DF 3: Phase Transitions

Time: Monday 10:40–12:20 Location: EB 407

DF 3.1 Mon 10:40 EB 407

Temperature-driven structural transformations in relaxor-ferroelectric $PbSc_{0.5}Ta_{0.5}O_3$ and $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ — Boriana Mihailova[1], •Bernd Maier[1], Carsten Paulmann[1], Thomas Malcherek[1], Jörg Ihringer[2], Martin Gospodinov[3], Rainer Stosch[4], Bernd Güttler[4], and Ulrich Bismayer[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Universität Tübingen, Tübingen, Germany — [3]Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

X-ray diffraction and Raman spectroscopic studies in a wide temperature range on perovskite-type relaxors $PbSc_{0.5}Ta_{0.5}O_3$ (PST) and $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST) are presented. The temperature evolution of phonon anomalies and the pseudo-cubic unit cell parameter for both PST and PBST reveals the existence of a critical temperature T^* between the Burns temperature T_B and the temperature of the dielectric-permittivity maximum T_m. T^* is associated with coupling of initially nucleated polar sub-clusters and their aggregation into larger polar nanoclusters. The temperature range between T_B and T^* is characterized by coupling between adjacent off-centered BO_6 octahedra to form initial polar clusters, while the range between T* and T_m is characterized by coupling between off-centered B-cations from adjacent polar clusters. Off-centered Pb atoms exist even above T_B and their coherence length governs the coupling between polar regions comprising B-cation off-centered shifts and directs the formation of proper or relaxor ferroelectric state.

DF 3.2 Mon 11:00 EB 407

Transformation from ferroelectric to relaxor state in $BaTiO_3$ based relaxor ferroelectrics — •Vladimir Shvartsman[1], Wolfgang Kleemann[1], Jan Dec[2], Sheng-Guo Lu[3], Zheng Kui Xu[3], and Jiwei Zhai[4] — [1]Angewandte Physik, Universität Duisburg-Essen. Duisburg, Germany — [2]Institute of Physics, University of Silesia, Katowice, Poland — [3]Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, China — [4]Functional Materrials Research Laboratory, Tongji University, Shanghai, China

Presently considerable interest is focused onto the investigation of environment-friendly lead-free relaxors, in particular those based on the ferroelectric $BaTiO_3$. In these materials relaxor properties are observed not only at heterovalent cation substitution as in most relaxors, but also at isovalent substitution. We report on results of investigations of $Ba(Ti_{1-x}Sn_x)O_3$ (BTSn) and $Ba(Ti_{1-x}Zr_x)O_3$ (BTZ), x=0.1-0.4, ceramics which show a gradual transformation from ferroelectric to relaxor behavior at decreasing titanium content. Low-frequency dielectric spectroscopy and piezoresponse force microscopy were applied in order to distinguish the ferroelectric and relaxor features. The ferroelectric state is evidenced in BTSn and BTZ with $x < 0.175$ and 0.25, respectively. The broadening of the peak of the dielectric permittivity ("diffuse phase transition") is due to the coexistence of ferroelectric domains and paraelectric regions related to a nanoscale compositional segregation into Ti-rich and Ti-depleted regions. Further decrease of Ti-content results in relaxor behavior, which is supposed to be related both to weak random fields and to disorder inherent in pure $BaTiO_3$.

DF 3.3 Mon 11:20 EB 407

Pressure-induced phase transition in $PbSc_{0.5}Ta_{0.5}O_3$ — Boriana Mihailova[1], Ross J. Angel[2], •Anna-Maria Welsch[1], Jing Zhao[2], Jens Engel[2], Carsten Paulmann[1], Mihail Gospodinov[3], Rainer Stosch[4], Bernd Güttler[4], and Ulrich Bismayer[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Virginia Tech, Blacksburg, USA — [3]Institute of Solid State Physics, Sofia, Bulgaria — [4]PTB Braunschweig, Germany

