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Local structure of disordered Bi0.5K0.5TiO3 investigated by pair distribution function analysis and first principles calculations BO JIANG, Norwegian Univ Tech (NTNU), ANDY FITCH, European Synchrotron Radiation Facility, TOR GRANDE, SVERRE SELBACH, Norwegian Univ Tech (NTNU) — We investigate the A-site cation ordering in the ferroelectric perovskite Bi0.5K0.5TiO3 (BKT) by Density Functional Theory (DFT) calculations and synchrotron X-ray total scattering. Using BKT as a prototypical lead-free ferroelectric perovskite with multiple A-site cations, we use a combination of theory and experiments to assess the energetics and resulting physical properties of cation ordering. Ten different cation orders in a 2x2x2 supercell were investigated by fitting real space pair distribution functions (PDF), and by calculating the relative energies with DFT. No particularly favourable cation order could be inferred from neither experiment nor theory. Ferroelectric polarization calculated by the Berry phase method and the point charge model yield values in the order of 50-100 C/cm2 for all possible cation orders, which is much larger than previously reported experimental values of about 30 C/cm2. This indicates that BKT does not possess long range A-site cation order. Reverse Monte Carlo (RMC) modelling of the total scattering data also support A-site disorder in BKT. Finally, the ferroelectric polarization calculated for structural models with local cation displacements in a pseudo-disordered A-site sublattice agrees with experimental observations.

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