Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-Principles Study of Diffuse Scattering in $Pb(Sc_{1/2}Nb_{1/2})O_3$

P. GANESH, M. AHART, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, E. COCKAYNE, B. BURTON, Materials Science and Engineering Laboratory, NIST — Recent X-ray and neutron experiments show diffuse scattering with characteristic butterfly and rod shapes in relaxor ferroelectrics $Pb(Sc_{1/2}Nb_{1/2})O_3$(PSN) and $Pb(Zn_{1/2}Nb_{1/2})O_3$(PZN) [1]. We have simulated diffuse scattering in PSN using first-principles based simulations in the ferroelectric, relaxor and the paraelectric phases [2]. The model assumes quenched chemical order in the form of chemically ordered regions in a chemically disordered matrix. Below the Burns temperature, polar nanoregions (PNR) form, pinned spatially to the COR, but whose polarization evolve dynamically. In the relaxor phase we find "butterfly" shaped diffuse scattering around the [100] peaks and around the [110] peaks we find "rod" shaped diffuse scattering similar to experiments. As the system is driven towards the paraelectric phase, the diffuse patterns around all the Bragg peaks display radial streaks elongated towards the origin. We have determined that the rods and butterflies below the Burns temperature originate from the PNR, while the radial streaks above it arise from atomic displacements associated with chemical disorder. References: [1] G. Xu, Z. Zhong, H. Hiraka and G. Shirane, Phys. Rev. B, **70**, 174109 (2004) [2] S. Tinte, B. P. Burton, E. Cockayne and U. V. Waghmare, Phys. Rev. Lett., **97**, 137601 (2006)

Aihaiti Muhetaer
Geophysical Laboratory, Carnegie Institution of Washington

Date submitted: 09 Dec 2008 Electronic form version 1.4