Ferroelectric Domain Continuity over Grain Boundaries

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Grain boundaries limit the macroscopic ferroelectric properties of bulk polycrystalline ferroelectrics by limiting the mobility of domain walls. Domain wall continuity across grain boundaries has been observed since the 1950's and is speculated to change these grain boundary-domain wall interactions. The collective ferroelectric response of neighbouring grains confirmed in thin films might also be due to correlated domains structures. This paper pertains to the computational study on possibility of such correlated domain structures across grain boundaries.
In order to understand domain wall interactions at grain boundaries, the full 5-dimentional nature of a grain boundary must be accounted for, i.e. 3 variables for the crystallographic misorientation of the grains, and 2 variables for the grain boundary plane orientation. In this work, we have developed the mathematical requirements for domain wall plane matching at grain boundaries. We have also incorporated the grain boundary ferroelectric polarization charge that is caused when any two domains meet at the grain boundary plane. By utilising 3D microstructural mapping methods like sectioned EBSD and 3D-XRD, and calculating the 5-dimensional grain boundary character, we can apply this knowledge to optimize processing techniques to result in desired interactions between grain boundaries and domain walls.