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Atomic Mapping of Domain Configurations in Ferroelectric Thin Films

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Atomic-scale information is of critical importance for understanding intrinsic characteristics of advanced functional materials such as ferroelectrics, magnets, superconductors and catalysts. For example, it is often the small deviations from symmetry in atom positions and the resultant strains that allow ferroelectric oxides, used in computer memory chips, to store charge/information or to resonate with magnets as composite multiferroics. Ferroelectric crystals feature asymmetric or polar structures that are switchable under an external field, holding promise for random access memories, thin-film capacitors and actuators [1].

$PbTiO_3$ is a ferroelectric with a tetragonal structure. We have grown a number of $PbTiO_3/SrTiO_3$ multilayered samples on orthorhombic $GdScO_3$(110) substrates by pulsed laser deposition (PLD), using a Lambda Physik LPX 305i KrF (λ=248 nm) excimer laser. We observe the as-grown epitaxial $PbTiO_3/SrTiO_3$ multilayer films in which the electric dipoles at domain-walls of ferroelectric $PbTiO_3$ are characterized by means of aberration-corrected scanning transmission electron microscopy (AC-STEM) [2-6]. We also rationalize the experimental observation via phase-field modeling [3].

Besides the well-accepted head-to-tail 90º uncharged domain-walls (UCDWs), we have identified not only head-to-head positively charged but also tail-to-tail negatively charged domain-walls (CDWs). The widths, polarization distributions, and strains across these charged domain-walls are mapped quantitatively at atomic scale, where remarkable difference between these domain-walls is presented [4].

We observe not only the atomic morphology of the flux-closure quadrant but also a periodic array of flux-closures in ferroelectric $PbTiO_3$ films, mediated by tensile strain on a $GdScO_3$ substrate. We directly visualize an alternating array of clockwise and counter-clockwise flux-closures, whose periodicity depends on the $PbTiO_3$ film thickness. In the vicinity of the core, the strain is sufficient to rupture the lattice, with strain gradients up to 10^9/m [5]. We also observe a 3D polarization texture of a four-fold flux closure domain. Ferroelectric displacement analysis based on aberration-corrected scanning transmission electron microscopic imaging reveals highly inhomogeneous strains with strain gradient above 10^7/m. These giant disclination strains significantly broaden the 90° domain walls, while the flexoelectric coupling at 180° domain wall is less affected [3].

We find that the coupling of 90° and 180° domain walls with dislocations may induce the formation of 90° charged domain walls and some other novel metastable domain configurations. Such domain patterns are observed to relax with 180° domain walls annihilation and the reversal of polarization directions of *a*- and *c*-domain. The configurations of both dislocations and stacking faults may lead to a dramatic change of the domain patterns. Unusual dislocation strain field is identified for a dislocation with the burgers vector 45° apart from a 90° domain wall [6]. In addition, we perform large-scale strain analysis by employing the combinations of geometrical phase analysis (GPA) and AC-STEM imaging, which makes the investigation of ferroelectric domain structures accurate and straightforward [7,8].

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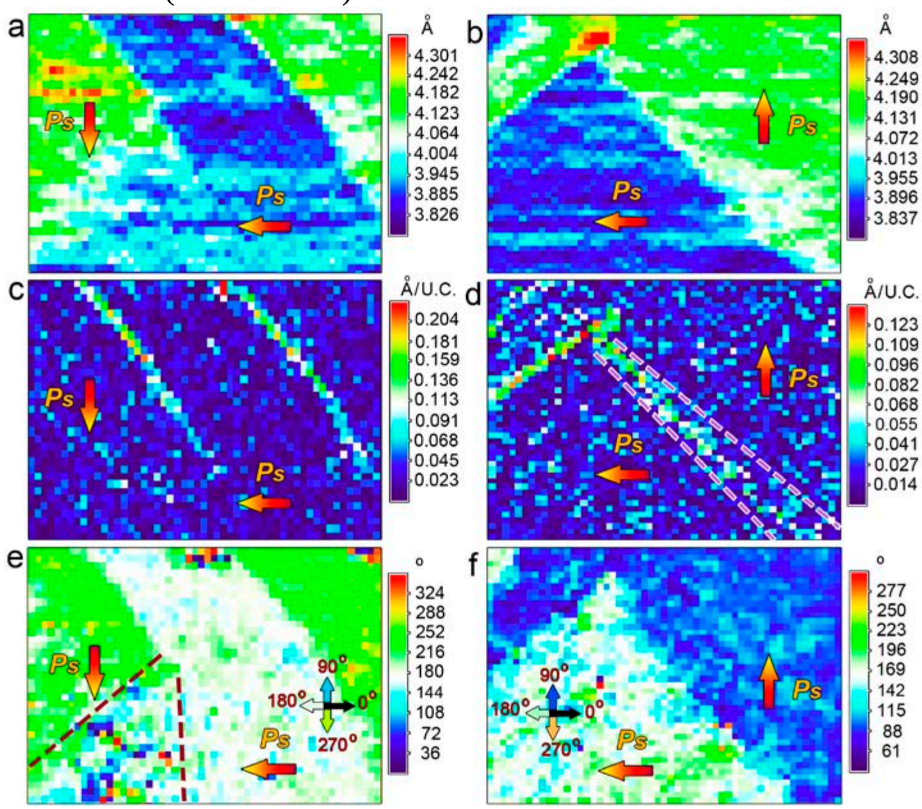

Figure 1. Two-Dimensional mappings of structural and electric behaviors showing the differences between 90º CDWs and 90º UCDWs. (a, b) Out-of-plane lattice spacing mapping for the 90º PCDW and NCDW. (c, d) Lattice gradient mappings (lattice gradient of the out-of-plane lattice mappings along in-plane direction, mapped unit-cell by unit-cell) for the two types of domains. Note the alleviated lattice gradient across the 90º CDWs, especially of the 90º PCDW, compared with sharp lattice gradient across the 90º UCDWs. (e, f) *Ps* angle mappings for the two types of domains. The definition of 0º, 90º, 180º, and 270º are marked with colored arrows with corresponding color-scale. In case of the 90º PCDW, the *Ps* angles are markedly disordered.