Geometrical frustration and piezoelectric response in oxide ferroics

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Materials with increased functionality are often based on crystalline structures with significant local disorder. Typical examples are ferrroic oxides exhibiting large spontaneous polarization that can be rotated by an applied electric field, finding use in many important applications. Despite years of investigation, the exact structural origin of the increased piezoelectric response of oxide ferroics is still unclear. We will show results from a study on the relationship between the local structure and piezoelectric properties of exemplary sodium-potassium niobate ferroics. The results indicate that their increased piezoelectric response is primarily due to a geometrical frustration in the underlying perovskite lattice induced by local fluctuations in the tilt pattern of the constituent niobium-oxygen octahedra (**Figure 1**), and not to a crystal-crystal phase transition or distinct nanodomains as considered by many. The study involves both conventional and resonant high-energy x-ray diffraction coupled to atomic pair distribution function analysis and large-scale 3D structure modeling. The advantages of this experimental approach will also be discussed.

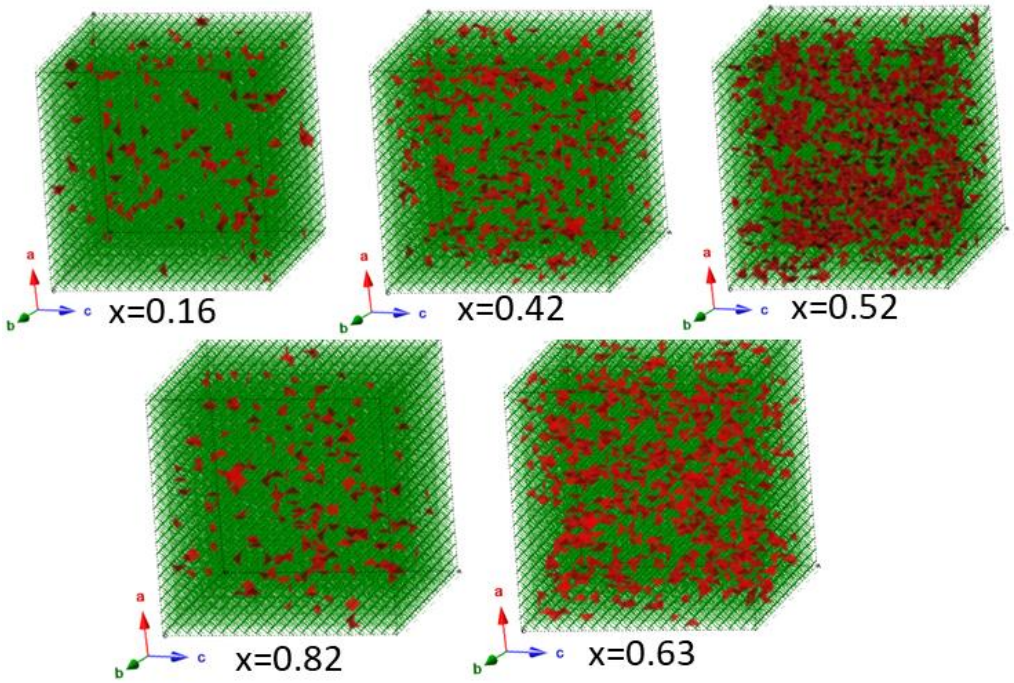

Figure 1. 120,000-atom models of the octahedral framework (green) of mixed $Na_{1-x}K_xNbO_3$ oxide ferroics (x=0.16, 0.42, 0.52, 0.63, 0.82). The models are refined against experimental total and Nb-differential atomic pair distribution functions. Configurations of Nb-O_6 octahedra tilted differently from the majority octahedra in the respective model structure are given in brown. Tilts are determined using relevant bond angles and distances between nearby Nb and O atoms.