Unravelling the Giant Piezoelectric Effect in ferroics under *in situ* external stimuli using Diffuse Multiple Scattering

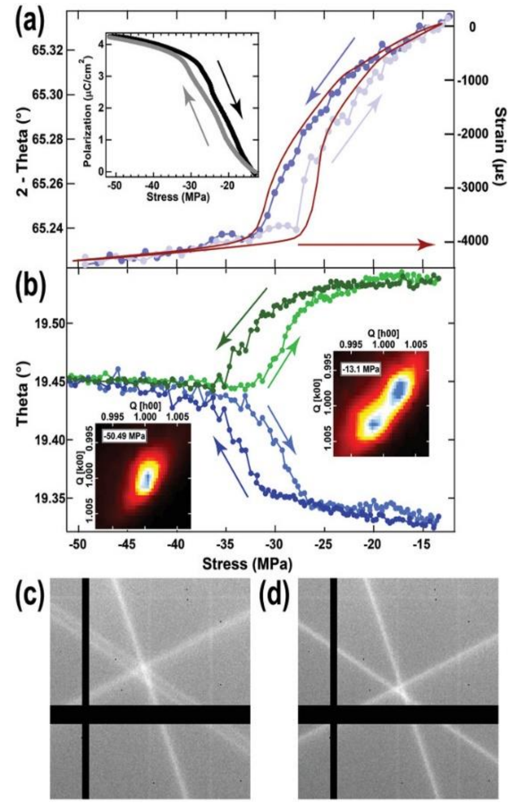

Fig. 1: a,b) Evolution of the (220) (a) and (111) (b) diffraction peaks during loading and unloading cycles. Also included in (a) is the stress–strain curve (inset). Reciprocal space maps for the (111) peak at low and high stress are shown as insets in (b). c, d) DMS results at low stress, zero-field (−7 MPa) (c) and high stress, high field −24 MPa, 2.5 kV cm^{-1} (d) states.

The interplay between stress, strain and electric field in complex multiphase oxides provides the technological underpinning of a plethora of technological applications ranging from sonar emitters, electrical and optical switches to new transistors. The challenge is to correlate macroscopic observables with the crystal structure itself. In these systems, with chemical compositions close to the morphotropic phase boundary, small changes induced by external stimuli cause the system to undergo phase transitions whereby both the physical properties and the crystal structure change (fig. 1) as demonstrated in recent work carried out on the XMaS (ESRF) [1], and I16 beamlines (Diamond Light Source) [2].

It is the exact pathways over which the structural properties change that underpin the functional properties such as the giant piezoelectric effect (GPE), the origin of which remains controversial. This ambiguity is because the evolution pathways of the small domains are complex and exhibit both spatial and temporal variations which cannot be probed using established experimental metrologies. This project exploits a new X-ray method designed to overcome this, taking advantage of "single-shot" measurements which allow the lattices from multiple domains to be determined simultaneously. To do this we will use Diffuse Multiple Scattering (DMS), a technique developed at Diamond Light Source (DLS), using beams as small as 1 μm and a new sample environment developed by Electrosciences Ltd. which will enable us to apply a range of external stimuli to the sample.

The project is embedded on the I16 beamline at DLS and the PhD studies will be based primarily at the synchrotron. You will work with the beamline team as well as collaborators from the USA and Europe to exploit artificial intelligence and machine learning algorithms to realise fast and accurate analysis of the DMS data. This requires modelling the conic projections onto the detector and designing data reduction pathways to make DMS an accessible user option at I16. The project will benchmark the new approach using crystals and thin films of PMN-PT and PIN-PMN-PT and extend studies to spatially resolved analysis as well as explore the dynamics of the system under external stimuli. Using commissioning and experimental time on I16, X-ray data will be recorded simultaneously with any applied optical, stress/strain and electric fields applied to correlate the atomic and the macroscopic responses. The DMS work will be supported with conventional diffraction studies at other beamlines including XMaS at the ESRF and offline at Warwick using the new sample environment. Whilst the project is multi-stranded and comprises many disciplines, the exact direction taken will be determined by the successful candidate's strengths and interests.

(1) Finkel P, *et al.* "Simultaneous Large Optical and Piezoelectric Effects Induced by Domain Reconfiguration Related to Ferroelectric Phase Transitions". *Adv Mater* 2106827 (2021) doi:10.1002/adma.202106827.

(2) Nisbet A G A, *et al.* "Intrinsic and extrinsic nature of the giant piezoelectric effect in the initial poling of PMN-PT *Phys Rev Mater* **5** L120601 (2021)." doi: 10.1103/PhysRevMaterials.5.L120601