Structural Disorder of $Bi_{0.5}K_{0.5}TiO_3$ Studied by Total Scattering and DFT

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We study local structural distortions in $Bi_{0.5}K_{0.5}TiO_3$ (BKT) by first principles electronic structure calculations and synchrotron X-ray total scattering at ambient and elevated temperatures. BKT and related solid solutions show promising electromechanical properties, but a fundamental understanding of the relationship between local structure and functional properties is missing, hampering rational design of BKT-based piezo- and ferroelectrics. We analyze pair distribution functions (PDF) collected from room temperature to 773K by small-box modelling with PDFGUI and large-box modelling with reverse Monte Carlo simulations (RMCProfile) to characterize the temperature dependent structural coherence length. Density functional theory (DFT) calculations were performed for all the 10 principle Bi/K cation configurations possible in a 2×2×2 *P*4*mm* supercell and we find that the Berry phase calculated polarization is larger than experimental values. This indicates that BKT is a disordered material where no local Bi/K configuration is particularly energetically favoured, hence the measured polarization of a BKT sample can be understood as the spatial average of a large number of polar regions with partly cancelling polarization. Combining RMC simulations with DFT calculations we construct a pseudo-disordered structural model with a point charge model calculated polarization in accordance with experimental findings. From the high temperature PDF analysis we find that the Ti displacements in the *P*4*mm* phase prevail into the high temperature *Pm*-3*m* phase, suggesting that the ferroelectric phase transition is predominantly of order-disorder character.