DF 7: Advanced Dielectrics

Time: Tuesday 14:00–16:20 Location: WIL A317

Invited Talk DF 7.1 Tue 14:00 WIL A317

Origins of large piezoelectric response and lead-free alternatives to PZT — •Dragan Damjanovic — Ceramics Laboratory, Swiss Federal Institute of Technology - EPFL

One of the hottest topics in the field of piezoelectricity is replacement of ubiquitous $Pb(Zr,Ti)O_3$ ceramics (or PZT) with lead-free materials. The most widely adopted approach in this search for new materials is to look for systems exhibiting the same salient features as good lead-based piezoelectrics: a morphotropic phase boundary (MPB), a tendency for a large polarization rotation, and a monoclinic phase. The term *polarization rotation* has been employed only recently and has now become a synonym, together with monoclinic phases, for large piezoelectric properties. It is suggested here that *polarization rotation* is an old concept proposed over thirty years ago to explain enhanced properties of PZT in the MPB region. It is shown, using an example of lead-free material, that in addition to polarization rotation polarization extension can also lead to large electro-mechanical properties. Substantial theoretical and experimental evidence exist to show that the highest piezoelectric response does not appear in monoclinic phases but in the phase transition regions where polarization either changes direction or appears from the non-polar state. It is proposed that concept of structural instability and associated free energy instability is the most general approach that underlies theoretical results and consistently interprets experimental observations on enhancement of piezoelectric properties. Finally, perspectives of finding lead-free alternatives to PZT among presently investigated systems are discussed.

5 min. break

DF 7.2 Tue 14:40 WIL A317

Electronic transport across single metallic nanowires fabricated through ferroelectric lithography — •Alexander Haussmann and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

The presence of different surface charges and thus different surface reactivities offers the possibility of exploiting domain-structured ferroelectrics as templates for the assembling of various functional nanostructures. This technique therefore is claimed ferroelectric lithography [1], bearing the power for the controlled bottom-up assembly and integration over large sample areas.

Here, we report on both the assembly and characterisation of noble-metal nanowires that were deposited photochemically at 180° domain walls on 5 mol% Mg-doped congruent $LiNbO_3$ single crystal templates. After connecting these wires to macroscopic contact leads, ohmic conduction properties were revealed in such wires by recording I-V-characteristics in conjunction to Kelvin probe force microscopy (KPFM) [2]. Furthermore, investigations at high spatial resolution were performed in order to quantify a possible spatial separation between the domain wall and the photochemically reactive zone.

[1] S.V. Kalinin, et al., Nano Letters **2**, 589 (2002)
[2] U. Zerweck, et al., Phys. Rev. B **71**, 125424 (2005)

DF 7.3 Tue 15:00 WIL A317

Low voltage electron emission from $[Pb(Mg_{1/3}Nb_{2/3})O_3]_{0.72}$ $[PbTiO_3]_{0.28}$ single crystals induced by ferroelectric polarization switching — •Oliver Mieth[1], Vinay S. Vidyarthi[2], Gerald Gerlach[2], Kathrin Dörr[3], and Lukas M. Eng[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Institute for Solid State Electronics, Technische Universität Dresden, Germany — [3]Institute for Metallic Materials, IFW Dresden, D-01069 Dresden, Germany

Here we report on electron emission from $[Pb(Mg_{1/3}Nb_{2/3})O_3]_{0.72}$ $[PbTiO_3]_{0.28}$ (PMN-PT) thin ferroelectric single crystals at ultra-low voltages down to 20 V per 400 μm thickness, and for up to 10^9 switching cycles. PMN-PT samples were prepared with split gold top electrodes exhibiting a 25 μm wide gap region. Applying a sinusoidal voltage between the two top electrodes and the bottom electrode initiated electron emission from the gap region. The emitted electrons were collected under UHV conditions using two single electron counters arranged under an angle of 90°. Two emission regimes have been identified, which are clearly separated by the onset of complete ferroelectric polarization switching. This is also confirmed by recording nanoscale ferroelectric hysteresis loops by means of Piezoresponse Force Microscopy. The emitted electrons are found to have a broad energy distribution with the maximum kinetic energies reaching 110 eV and 50 eV for applied switching voltages of 140 V and 110 V, respectively. Our results confirm that polarization reversal is the governing mechanism behind the electron emission process.

