Oral presentation

Spatially resolved crystallography’: 3DXRD for discovering ferroic domain structures

E. Ladbrook[1], J. Wright[2], M. Senn[1]

[1]*Department of Chemistry, University of Warwick, Coventry, U.K.* [2]*European Synchrotron Radiation Facility, Grenoble, France*

Evie.ladbrook@warwick.ac.uk

Domain walls, which separate regions of differing polarisation in ferroic materials, are not only mobile but often exhibit properties different to that of the domains themselves. This includes phenomena such as increased conductivity at the domain walls or displaying polar domain walls in otherwise non-polar materials, which may find applications in nanoelectronics and memristive technologies. Despite being energetically unfavourable in proper ferroelectrics such as $BaTiO_3$, charged domain walls are abundant in hybrid improper ferroelectric, $(Ca, Sr)_3Ti_2O_7$, as shown by TEM [1] and IP-PFM [2], which is believed to result in a polarisation switching barrier that is significantly lower than theoretically predicted. Understanding the domain structure is fundamental to revealing the polarisation switching mechanism which will, in turn, aid in the development of devices that utilise domain walls as a key component in order to meet the demand for fast high-density data storage.

3DXRD is a versatile, non-destructive tomographic technique that can image through the bulk of polycrystalline or single crystal samples, with the image contrast given by diffraction intensities. We utilised scanning 3-dimensional X-ray diffraction (3DXRD) to visualise the domain structure within a single crystal of $Ca_{2.15}Sr_{0.85}Ti_2O_7$, as shown in Fig. 1. In these materials, as polarisation arises as a secondary effect driven by the primary order parameters associated with rotations and tilts of the TiO_6 octahedra, which produce superstructure diffraction peaks, 3DXRD provides a particularly powerful tool for probing the domain boundary structures. From our measurements and in combination with symmetry mode refinements, we can extract the strains and the atomic displacements that underpin the domains to further our understanding of the ferroelastic and ferroelectric domain structure.

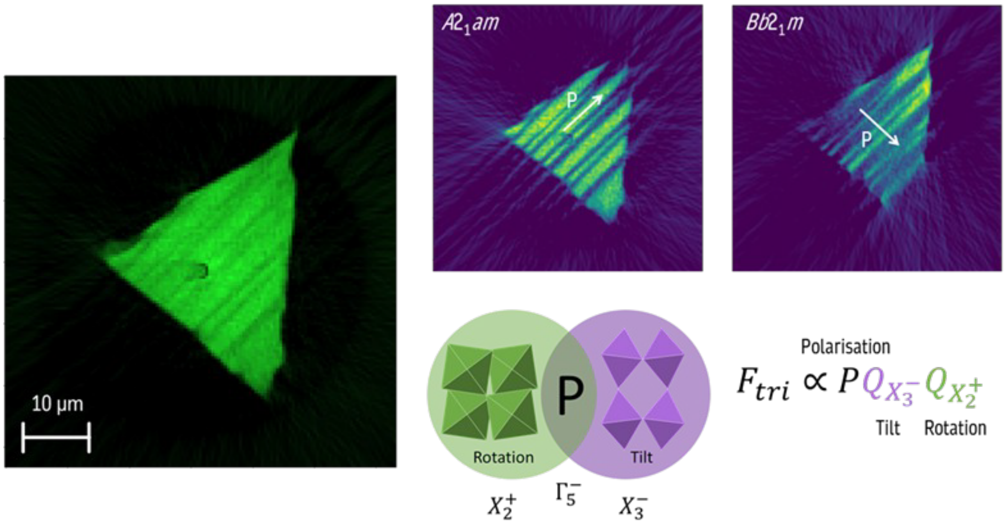

Figure 1. Reconstruction of a slice through a 30 μm sized crystal of $Ca_{2.15}Sr_{0.85}Ti_2O_7$, showing the ferroelastic ($A2_1am$ and $Bb2_1m$ orthorhombic twin) domain structure. Polarisation arises due to the trilinear coupling between rotations and tilts of the TiO_6 octahedra with a polar mode, which transform as irreducible representations X_2^+, X_3^- and Γ_5^-, respectively.

[1] F. -T. Huang *et al*. (2016). *Nature Communications*, **7**, 11602.

[2] Y. S. Oh, X. Luo, F. -T. Huang, Y. Wang, S. -W. Cheong. (2015). *Nature Materials*, **14**, 407-413.