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“Dynamical mechanism of phase transitions in Na$_{0.5}$Bi$_{0.5}$TiO$_3$-x%BaTiO$_3$ single crystals near MPB”

**Abstract**

Lead-free Na$_{1/2}$Bi$_{1/2}$TiO$_3$ (NBT) piezoelectrics have received much attention due to environmental concerns associated with traditional lead-containing piezoelectric compounds. Structural investigations by x-ray diffraction (XRD) and neutron diffraction have revealed a morphotropic phase boundary (MPB) in the NBT-x%BaTiO$_3$ (NBT-x%BT) solid solution for 6<x<7, where piezoelectric coefficients as high as 480 pC/N have been reported. This overall behavior is reminiscent of that seen in lead-containing compounds such as Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$–PbTiO$_3$ (PMN-PT) and Pb(Zn$_{1/3}$Nb$_{2/3}$)O$_3$–PbTiO$_3$ (PZN-PT), which have been thoroughly studied owing to their excellent piezoelectric properties. However, the fundamental properties and microscopic mechanisms leading to the large piezoelectric response of NBT-BT have been much less studied. In addition, there is a fundamental difference between the lead-based compounds, in which cation disorder is on the B-site of the ABO$_3$ perovskite structure, while the lead-free NBT-BT exhibits cation disorder in the A-site. The impact of this fundamental difference on the lattice dynamics and the ferroelectric properties are currently not well understood.

Neutron diffuse scattering and inelastic scattering measurements are powerful techniques to unravel the microstructure and mechanisms underpinning the bulk piezoelectric behavior. In this work, we focused on low-energy optic and acoustic phonons, which are the dominant contributors to the diffuse scattering signal. Specifically, we have mapped the phonons into three datasets-NBT-5%BT-300K, NBT-5%BT-600K, NBT-6.5%BT-300K, in order to find the dynamical mechanism in both axis of phase diagram.

**Biosketch**

Chengtao Luo is currently a PhD candidate supervised by Dr. Dwight Viehland in department of materials science and engineering at Virginia Tech. His research is mainly focused on the non-lead high-performance piezoelectric materials, especially the nano-structure and dynamical mechanism of the phase transitions and phase diagram. He received his B.S. degree in Materials Science and Engineering in Fudan University, China in 2011 and started his graduate study at Virginia Tech since then.