DF 7.4 Tue 15:20 WIL A317

Ab initio and atomistic simulation of copper doping in the lead–free ferroelectric perovskite potassium sodium niobate — •Sabine Körbel and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Recently lead–free ferroelectric ceramics, one of them the perovskite potassium sodium niobate (KNN), have attracted strong scientific interest for being environmentally friendly materials suitable for piezoelectric devices in applications like actuators and sensors. Various doping elements, for instance copper, have been found to improve the ceramic processing conditions and the piezoelectric properties of KNN significantly. Therefore a theoretical understanding of the effects of these impurities is important.

We employed density functional theory in the local density approximation and atomistic simulations with empirical interatomic potentials to determine the preferred lattice site for copper impurities in KNN, and the influence of the impurities on the energy barriers associated with switching the ferroelectric polarization.

DF 7.5 Tue 15:40 WIL A317

Lead-free ferroelectric solid solutions from first-principles calculations — •Silke Hayn, Melanie Gröting, and Karsten Albe — Materialwissenschaften, TU Darmstadt, Deutschland

Ferroelectric materials provide a link between electricity and mechanical movement. The technologically relevant materials, like PZT, are solid solutions which exhibit a morphotropic phase boundary (MPB). In an attempt to replace PZT by materials that do not contain toxic lead, a wide variety of solid solutions of lead-free perovskites is under investigation. First-principles calculations can be used to assist or even guide this search involving an enormous number of candidate materials.

In this contribution we present DFT calculations on $K_xNa_{1-x}NbO_3$, $Bi_{1/2}Na_{1/2}TiO_3$ (pure and doped with $BaTiO_3$), $BaTiO_3$ (pure and doped with $BaZrO_3$), and $PbMg_{1/3}Nb_{2/3}O_3$ and compare them with the standard material PZT. For all these materials cation displacements, tilt angles of oxygen octahedra and electronic transfer are evaluated. Further we investigate substitution effects, ordering and local distortion in detail and compare the results to experimental findings.

DF 7.6 Tue 16:00 WIL A317

Stretchable pressure sensor made of ferroelectret-elastomer-composite and elastic gold electrodes — •Markus Krause[1], Ingrid M. Graz[1,2], Petr Bartu[1], Simona Bauer-Gogonea[1], Sigurd Wagner[3], Stéphanie P. Lacour[2], and Siegfried Bauer[1] — [1]Soft Matter Physics, Johannes Kepler University, Linz, Austria — [2]Nanoscience Centre, Dept. Of Engineering, University of Cambridge, Cambridge, U.K. — [3]Department of Electrical Engineering, Princeton University, Princeton, NJ, USA

Stretchable electronics recently emerged as a new area of macroelectronics, with applications in consumer goods, mobile appliances and artificial skin for full body tactile sensors. Challenges in research are the development of stretchable sensing materials, capable of recording changes in physical parameters such as temperature or pressure. Here we describe a reversibly stretchable pressure sensor material, where charged polypropylene ferroelectret foams as pressure-sensitive part are embedded in a 1mm thick matrix of a surface microstructured silicone elastomer. For electrical readout, 75 nm thick elastic gold electrodes were evaporated on it. The sensor was fabricated and tested as standalone system and combined with an a-Si:H TFT. Modulations in the source-drain-current reflect the periodically applied pressure signal. Pressure in a range from 10 to 1000 kPa was detected, while the sensor was uniaxially streched up to 40%. The signal remained stable over the described pressure and stretch ranges and is even high enough to switch the TFT from the OFF to the ON-state. Financial support

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