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Dynamical Mechanism of Phase Transitions in A-site Ferroelectric Relaxor (Na_{1/2}Bi_{1/2})TiO₃

The dynamical phase transition mechanism of (Na_{1/2}Bi_{1/2})TiO₃ (NBT) was studied using inelastic neutron scattering. Softening of multiple phonon modes were observed to correlate with the phase transition sequence of NBT. As usual, the softening of the zone centre transverse optic (TO) modes Δ_5 and Σ_3 was observed in (200) and (220) zone, showing the Ti vibration instabilities in TiO₆ octahera for both cubic-tetragonal (C-T) and tetragonal-rhombohedral (T-R) phase transitions. In this two phase transitions, however, Ti⁴⁺ has different preferential displacement directions. Surprisingly, the longitudinal optic (LO) mode also soften significantly toward zone centre in the vicinity range of the transition temperature, indicating the Na⁺/Bi³⁺ vibration instability against TiO₆ octahera during the R-T phase transition. Strong inelastic diffuse scattering shows up near M(1.5, 0.5, 0) and R(1.5, 1.5, 0.5) in the tetragonal and rhombohedral phases, respectively, indicating the condensations of the M₃ and R₂₅ optic modes for the corresponding phase transitions. This reveals the rotation instabilities of TiO₆ in the corresponding phase transition temperature range. Bottleneck or waterfall features were observed in the dispersion curves at certain temperatures, but did not show the close correlations to the formation of polar nanoregions (PNRs). Additional instabilities are the origin of the complexity of phase transitions and crystallographic structures in NBT.

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