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Domain and superdomain structures in ferroelectric $PbTiO_3$ based heterostructures

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$PbTiO_3$ is a ferroelectric material that undergoes a bulk paraelectric-to-ferroelectric phase transition at a critical temperature (T_c) of 765 K, with a polarization that develops along the c-axis primarily driven by ionic displacements. Theoretical studies of domain structures in $PbTiO_3$ thin films reveal complex phase diagrams, with distinct domain configurations as a function of different parameters such as epitaxial strain, film thickness, electrostatic boundary conditions, and deposition temperature [1].

In prior work on $PbTiO_3$ heterostructures grown epitaxially on $(110)_o$-oriented $DyScO_3$ substrates with both top and bottom $SrRuO_3$ electrodes [2,3], we demonstrated an evolution in domain structure—from flux-closure configurations to an a/c-phase—as the film thickness increased. Beyond a critical $PbTiO_3$ thickness, these domains were observed to organize into larger-scale superdomain structures [2,3].

In the present study, we examine a series of heterostructures with $PbTiO_3$ layer thicknesses ranging from 18 to 720 unit cells, with a 22 nm-thick $SrRuO_3$ bottom electrode [4]. Using a combination of atomic force microscopy, vertical and lateral piezoresponse force microscopy, scanning transmission electron microscopy, and x-ray diffraction, we reconstruct the three-dimensional domain configurations and identify distinct superdomain types. Our analysis reveals that the superdomain periodicity scales with film thickness, and we observe the formation of superdomain walls. These walls exhibit potentially unique switching characteristics compared to conventional domain walls, suggesting a route toward enhanced functional properties in ferroelectric heterostructures.

References:

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