DF 2: Nonlinear dielectrics, phase transitions, relaxors

Time: Monday 11:00–12:40 Location: KÖN Farb

DF 2.1 Mon 11:00 KÖN Farb

Pressure induced Griffiths-like phase in $Sn_2P_2S_6$ ferroelectrics with three-well potential — •Konstantin Z. Rushchanskii[1], M. Kempa[2], P. Ondrejkovic[2], J. Hlinka[2], P. Saint-Grégoire[3], Ph. Bourges[4], and Yu. M. Vysochanskii[5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics AVCR, Prague, Czech Republic — [3]University de Nimes, Nimes, France — [4]Laboratoire Leon Brillouin, Saclay, France — [5]Uzhgorod National University, Uzhgorod, Ukraine

The origin of the second-order phase transition in uniaxial $Sn_2P_2S_6$ (SPS) monoclinic ferroelectrics is the relaxation of a lone-pair electron localized on Sn^{2+} cations, which results in nonlinear interaction of the soft polar and fully symmetrical optic modes and leads to a three-well potential in corresponding energy surface [1]. It is known [2] that systems with three-well potential, which are described by two order parameters (dipolar and quadrupolar), present a variety of stable, unstable and metastable phases at different temperatures. Combining *ab initio* derived effective Hamiltonian with Monte Carlo statistical simulations on large supercells, we first predict and then confirm experimentally by neutron diffuse scattering an existence of a pressure induced Griffiths-like phase in the PT-diagram near 0.6 GPa. KZR gratefully acknowledge the support from HGF Nachwuchsgruppe Programme VH-NG-409. [1] K.Z. Rushchanskii *et al*, Phys. Rev. Lett. **99**, 207601 (2007); [2] C. Ekiz *et al*, Physica A 293, 215 (2001).

DF 2.2 Mon 11:20 KÖN Farb

Effect of the substrate on the insulator-metal transition of vanadium dioxide films — •Gyoergy Kovacs, Danilo Buerger, Ilona Skorupa, Helfried Reuther, and Heidemarie Schmidt — HZDR, Dresden-Rossendorf

Vanadium dioxide is a potential candidate for on-chip memristive applications due to its hysteretic insulator-metal transition, which can be triggered by electronic pulses. Therefore it is interesting to investigate the details of the growth of VO2 on different substrates to see how the film structure and the electronic properties [1] depend on the underlying substrate. Here we show that single-phase vanadium dioxide films grown on (0001) sapphire and (001) silicon show a very different hysteretic insulator-metal electronic transition. The reason for this difference is that (tri-)epitaxy-stabilized columnar growth of VO2 takes place on the sapphire substrate, while on silicon the expected Zone II growth is identified [2]. The former ensures high crystalline quality so a narrow and high amplitude hysteresis loop, while in the latter case material transport between the substrate and the growing film alters the structure, resulting in a wider and lower amplitude hysteresis loop.

[1] V. A. Klimov, I. O. Timofeeva, S. D. Khanin, E. B. Shadrin, A. V. Ilinskii, and F. Silva-Andrade, Technical Physics 47, 1134 (2002). [2] György J. Kovács, D. Bürger, I. Skorupa, H. Schmidt, submitted

DF 2.3 Mon 11:40 KÖN Farb

Structural transformations in relaxor ferroelectrics on the mesoscopic scale — •Bernd J. Maier[1], Boriana Mihailova[1], Evgeniy A. Dul'kin[2], Tim Prüssmann[1], Carsten Paulmann[1], Marin Gospodinov[3], and Ulrich Bismayer[1] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg — [2]Faculty of Science, The Hebrew University of Jerusalem, Israel — [3]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

$Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST) is a canonical relaxor, undergoing on cooling a series of structural transformations without developing long-range ferroelectric order. Recently, it has been established that perovskite-type relaxors exhibit a characteristic temperature $T^\star$, at which initially formed polar clusters slow down and merge into larger polar nanoregions (PNRs). For PBST the temperature $T^\star$ is near 490 K as revealed by Raman scattering (RS) and acoustic emission (AE). RS data indicate that the transformation processes near $T^\star$ are realized via coupling of off-centred octahedral cations from adjacent polar clusters. AE experiments reveal that the coupling is highly anisotropic and is strongest along $\langle 110 \rangle$ cubic directions. AE measurements also demonstrate a temperature hysteresis of ∼15 K. Since PNRs generate strong x-ray diffuse scattering (XDS) along the $\langle 110 \rangle^\star$ directions, the XDS intensity was used as an order parameter to determine the thermodynamical character of the phase transformation occurring at $T^\star$. The temperature evolution of XDS in PBST measured with synchrotron radiation reveals a near-tricritical behaviour in terms of the Landau theory.

DF 2.4 Mon 12:00 KÖN Farb

Origin of polar nano regions (PNR) in relaxor ferroelectrics: nonlinearity, polaron formation and charge transfer — •Annette Bussmann-Holder — Max-Planck-Institut für Festkörperforschung, Heisenbersgtr. 1, D-70569 Stuttgart, Germany

A central issue in the physics of relaxor ferroelectrics is the origin of the formation of PNRs below some characteristic temperature scale. While it is often attributed to chemical disorder, random bond * random field appearance, local symmetry lowering, it is shown here that the huge intrinsic nonlinearity of ferroelectrics gives rise to spatially limited solutions of discrete breather type, which interact strongly with the remaining lattice. This scenario corresponds to a two-component approach to relaxor physics with decisive signatures in the dielectric spectra and strong charge transfer.

DF 2.5 Mon 12:20 KÖN Farb

Complex polarization ordering in PbTiO3 nanowires: A first-principles computational study — Ghanshyam Pilania[1] and •Rampi Ramprasad[2] — [1]University of Connecticut, Storrs, USA — [2]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany

Based on parameter-free density-functional-theory calculations, we demonstrate the possibility of nonrectilinear curling vortex electric dipole configurations in PbTiO3 nanowires [1]. We predict that the critical size for the genesis of the vortex polarization instability with an axial toroidal moment is 16 Å. We also report previously unknown phase transitions between the nonrectilinear vortex and conventional rectilinear axial polarization configurations mediated by strain and surface terminations. The ability to switch reversibly between the vortex clockwise/counterclockwise and axial positive/negative polarization states may open up transformative technological possibilities.

[1] G. Pilania and R. Ramprasad, Phys. Rev. B 82, 155442 (2010).