Poster Presentation

MS55.P06

Tracking morphotropic phase boundary through total scattering technique

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Morphotropic phase boundary (MPB) is an important theme in the research of ferroelectric materials since materials often exhibit enhanced physical properties at MPB. 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 cations as evidences found in recent diffuse scattering studies [2] on both lead-based and lead-free systems. We have studied an important and popular ferroelectric system xBiScO3-(1-x) PbTiO3 (BS-PT), which was first reported in 2001 with MPB characteristics [3], through total scattering technique to understand its structural evolution as a function composition 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. Both x-ray and neutron powder diffraction experiments were carried out on six different compositions of BS-PT 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 sigmas of individual cationic displacements where the reported MPB composition show a minimum.

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Keywords: Ferroelectric material, Pair distribution function, Morphotropic phase boundary