DF 4: Internal Symposium "Order/Disorder versus/with Displacive Behaviour"

Time: Tuesday 10:00–13:00 Location: H11

Invited Talk DF 4.1 Tue 10:00 H11

Intrinsically Heterogeneous Ferroelectrics: Origins and Consequences — •A. R. Bishop — Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

We describe expectations of intrinsic heterogeneity and coexistence of phases in some classes of ferroelectric materials. Understanding such behavior is essential to rationalize and motivate experiments, and to optimize materials for applications. We emphasize ferroelectrics as highly anisotropic, polarizable materials. We suggest modeling approaches based on coexisting anisotropic short- and long-range interactions arising from the coupling of spin, charge and lattice (strain) in multi-orbital situations, and the sympathetic proximity of solid-solid structural phase transitions with extended multiscale precursor regimes of twinning, tweed,etc.

DF 4.2 Tue 10:40 H11

High resolution NMR of phase transitions: experimental criteria for order/disorder vs. displacive behaviour — •Naresh Dalal — Florida State University and National High Magnetic Field Laboratory

Traditionally, phase transitions have been classified as of either 'order-disorder' or 'displacive' type. Recently, however, there has been increasing evidence that this classification should be reexamined, and that many systems that were considered as proto-types of order-disorder type, actually exhibit strong features indicating the role of 'displacive' mechanism as well. We have found that among other techniques for probing this question, the modern high-field, high-resolution nuclear magnetic resonance (NMR) could prove to be perhaps the most sensitive and easily accessible method. This presentation will discuss the basics of this tenet, experimental details and recent data, with a conclusion that perhaps most such transitions involve both types of features, and should thus be reclassified as such.

DF 4.3 Tue 11:00 H11

Peculiarities in the dielectric and heat capacity responses of strontium barium niobate — •Jan Dec[1], Zdravko Kutnjak[2], Severyn Miga[1], Wolfgang Kleemann[3], George Cordoyiannis[2], Vladimir Shvartsman[3], Tadeusz Łukasiewicz[4], and Marek Świrkowicz[4] — [1]Institute of Physics, University of Silesia, Pl-40-007 Katowice, Poland — [2]Josef Stefan Institute, P. O. Box 3000, SV 1001 Ljubljana, Slovenia — [3]Angewandte Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [4]Institute of Electronics Materials Technology, Pl-01-919 Warsaw, Poland

The ferroelectric materials SrxBa1-xNb2O6 (SBN) are particular among ferroelectrics since investigations of the c-axis linear dielectric response of SBN single crystals with x = 0.40, 0.50, 0.61 and 0.75, (SBN40, SBN50, SBN61, SBN75) reveal a crossover from conventional ferroelectric (SBN40) to relaxor (SBN75). The temperature dependencies of the dielectric susceptibility were measured in the range 10-2 - 10-5 Hz. Analysis of the data shows that the Curie point TC of SBN40 lies on a linear extrapolation of the "estimated" TC*s of the other SBN crystals. Correspondingly, a change from "normal" domains (SBN40) to smaller ones with fractal-like boundaries was observed by piezoresponse microscopy. The estimated TC*s correspond with anomalies in heat capacity runs. A difference in these around TC shows a non-vanishing latent heat. This complies with the positive sign of the third order nonlinear dielectric susceptibility which decreases when increasing the amplitude of the probing field. Thus, the phase transition in SBN is first order and converts into critical at higher fields.

DF 4.4 Tue 11:20 H11

Is the observation of a soft mode sufficient to characterize a transition as displacive? The case of SrTi18O3 — •Annette Bussmann-Holder — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Deutschland

For many years it has been believed that ferroelectric phase transitions can be strictly classified as either being of displacive or of order / disorder type. First doubts about this clear cut distinction came from local probes like EPR and NMR, where evidence for order / disorder behaviour was obtained in systems exhibiting classical soft mode behaviour. A similar seemingly controversial situation is now also encountered in the isotope induced ferroelectric system SrTi18O3 where long wave length testing experiments reveal classical mode softening whereas NMR and nonlinear dielectric response support order / disorder dynamics. It is shown here that displacive and order / disorder dynamics coexist in SrTi18O3, however obeying different length and time scales. Far above the actual lattice instability self-induced polar nano-domains are formed which stem from optic-acoustic mode coupling and are characterized by order / disorder dynamics, whereas simultaneously a classical soft mode exists in the long wave length limit. The polar state is novel in this compound since an incomplete ferroelectric state forms below Tc.

