth, Matthias Brandt, Michael Lorenz und Marius Grundmann — Fakultät für Physik und Geowissenschaften, Institut für experimentelle Physik II, Universität Leipzig

Aufgrund diverser Anwendungsmöglichkeiten in Elektronik, Elektromechanik und Elektrooptik sind ferroelektrische Oxide zentraler Bestandteil aktueller Forschung. Insbesondere für optische Anwendungen, ist eine genaue Kenntnis der dielektrischen Funktion (DF) über einen weiten Spektralbereich erforderlich.

Wir präsentieren eine detaillierte Untersuchung der DF epitaktischer $BaTiO_3$ (BTO)-Dünnfilme, abgeschieden auf (100)-, (110)- und (111)-orientierten $SrTiO_3$ (STO)-Substraten mittels gepulster Laserablation (PLD). Es wurden spektroskopische Ellipsometrie-Messungen im Spektralbereich $0.03-0.4$ eV bzw. $0.8-5$ eV durchgeführt und mit Ergebnissen von struktursensitiven Messmethoden wie Rasterkraftmikroskopie und Röntgenbeugung korreliert.

Zur Analyse der Ellipsometriedaten wurde ein Schichtstapel-Modell erstellt, bestehend aus parametrisierten DF des STO-Substrats, der BTO-Schicht und einer Oberflächenschicht. Daraus wurden Eigenschaften der Band-Band-Übergänge im Bereich der fundamentalen Bandlücke und höherer kritischer Punkte, sowie Phononenmoden erstmalig für dünne Schichten abgeleitet.

DF 16.3 Thu 15:30 WIL B321

The Local Field Method for Dielectric Nanocomposites — •Markus Kühn and Herbert Kliem — Saarland University, Germany

We focus on nanodielectrics consisting of two different phases. The systems are embedded between coplanar conducting electrodes which are taken into account by the method of image dipoles. Binary mixtures are modelled by neutral atoms with polarizabilities α and β, respectively. The different atoms are statistically arranged on cubic lattice sites. For different volume ratios and different dielectric contrasts of the two phases the dipole moments and local fields are calculated. For vanishing α- or rather β-phase the corresponding Lorentz fields are obtained, respectively. The simulation results are compared to the common Maxwell-Garnett mixing rule. In contrast to the local field method which also inherently takes into account all depolarization effects, macroscopic mixing rules are based on a homogenization of heterogeneous systems. This simplified description of the dielectric neglects the real microstructure and the varying local fields. In addition, we investigated two-dimensional nanodielectrics where we have a polar inclusion modelled by permanent bidirectional dipoles at cubic lattice sites. The shape of the inclusion is random and it is surrounded by a matrix of induced dipoles placed at cubic lattice sites. Again, the local field method yields the locally varying dipole moments due to the microstructure.

DF 16.4 Thu 15:50 WIL B321

Impact of high interface density on ferroelectric and structural properties of $PbZr_{0.2}Ti_{0.8}O_3$ / $PbZr_{0.4}Ti_{0.6}O_3$ epitaxial multilayers — •Ludwig Feigl[1], Shijian Zheng[2], Balaji I. Birajdar[1], Brian J. Rodriguez[1], Yinlian Zhu[1,2], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, 110016 Shenyang, China

Multilayers consisting of the two tetragonal compositions $PbZr_{0.2}Ti_{0.8}O_3$ and $PbZr_{0.4}Ti_{0.6}O_3$ were deposited onto a $SrRuO_3$ electrode grown on a vicinal (100) $SrTiO_3$ substrate. It has been shown by extensive structural investigations comprising transmission electron microscopy in conventional and high resolution mode, reciprocal space mapping and piezoresponse force microscopy that with decreasing layer thickness a transition from a-domains confined to individual layers to a-domains propagating through the whole film takes place. This is caused by the formation of a common strain state of all layers which is responsible for the observed enhancement of the electrical properties. These show a maximum in the product of remanent polarization and dielectric constant at a certain density of interfaces. If the interface density becomes too high the lattice distortion accompanying each interface deteriorates the properties of the multilayer structure.

DF 16.5 Thu 16:10 WIL B321

Nonlinear Frequency Response of Metal/Ferroelectric/Metal and Metal/Ferroelectric/Semiconductor Heterostructures — •Kay Barz, Martin Diestelhorst, and Horst Beige — Martin Luther-Universität Halle-Wittenberg

By investigating the dynamic behavior of a ferroelectric-semiconductor heterostructure we observed a torus doubling bifurcation together with other interesting frequency responses obviously driven by the nonlinear nature of the sample.[1] In the talk, some of these experimental findings will be presented, mainly focusing on the amplitude-frequency-characteristics observed at different structure types (metal/ferroelectric/metal (MFM) and metal/ferroelectric/semiconductor (MFS)). Concerning the MFS heterostructures it was to clarify, whether the observed nonlinear phenomena can be attributed to the ferroelectric thin film or the semiconductor substrate or if it is an emergent property (i.e. spontaneously arising owing to the system's complexity). Therefore the behavior of the MFS structures was compared to simple MOS-capacitors (metal/oxide/semiconductor). The results on MFM structures show, how hysteresis and its transient alterations due to fatigue manifest in the frequency response. It turns out that ferroelectric thin films and ferroelectric/semiconductor heterostructures provide easy experimental access to interesting phenomena known from theory of nonlinear dynamics.

[1] M. Diestelhorst et.al.; *Phil.Trans.Roy.Soc.A*; 366; 437-446; 2008.