Relaxors are ferroelectrics with peculiar structural and physical features having various technological applications. The relaxor structural state consists of polar nanoclusters incorporated into a paraelctric matrix. The temperature evolution of polar nanodomains has been extensively analyzed but up to now only few structural studies have been performed under high pressures.$PbSc_{0.5}Ta_{0.5}O_3$ (PST) is a model representative of Pb-based perovskite-type relaxors. High-pressure studies on PST are rather fruitful to give deeper insights on relaxor structure in general, because: (i) PST shows long-range compositional B-site cation ordering of variable degree; (ii) the temperature of dielectric-permitivitty maximum is near 280 K, suggesting well pronounced polar nanoclusters at room temperature. We report on pressure-induced structural transformations in single-crystal PST samples up to 10 GPa. The structural changes were followed by in-house and synchrotron single-crystal X-ray diffraction and Raman scattering. A continuous phase transition was revealed by the appearance of a soft mode, change in the volume compressibility, broadening of the diffraction maxima and suppression of the x-ray diffuse scattering.

DF 3.4 Mon 11:40 EB 407

Pressure-induced phase transitions in the multiferroic $BiFeO_3$ studied by infrared spectroscopy — •Alexej Pashkin[1], Kaneez Rabia[1], Simone Frank[1], Raphael Haumont[2], Jens Kreisel[3], and Christine A. Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, , 86159 Augsburg, Germany — [2]Laboratoire de Physico-Chimie de l'Etat Solide ICMMO - UMR CNRS, Université Paris Sud, 91405 Orsay Cedex, France — [3]Laboratoire des Matériaux et du Génie Physique (CNRS), INP Grenoble - MINATEC 38016 Grenoble, France

$BiFeO_3$ is considered to be one of the model multiferroic materials with unusually high temperatures of antiferromagnetic ($T_N \sim 370$ °C) and ferroelectric ($T_C \sim 830$ °C) ordering. Recently, an extremely high spontaneous polarization has been reported for $BiFeO_3$ thin films, ceramics and crystals making this material very attractive for applications. $BiFeO_3$ presents a complex interplay between the magnetic, ferroelectric and ferroelastic order parameters. Thus, a particularly rich phase diagram is expected for this material.

We report a high-pressure infrared spectroscopic study of high-quality $BiFeO_3$ single crystals in the far-infrared range up to 10 GPa. The observed behavior of the infrared phonon modes under pressure clearly reveals two structural phase transitions around 3.0 and 7.5 GPa supporting the results of recent Raman and x-ray diffraction studies under pressure. *Financially supported by the DFG (Emmy Noether-program, SFB 484). Provision of beamtime at the ANKA (Karlsruhe) is acknowledged.*

DF 3.5 Mon 12:00 EB 407

Novel complexity in the phase diagram of ferroelectrics — •Annette Bussmann-Holder[1], Helmut Büttner[2], and Alan R. Bishop[3] — [1]Max-Planck-Institut Für Festköroerforschung, Heisenbergstr.1, D-70569 Stuttgart, Deutschland — [2]Lehrstuhl für Theoretische Physik, Universität Bayreuth, Bayreuth, Deutschland — [3]Los Alamos National Laboratory, Los Alamos, NM 87545, USA

The temperature/ doping dependent phase diagram of ferroelectric perovskite oxides is shown to be characterized by six different temperature scales: At high temperatures a crossover from paraelectric to paraelectric / ferroelastic behavior sets in followed by the onset of fluctuating ferroelastic clusters with doping and temperature dependent size. The cluster size anti correlates with their volume which defines another transition line. The onset of ferroelectricity is not sharp since para- and ferroelectric solutions coexist in a small temperature regime. The ferroelectric phase shows novel effects since from a certain transition temperature on this state is incomplete, i.e., ferroelastic clusters fluctuate in a polar matrix. Finally ferroelectricity is completely suppressed by quantum fluctuations. In addition, a novel phenomenon is discussed, where it is shown that the ferroelectric soft modes controls preceding structural instabilities