DF 4.5 Tue 11:40 H11

Domain states and critical behaviour of random field Ising model systems — •Wolfgang Kleemann — Angewandte Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

The charge-disordered three-dimensional uniaxial relaxor ferroelectric Sr0.61Ba0.39Nb2O6 splits up into metastable polar nanoregions (PNRs) and paraelectric interfaces upon cooling from above Tc. The frozen PNRs are verified by piezoresponse force microscopy, respond domain-like to dynamic light scattering and dielectric excitation, reveal non-ergodicity at via global aging, and coalesce into polar nanodomains below Tc. Contrastingly, the percolating system of unperturbed interfaces becomes ferroelectric with two-dimensional Ising model-like non-asymptotic critical exponents, , and , as corroborated by ac calorimetry, second harmonic generation, and susceptometry, respectively [1,2]. Signatures of the crossover into the asymptotic critical behavior of the three-dimensional random-field Ising model (RFIM) will be discussed and compared to corresponding features of the dilute axial antiferromagnet in an external magnetic field (DAFF). [1] W. Kleemann, J. Dec, V. V. Shvartsman, Z. Kutnjak, Th. Braun, Phys. Rev. Lett. 97 (2006) 065702. [2] W. Kleemann, J. Phys.: Cond. Matter 18 (2006) L253.

DF 4.6 Tue 12:00 H11

Possible frustrated ferroelectricity and very high K of oxide perovskites — •Francois Gervais, Virginie Brizé, Cécile Autret, Jérôme Wolfman und Monique Gervais — LEMA UMR 6157 CNRS/CEA Universite François Rabelais Tours (France)

The integration of capacitors on silicon with the highest possible capacity per surface unit is a challenge of mobile microelectronics. One way to achieve this task is to use materials with very high dielectric constant. The origin of the dielectric constant in barium titanate takes place in displacive-order-disorder crossover mechanisms. CaCu3Ti4O12 (CCTO) opens a new way to still better properties with a dielectric constant in excess of 10,000 in the single crystal. In addition, the property little varies with temperature around room temperature. The observation of diffuse scattering in CCTO was recently observed and a frustrated ferroelectricity mechanism was proposed. When CCTO is substituted with only 0.5 % of transition metal element such as Fe or Mn, the permittivity drops down to 100, the contribution due to phonons. Electron spin resonance displays a rapid downshift of the resonance line of copper towards low magnetic field below 30 K when substituted, correlated with dielectric data. The downshift is the signature of local magnetic field. A possible multiferroic character is therefore evidenced. These results will be discussed in terms of frustrated ferroelectrics scenarios.

Invited Talk DF 4.7 Tue 12:20 H11

Order - disorder versus displacive behaviour of ferroelectric perovskites — •Robert Blinc — J. Stefan Institute, Ljubljana, Slovenia

Whereas the first microscopic theory of BaTiO3 was based on order-disorder behavior, later on BaTiO3 has been considered as a classiacal example of displacive soft mode transitions, which can be described by anharmonic lattice dynamics. Already more than twenty years ago, electron paramagnetic resonance (EPR) measurements performed on Mn4+, Cr3+, and Fe3+ doped BaTiO3 by Müller et. al. seriously questioned the pure displacive character of the phase transitions. Recently, the problem has been studied by quadrupole perturbed 47Ti and 49Ti NMR. It was clearly shown that the Ti sits off-center not only in the tetragonal but also in the cubic phase. This off-center scenario confirms theoretical studies which showed a combined displacive

and order-disorder character of the transitions in BaTiO3. The model clearly shows the characteristics of a displacive transition, but with a simultaneous partial ordering of the Ti subsystem as an additional order-disorder feature. Similar results were obtained for SrTiO3 and 18O enriched SrTiO3. Here we present quadrupole perturbed 17O NMR data of both BaTiO3 and SrTiO3 which throw some new light on the role of the oxygen network as well as the A and B ions at the phase transitions in ABO3 perovskite lattices.