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Insights on the structural tranformations in NBT-xBT from polarized Raman

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Lead-based ferroelectric materials are currently the technologically important ferroelectrics due to their remarkably strong dielectric, electrostrictive, pyroelectric and optoelectric responses and their applications in electronic devices such as capacitors, sensors, medical imaging, filters, information storage processing devices, etc. In particular, binary and ternary ferroelectric solid solutions of type (1-x)PbB'1/3B''2/3O3-xPbTiO3 and (1-y)PbB'1/2B''1/2O3-y[(1-x)PbB'1/3B''2/3O3-xPbTiO3] were considered very promising for industrial applications. However, the restrictions on the use of lead have increased over the past years, due to its potential environmental toxicity during disposure. As a consequence, a huge amount of research is currently being dedicated to find "green" Pb-free or Pb-poor ferroelectric solid solutions with properties comparable to the exemplar Pb-based systems. Bi-based ferroelectric solid solutions are anticipated to be a suitable replacement and they have a great potential to be used in high-performance ecologically friendly devices. In particular, the solid solution (1-x)Na0.5Bi0.5TiO3-xBaTiO3 (NBT-xBT) receives much attention due to its similarities with PbZr1-xTixO3 and (1-x)PbB'1/3B''2/3O3-xPbTiO3 in terms of the existence of a morphotropic phase boundary (MPB, composition xMPB at which the symmetry of the ferroelectric long-range order is changed) with weak temperature dependence and strong enhancement of the dielectric permittivity and piezoelectric response. Additionally, NBT-xBT has a rather complex phase diagram and exhibits a relaxors behavior for $x \leq x_{MPB}$ similar to (1-x)PbB'1/3B''2/3O3-xPbTiO3. The aim of this contribution is to study the mesoscopic-scale coupling processes and dynamics in ferroelectric solid solution (1-x)Na0.5Bi0.5TiO3-xBaTiO3 (NBT-xBT) by in situ polarized Raman spectroscopy on single crystals. The use of single crystals instead of ceramics provides much better opportunity to follow the temporal composition-driven transformation process on the crystal bulk. For that purpose, a series of NBT-xBT single crystals with $x = 0$, $x < x_{MPB}$, $x \sim x_{MPB}$ and $x > x_{MPB}$ (x=0, 0.013, 0.048, 0.053 and 0.074) have been studied at different temperatures. The Raman spectra were collected in parallel and cross-polarized scattering geometries between 100 K and 870 K with a small temperature step of 10 K. The temperature evolutions of specific phonon modes clearly reveal all critical temperatures, including the depoling temperature, which cannot be detected via conventional Bragg diffraction analysis, and reveal the local ferroic distortion responsible for the corresponding structural transformation. The comparison between the temperature trends of the same phonon mode for different compounds further elucidates the atomistic mechanism of the composition-driven crossover from monoclinic to tetragonal ferroelectric long-range order.

Keywords: NBT-xBT, morphotrophic phase boundary, Raman spectroscopy