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Local Structure Study of the Diffuse Phase Transitions in $0.75Pb(Mg_{1/3},Nb_{2/3})O_3$-$0.25PbTiO_3$ HIROYUKI TAKENAKA, ILYA GRINBERG, ANDREW M. RAPPE, University of Pennsylvania, THE MAKINENI THEORETICAL LABORATORIES TEAM — Relaxor ferroelectrics have been of scientific interest and importance due to their fascinating properties such as a giant piezoelectric response, high permittivity over a broad temperature range, and unique dielectric response with frequency dispersion with the diffuse phase transitions. The experimental results undoubtedly explain the transitions with the widely accepted model of polar nanoregions (PNRs), appear at T_b, in a non-polar matrix. Local structure distortions using diffuse scattering (DS) technique had been reported already. Intensities of DS raise up below the intermediate temperature $T*$, a few hundreds degrees below T_b, and can be seen even at low temperature where system undergoes the frozen phase. Formations of local dipoles which give rise to the DS intensities are still unclear. We study DS by performing molecular dynamics simulations with the first-principle-based potential for $0.75Pb(Mg_{1/3},Nb_{2/3})O_3$-$0.25PbTiO_3$ without invoking the PNRs. Our results show that DS patterns form the experimentally reported shapes and integrated DS intensities as a function of temperature reveal a similar trend to the experimental results. Our results indicate that the local structure correlations in lead-based relaxors can arise from local random fields without PNRs. Instead, we find that the DS patterns are due to formations of slush-local-dipole multidomains..

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