Exploring domain continuity in polycrystalline ferroics

First Supervisor: Dr. Miryam Arredondo
Facilities: Ewald Microscopy Facilities
Funding: TBC
Contact details to discuss project: m.arredondo@qub.ac.uk.

Project background and description

Polycrystalline ferroelectrics belong to a strong and well-defined class of advanced functional materials, with remarkable piezoelectric, ferroelectric, dielectric and electrical properties. They are widely used for devices such as actuators, sensors, ultrasonic devices, transducers, high precision positioning equipment and in ceramic capacitors, which are ubiquitous throughout all electronics and electrical engineering (>10^{13} units p.a.; e.g., >1000 units per smartphone). Their low cost and accessible fabrication, compared to their single crystal counterparts, present exceptional opportunities for microstructure engineering. However, there are still theoretical and experimental challenges that limit our ability to exploit their functionality, particularly important is the relationship between microstructure and properties, where domain engineering, texturing and domain wall continuity can be crucial to tailor and enhance functional properties. Domain wall (DW) continuity (also known as domain continuity) is the phenomenon referred to when domains are observed to cross grain boundaries. This is speculated to affect the domain wall – grain boundary interaction, which could have a contribution on the collective response of domains in adjacent or neighbouring grains, especially during domain switching. The most exciting possibility is that DW continuity could allow a collective switching response over several grains, meaning that the domain structure within one grain would change due to the switching of domains from neighbouring grains. In this picture, those grain boundaries that do not promote DW continuity could be considered as pinning sites, reducing the bulk polarisation during switching. Up to date DW continuity has been elucidated to be key in developing novel ferroelectric ceramics, as an alternative route to tailor (and enhance) properties such as piezoelectricity. However, the true impact of this phenomenon on ferroelectric properties, and the conditions under which DW continuity develops, are not yet fully understood, with limited theoretical[1, 2] and experimental reports.[3, 4] Recently, we established an extension of the crystallographic theory of martensite and provided good predictions of the conditions needed for DW continuity between adjacent grains where an agreement of minimal strain and polarisation mismatch for a pair of domain variants were found in cases where domain wall continuity across grain boundaries was observed.[5] The theory was tested on experimental data for tetragonal BTO. However, its wider applicability to important commercial systems, remains speculative and requires experimental confirmation.
In summary, the relationship between domain continuity, texturing, and functional properties has not been yet addressed. This project aims to use experimental methods to investigate DW continuity in polycrystalline ferroelectrics, evaluate its effect on key functional properties and explore its relationship to texturing.

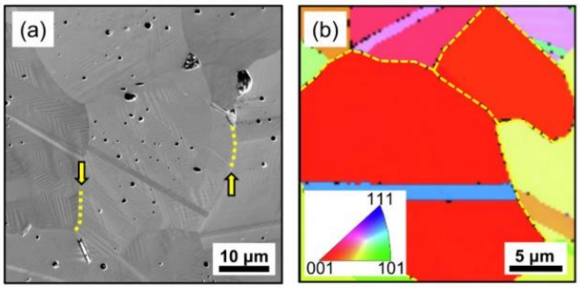

Fig. 1. a) SEM image of a polished ceramic indicating areas where DW continuity has been identified. b) representative EBSD map.

This project involves characterization by electron backscatter diffraction (EBSD), as shown in figure 1, thin lamellae fabrication of selected grains by focused ion beam (FIB) and transmission electron microscopy (TEM), including in-situ heating.
Furthermore, specific parts of the project will be carried out in collaboration with world-leading advanced electron microscopy centres such as the Ernst Ruska-Centre, leading experts in the field of ferroelectrics and modelling.

Entry requirements: Applicants are expected to possess a first or upper-second class degree in physics, chemistry, mathematics, or a relevant discipline (or an equivalent overseas qualification), or a lower second-class degree along with a Master's degree.
How to apply: Applications should be submitted via the Direct Applications Portal.

References

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[3] D. M. Marincel, H. Zhang, A. Kumar, S. Jesse, S. V. Kalinin, W. M. Rainforth, I. M. Reaney, C. A. Randall, S. Trolier-McKinstry, *Advanced Functional Materials* **2014**, 24, 1409.
[4] D. M. Marincel, H. Zhang, S. Jesse, A. Belianinov, M. B. Okatan, S. V. Kalinin, W. M. Rainforth, I. M. Reaney, C. A. Randall, S. Trolier-McKinstry, *Journal of the American Ceramic Society* **2015**, 98, 1848.
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