Domain evolution mechanisms of ferroelectric ceramics elucidated by a novel EBSD indexing method

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Abstract

Ferroelectric ceramics are widely used within actuators, sensors, transistors, and solar cells due to their coupled thermo-electro-mechanical properties. Despite their widespread use, the domain nucleation and switching mechanisms within ferroelectric ceramics are not well understood due to the complexities in characterizing a polycrystalline microstructure containing intragranular nanodomains and defects such as pores and precipitates. Domain nucleation and switching mechanisms are hypothetically influenced by both structural features-including the grain orientation, misorientation to neighboring grains, proximity to defects, and the initial domain structure, and the loading configuration-including the boundary conditions, stress applied, and the electric field loading rate. To understand such effects, we have developed an in-house electrical testing setup capable of capturing the bulk ferroelectric response. To connect the bulk polarization hysteresis to the micro-scale evolution of domains, the microstructure is characterized both before and after electrical loading using electron backscatter diffraction (EBSD). We have developed a novel reindexing approach that accurately identifies domain variants in tetragonal ferroelectrics. Minute intensity differences produced by dynamical diffraction within a non-centrosymmetric crystal structure cannot be identified through traditional Hough-indexing, but they can be identified through weighted correlations to simulated patterns of all pseudosymmetric variants. This novel method provides a wealth of microstructural data, giving insight into condition-specific ferroelectric switching mechanisms. The new mechanistic understanding that our research provides will guide microstructural design strategies to yield a target bulk ferroelectric response.

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