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Generalised requirements for ferroelectric domain sharing over grain boundaries

Ferroelectric materials are utilised in a range of technologically important devices. For cost reasons, they are mostly used in the polycrystalline form. Observations of the microstructure and domain structure in polycrystalline ferroelectrics and its effect on ferroelectric performance has been extensively studied. Some of these observations show the frequent occurrence of continuous ferroelectric domain boundaries across grain boundaries. This continuity of domains is suspected to lead to collective dynamics behaviour, particularly during ferroelectric domain wall motion during material excitation. The presented research relates to this domain sharing between neighbouring grains. The requirements for plane matching across grain boundaries is studied, which in turn is used to analyse the proportion of grain boundaries that can allow for plane matching for various grain misorientations using simulations. These simulations are then compared to the microstructures recorded using near field 3D-XRD methods to understand the grain-scale heterogeneous response of these materials under applied electric field.

Primary author: Ms MANTRI, Sukriti (UNSW)

Co-author: Dr DANIELS, John (UNSW)

Presenter: Ms MANTRI, Sukriti (UNSW)