Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data - DTU Orbit (05/12/2018)

Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data

A method for the extension of the three-dimensional X-ray diffraction technique to allow the extraction of domain volume fractions in polycrystalline ferroic materials is presented. This method gives access to quantitative domain volume fractions of hundreds of independent embedded grains within a bulk sample. Such information is critical to furthering our understanding of the grainscale interactions of ferroic domains and their influence on bulk properties. The method also provides a validation tool for mesoscopic ferroic domain modelling efforts. The mathematical formulations presented here are applied to tetragonal coarse-grained $\text{Ba}_0.88\text{Ca}_{0.12}\text{Zr}_{0.06}\text{Ti}_{0.94}\text{O}_3$ and rhombohedral fine-grained $(0.82)\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3-(0.18)\text{Bi}_{0.5}\text{K}_{0.5}\text{TiO}_3$ electroceramic materials. The fitted volume fraction information is used to calculate grainscale non-180° ferroelectric domain switching strains. The absolute errors are found to be approximately 0.01 and 0.03% for the tetragonal and rhombohedral cases, which had maximum theoretical domain switching strains of 0.47 and 0.54%, respectively. Limitations and possible extensions of the technique are discussed.

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