MS16-O5 Imaging the dynamics of polar nanoregions in $PbSc_{0.5}Ta_{0.5}O_3$ using transmission electron microscopy and 'digital' electron diffraction

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The existence of dynamically fluctuating regions with a dipole moment (polar nanoregions, or PNRs) in some relaxor materials is now generally accepted as necessary to explain their dielectric response. However little, if any, direct experimental observations of such regions have been made.Here, we show that fluctuating contrast can be observed under appropriate imaging conditions in $PbSc_{0.5}Ta_{0.5}O_3$ (PST) at room temperature using transmission electron microscopy. Its appearanceconsistent with the existence of a domain or 'tweed' structure that is continuously altering on atime scale of milliseconds or less. We find that the domains become smaller and fluctuate morerapidly on heating as the Curie temperature is approached, while they enlarge and slow down uponcooling, switching over seconds or being completely frozen at liquid nitrogen temperature. They arelinked to the presence of additional spots visible in electron diffraction patterns. We use 'digital'large angle convergent beam electron diffraction (D-LACBED) to obtain information about thesymmetry of single frozen domains in PST.

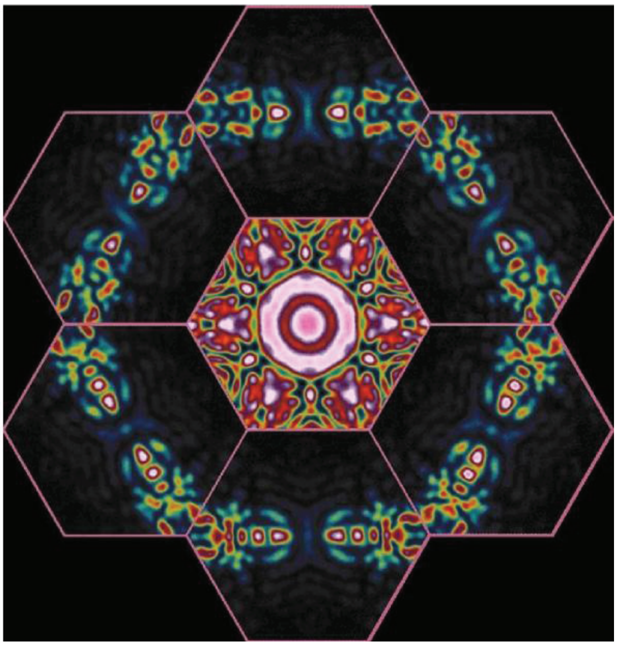

Figure 1. Digital large angle convergent beam electron diffraction (D-LACBED) pattern from a pseudo-cubic [111]zone axis from PST at 130K, showing mirror symmetry. This is incompatible with the nominal spacegroup of R3, but is consistent with R3m or R3c.

Keywords: Relaxor, ergodic, PNRs, tweed, digital diffraction

MS16-O6 Microstructural evolution of the ferroelectric solid solution xBiScO$_3$-(1-x)PbTiO$_3$ throughout its morphotropic phase boundary

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The structural state at the morphotropic phase boundary (MPB) is an important theme in the research of ferroelectric materials since ferroelectric solid solutions exhibit enhanced physical properties near MPB composition. Although an established understanding of creating MPB behaviour relies on invoking instability of average crystal structure or a low-symmetry monoclinic phase in the system driven by composition [1], the actual mechanism is far more complex and heavily dependent on the local ordering of the cations as evidences found in recent diffuse scattering studies [2] on either lead-free or lead-based based systems. We have studied an important and popular ferroelectric system xBiScO$_3$-(1-x) PbTiO$_3$, which was first reported in 2001 with MPB characteristics [3], using the total elastics scattering and Raman scattering methods to better understand its microstructural evolution as a function of composition and temperature in the vicinity of the MPB. Total scattering technique, which is essentially the analysis of the pair distribution function (PDF) of a system, provides crucial structural information at the microscopic level which are not easily available from conventional structural analysis like Rietveld refinement. Neutron powder diffraction experiments were carried out on six different compositions of xBiScO$_3$-(1-x) PbTiO$_3$ in the range $0.30 < x < 0.40$ and neutron PDFs were analysed through RMC simulations to extract the behaviour of individual cations. It was observed that locally there was no abrupt change in any of the cation-cation correlations to assign the MPB unambiguously, however a trend was noticed in the distribution of directions of Ti cation including an ordering between Ti and Sc. These observations were corroborated by the Raman scattering data which further distinguish the roles different cations in terms of composition-induced and temperature-induced phase transitions for this system [4].

Reference:

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Keywords: ferroeletric materials, morphotropic phase boundary, pair distribution function, Raman scattering