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Structural Characterization of Nanopolar Domains in PZN-PT[1]

VAYEE VUE, BRANTON CAMPBELL, Brigham Young University, Department of Physics & Astronomy — $Pb(Zn_{1/2}Nb_{2/3})O3$-PbTiO3 (abbreviated as PZN-PT) is of currently of great interest because of its potential as a ferroelectric-relaxor material and because it has the highest known piezoelectric constant. Piezoelectricity is the ability of a crystalline material to generate an electric potential difference when an external stress is applied, or conversely, to generate a physical strain (i.e. stretch or compress) when an external electric field is applied. The physical mechanism that facilitates the special properties of PZN-PT is not well understood. The existence of local structural distortions called nanopolar domains (NPDs) have been suggested as a likely mechanism. We present three-dimensional computer-generated defect models that embody all of the structural freedom an NPD is likely to possess. Individual defect models are evaluated by simulating the x-ray diffuse scattering distribution that results and comparing against experimental data collected at the Advanced Photon Source at Argonne National Laboratory. The DISCUS software package is used to generate the defect models and simulated diffuse scattering patterns, while Crystal Maker is used to visualize the results.

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