



	Experiment title: Strain mechanisms in lead-free piezoelectric ceramics investigated at the single grain level	Experiment number: MA-1919
Beamline: ID11	Date of experiment: from: 06/12/2013 to: 10/12/2013	Date of report: 01/06/2015
Shifts: 12	Local contact(s): Jon Wright	<i>Received at ESRF:</i>
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Report:

Based on the data collected at the beamtime a method for the extension of the 3D-XRD technique to allow the extraction of domain volume fractions in polycrystalline ferroic materials was developed and presented [1]. 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 grain-scale 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 in the publication 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 grain-scale 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.

[1] Jette Oddershede, Marta Majkut, Qinghua Cao, Søren Schmidt, Jonathan P. Wright, Peter Kenesei and John E. Daniels. *J. Appl. Cryst.* (2015). **48**, 882–889