DF 8: Dielectric and Ferroelectric Thin Films and Nanostructures II

Time: Wednesday 14:30–17:10 Location: H11

Invited Talk DF 8.1 Wed 14:30 H11

Piezoelectricity and pyroelectricity in amorphous perovskite thin films — •Alexander K. Tagantsev[1], Vera Lyahovitsky[2], David Ehre[2], Ellen Wachtel[2], Sidney R. Cohen[2], Konstantin Gartsman[2], and Igor Lubomirsky[2] — [1]Swiss Federal Institute of Technology (EPFL), Lausanne 1015, Switzerland — [2]Weizmann Institute of Science, Rehovot 76100, Israel

One customarily considers the crystallinity as a prerequisite for pyro- and piezoelectricity in a material. Though the theory does not impose such limitation, the long-standing experience in the field tells us that ionic structures exhibiting pyro- and piezoelectricity should be at least polycrystalline. In this paper, we demonstrate that the "common" behavior of perovskite dielectrics can be revolutionary influenced when thin films of these materials are treated with a specially tailored temperature gradient. Such treatment enables the transformation of non-polar amorphous films of $BaTiO_3$, $SrTiO_3$, and $BaZnO_3$ into a polar state that exhibits appreciable values of pyro- and piezoelectric coefficients. One should stress that, in the case of $SrTiO_3$ and $BaZnO_3$, the polar amorphous films are prepared from originally non-polar materials. This unusual phenomenon raises a body of intriguing questions concerning the physics behind it. In this paper we address two of these issues in detail: (i) the mechanism of temperature-gradient driven amorphous-to-amorphous-state transformation and (ii) the mechanism of polar-state formation in the amorphous materials.

DF 8.2 Wed 15:10 H11

Permittivity of sputtered thin films of TiO(2) — •Dieter Mergel, Janika Bolz, and Fred Fürtges — WG Thin Film Technology, Fb Physik, University Duisburg-Essen, 45117 Essen

Thin film capacitors have been prepared on Si substrates with bottom and top electrodes of RuO(2) or In(2)O(3):Sn. The deposition method was rf-diode sputtering. Depending on the details of the process (heating, grounded or floating substrate, sputter pressure, oxygen partial pressure) the TiO(2) films contained mainly anatase or mainly rutile grains or both.

Impedance spectroscopy delivered one semicircle in all cases. The dielectric permittivity at room temperature ranges between 80 and 300. The film stacks with RuO(2) disintegrated during the measurements at higher temperatures but were stable without electric field up to 300°C.

DF 8.3 Wed 15:30 H11

Electrostriction vs polarisation reversal in ferroelectric nanoislands — •Serge Röhrig and Andreas Rüdiger — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Piezoresponse Force Microscopy plays an important role in the investigation of ferroelectric nanostructures. The contrast mechanism for vertical PFM comprises piezoelectric and electrostatic contributions nurturing the discussions which one is dominating. Scanning over c-axis oriented nanoislands leads to a pronounced lateral signal at the slops of the islands. This signal is virtually free of electrostatic contributions. Detecting the second harmonic response, we observe a clear transition from quadratic (electrostriction) to linear (polarisation reversal) behaviour as we exceed the coercive field. The microscopic interpretation suggests a new type of non-volatile ferroelectric memory.

DF 8.4 Wed 15:50 H11

NMR Spectroscopy for Study of Size Effects in BaTiO3 fine particles and of Materials Embedded in Mesoporous Materials — P. Sedykh[1], E. V. Charnaya[2], G. Klotzsche[1], and •D. Michel[1] — [1]University of Leipzig, Institute for Experimental Physics II, Linnéstrasse 5, 04103 Leipzig — [2]Institute of Physics, St.Petersburg State University, St.Petersburg, 198904, Russia

Studies of size effects on ferroelectric properties have obtained a great impetus in recent years. Ultrafine BaTiO3 powders are prepared from a monomeric metallo-organic precursor through combined-solid state polymerization and pyrolysis (CPP) [1-3] with particle size (dm) in the range between 15 nm and 250 nm. The properties of BaTiO3 powders were characterized by various methods (FT-Raman, XRD, SEM and 137Ba NMR). Critical particle diameters for the disappearance of ferroelectricity are estimated. A structural model for a nanograin is derived. Moreover, we study the behavior of BaTiO3 and other ferroelectrics embedded into mesoporous MCM 41 materials and in porous glasses. An overview about our recent work will be given.

