Neutron and x-ray scattering study of phonon dispersion and diffuse scattering in (Na,Bi)TiO3-xBaTiO3 single crystals near the morphotropic phase boundary

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Neutron and x-ray scattering measurements were performed on (Na1/2Bi1/2)TiO3-x at%BaTiO3 (NBT-xBT) single crystals (x = 4, 5, 6.5, and 7.5) across the morphotropic phase boundary (MPB), as a function of both composition and temperature, and probing both structural and dynamical aspects. In addition to the known diffuse scattering pattern near the points, our measurements revealed new, faint superlattice peaks, as well as an extensive diffuse scattering network, revealing a short-range ordering of polar nanoregions (PNR) with a static stacking morphology. In samples with compositions closest to the MPB, our inelastic neutron scattering investigations of the phonon dynamics showed two unusual features in the acoustic phonon branches, between the superlattice points, and between the superlattice points and points, respectively. These critical elements are not present in the other compositions away from the MPB, which suggests that these features may be related to the tilt modes coupling behavior near the MPB.