Domain Pinning Near a Single-Grain Boundary in Tetragonal and Rhombohedral Lead Zirconate Titanate Films

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The interaction of grain boundaries with ferroelectric domain walls strongly influences the extrinsic contribution to piezoelectric activity in PbZr1−x ,TixO3 (PZT), ubiquitous in modern transducers and actuators. However, the fundamental understanding of these phenomena has been limited by complex mechanisms originating from the interplay of atomic-level domain wall pinning, collective domain wall dynamics, and emergent mesoscopic behavior. This contribution utilizes engineered grain boundaries created by depositing epitaxial PZT films with various Zr:Ti ratios onto 24° tilt SrTiO3 bicrystals. The nonlinear piezoelectric response and surface domain structure across the boundary are investigated using piezoresponse force microscopy while the cross-sectional domain structure is studied using transmission electron microscopy. The grain boundary reduces domain wall motion over a width of 800 °æ 70 nm for PZT 45:55 and 450°æ30 nm for PZT 52:48. Phase field modeling provides an understanding of the elastic and electric fields associated with the grain boundary and local domain configurations. This study demonstrates that complex mesoscopic behaviors can be explored to complement atomic-level pictures of the material system.