DF 20: Nonlinear dielectics, phase transitions, relaxors

Time: Thursday 10:30–11:50 Location: GER 37

DF 20.1 Thu 10:30 GER 37

Precursor dynamics, incipient ferroelectricity and huge anharmonicity in antiferroelectric lead zirconate PbZrO3 — •Annette Bussmann-Holder[1] and Krystian Roleder[2] — [1]Max Planck Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

To understand better the phase transition mechanism of PbZrO3 (PZO) the lattice dynamics of this antiferroelectric compound are investigated within the polarizability model, with emphasis on the cubic to orthorhombic phase transition. Similarly to ferroelectric phase transitions in ABO3 perovskites, polar dynamical clusters develop and grow in size upon approaching TC from the high temperature side and never form a homogeneous state. Simultaneously, elastic anomalies set in and compete with polar cluster dynamics. These unusual dynamics are responsible for precursor effects that drive the PZO lattice towards an incipient ferroelectric state. Comparison of the model calculations with the temperature dependences of elastic coefficients measured on PZO single crystals reveals striking similarity.

DF 20.2 Thu 10:50 GER 37

Tuning of the electrocaloric effect in $BaTiO_3$ and $PbTiO_3$-based relaxors by molecular dynamics simulations — •Anna Grünebohm[1], Peter Entel[1], Takeshi Nishimatsu[2], and Scott P. Beckman[3] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute for Materials Research (IMR), Tohoku University, Sendai 980-8577, Japan — [3]Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011, United States

The electrocaloric effect is an adiabatic temperature change of a material upon applying an external electrical field. Recently, this effect has been rediscovered as a promising candidate for solid state refrigeration as large temperature changes have been found in experiment and theoretical simulations.[1−3] However, the underlaying mechanisms for the large caloric response as well as possible obstacles are still not well understood. In addition, the effective temperature range in pure ferrolectric materials is narrow. We thus perform molecular dynamics simulations of an ab-initio based effective Hamiltonian as implemented in the feram package[3] in order to study the effect of local fields, defects, and alloying on the electro caloric response and its operation range. Our systematic study will focus on $BaTiO_3$, (Ba,Sr)TiO_3, $PbTiO_3$ and PNM-PT.

1 A. Mishenko, *et al*, Science **311**, 1270 (2006)
2 I. Ponomareva *et al*, Phys. Rev. Lett. **108**, 167604 (2012)
3 T. Nishimatsu *et al*, J. Phys. Soc. Jpn., **82**, 114605 (2013)

DF 20.3 Thu 11:10 GER 37

Optically induced switching and bistability of the insulator-metal phase transition in vanadium dioxide nanoclusters — •Thorben Jostmeier[1], Johannes Zimmer[2], Achim Wixforth[2], Helmut Karl[3], Hubert J. Krenner[2], and Markus Betz[1] — [1]Experimentelle Physik 2, TU Dortmund — [2]Lehrstuhl für Experimentalphysik 1 and Augsburg Centre for Innovative Technologies, Universität Augsburg — [3]Lehrstuhl für Experimentalphysik IV, Universität Augsburg

Bulk vanadium dioxide (VO_2) exhibits a insulator-metal phase transition (IMT) at a near ambient temperature of 68°C. Upon heating, VO_2 undergoes a structural and electronic change which is accompanied by a substantial change of the complex dielectric function. More specifically, the metallic phase features a strongly decreased transmission of near-infrared frequencies. A well known effect in nanoscopic VO_2 is a reversible thermal hysteresis of the IMT. Ion beam synthesised $VO_2:SiO_2$ nanoclusters show a more pronounced thermal hysteresis with an supercooled state at room temperature. Additionally, diffraction gratings formed by site selective ion beam implantation show giant switching contrasts exceeding one order of magnitude.

The IMT can be also controlled using femtosecond near-infrared laser pulses. We for the first time show a broad fully reversible hysteresis/bistability in the *optically* induced phase transition of $VO_2:SiO_2$ nanoclusters which allows for a permanent but still erasable switching of the IMT. These properties allow for the implementation of applications like ultrafast optical switches and optical storage devices.

DF 20.4 Thu 11:30 GER 37

Study of field induced critical point in relaxor ferroelectric single crystal and ceramics — •Nikola Novak[1,3], Raša Pirc[1], and Zdravko Kutnjak[1,2] — [1]Jožef Stefan Institute, Jamova 39, 1001 Ljubljana, Slovenia — [2]Jožef Stefan International Postgraduate School, Jamova 39, 1001 Ljubljana, Slovenia — [3]Institute of Materials Science, 64287 Darmstadt, Germany

Relaxor ferroelectrics represent a class of disordered ferroelectrics, which are characterized by the absence of long range ferroelectric order in zero applied field at any temperature. The study of the third-order nonlinear dielectric permittivity some time ago predict a first-order phase transition into a ferroelectric state by cooling a relaxor in an electric field E larger than some threshold electric field Ec.

In order to investigate the field-induced phase transition in relaxor ferroelectric a high-resolution calorimetric and polarization measurements were utilized along the Ec(T) transition line. The behavior of the heat capacity as a function of the temperature and electric field as well as the vanishing of the latent heat gives a sharp defined critical point in [110] relaxor ferroelectric single crystal $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN). On the other hand in 9/65/35 PLZT ceramic the heat capacity as a function of electric field shows a crossover from a discontinuous to continuous step, however, the sample temperature change as a consequence of released latent heat does not vanishes completely. The persisting of the sample temperature anomaly at high temperature can be attributed to two effects: i) the anisotropy of the critical point and ii) electrocaloric effect (ECE).