[1] H. J. Gläsel, E. Hartmann, R. Böttcher, C. Klimm, B. Milsch, D. Michel, H.-C. Semmel-hack, J. Hormes, J. Materials Science 34(1999)1-5 [2] E. Erdem, R. Böttcher, H.-C. Semmelhack, H.-J. Gläsel, E. Hartmann, D. Hirsch, J. Mater. Sci. 38 (2003) 3211-3217 [3] E. Erdem, PhD Thesis, University of Leipzig, 2006

DF 8.5 Wed 16:10 H11

Ultrafast Structure and Polarization Dynamics in Nanolayered Perovskites Studied by Femtosecond X-Ray Diffraction — •Clemens von Korff Schmising[1], Matias Bargheer[1], Mareike Kiel[1], Nicolai Zhavoronkov[1], Michael Woerner[1], Thomas Elsaesser[1], Ionela Vrejoiu[2], Dietrich Hesse[2], and Marin Alexe[2] — [1]Max Born Institut, Berlin — [2]Max Planck Institut, Halle

We apply ultrafast x-ray diffraction with 100 femtosecond temporal and 100 femtometer spatial resolution to study optically induced polarization dynamics in a nanolayered $PbZr_{0.2}Ti_{0.8}O_3/SrTiO_3$ (PZT/SRO) superlattice. Displacive ferroelectricity of crystals with a perovskite structure is essentially determined by two lattice coordinates, the tetragonal distortion η (i.e. the ratio of the out- and in-of-plane lattice constant) and the ion displacement ξ within the unit cell, which directly causes the macroscopic polarization P. Optical excitation of the metallic SRO layers generates ultrafast giant stress at the 1 GPa level, which compresses the ferroelectric PZT layers by up to 2%, thus directly modulating the tetragonal distortion η. The measured time-dependent x-ray intensity changes of two Bragg reflections provide complementary information on the coupled dynamics of the tetragonal distortion η and the ion displacement ξ. The evaluation of these transient Bragg reflections yield a maximal change of η after 1.5 ps. As a result, the ferroelectric polarization P is reduced by up to 100 percent with a slight delay that is due to the pronounced anharmonic coupling of the two modes. The resulting change of ξ reaches a maximum after 2 ps.

DF 8.6 Wed 16:30 H11

Computer simulation of ultralow-k dielectric materials based on C_{60}: Structural, mechanical and dielectric properties — •Kostyantyn Zagorodniy, Helmut Hermann, and Manfred Taut — IFW-Dresden, PF 270116, D-01171 Dresden, Germany

The International Technology Roadmap for Semiconductors (ITRS) predicts that continued scaling of devices will require materials with ultralow dielectric constant. In the present work we propose novel interlayer dielectric materials with ultralow dielectric constants and reasonable mechanical properties for future microelectronic applications. The model structure of the material for investigation consists of fullerene molecule C_{60} connected by bridge molecules. Classical and quantum-chemical methods are used to optimize the structures and to calculate dielectric and mechanical properties. The dependencies of structural, mechanical and dielectric properties on the bridge length and its realization have been investigated. The (static) dielectric constants, k, and elastic bulk moduli, B, of the proposed materials are in the range of $k = 1.7$ to 2.2 and $B = 5$ to 23 GPa, respectively. These values meet the demands of future microelectronic devices.

DF 8.7 Wed 16:50 H11

Optimization of porous low-k dielectrics by simulated sphere packings — •Antje Elsner and Helmut Hermann — Institute for Solid State and Materials Research, IFW Dresden, PF 260116, D-01171 Dresden, Germany

Computer generated dense random packings were used as model for porous low-k dielectrics. In this case the pores are represented by spheres whereas the space around spheres stands for the base dielectric material. Main task was to find an optimum parameter set for pore size distributions to get a low dielectric constant. The dielectric constant decreases with increasing porosity but mechanical properties may get worse therefore. The main challenge is to optimize the porous structure so that mechanical properties are acceptable at preferably highest possible porosity. The model of dense packed spheres was then extended to simulate open pore systems with controllable parameters. Properties of open pore systems differ from closed pore systems.

Simulations of models with different degree of open porosity and size distributions were analyzed in terms of specific surface, particle penetrability and other properties.