doi:10.1017/S1431927611007690
Microsc. Microanal. 17 (Suppl 2), 2011

Electron Microscopy of Ferroelectric Domain Switching in $PbZr_{0.2}Ti_{0.8}O_3$ Thin Films

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Domain switching dynamics in ferroelectric materials involving domain wall motion and its interaction with defects is the key process for practical applications. Complex domain structures found in epitaxial ferroelectric thin films mostly are due to the presence of structural defects such as in-plane domains and misfit and threading dislocations formed during the growth. Because these defects alter local strains by distorting nearby lattices and electrostatic potentials due to their charge unbalances, local polarization switching is not readily understood by general thermodynamic theory.

Fig.1 illustrates, for the first time, our direct TEM observations of out-of-plane polarizations and domain dynamics of ferroelectric thin films ($PbZr_{0.2}Ti_{0.8}O_3$ (PZT) grown on Nb-doped $SrTiO_3$ (Nb-STO)) under various applied biases. Domain contrasts are due to violation of Friedel's for 180^o domain structures, which reported previously [1]. Our results suggest that the PZT film, initially, possesses a nearly single-domain (c_{down} domain) with the out-of-plane polarization pointing towards the film/substrate interface except some minor in-plane components. Upon application of positive bias to the substrate, nucleation of new domain (c_{up} domain) with the out-of-plane polarization pointing towards the metal/PZT film interface was followed by fast forward and relatively-slow lateral growth. The speed of domain wall propagation is found to be similar to that of sound wave in the material, thus Young's modulus in the propagation direction determines the speed. In PZT material, Young's modulus in *c*-axis ([001]) is about 3 times faster than that in *a*-axis (100), which results in a trapezoidal shape of domains, as shown in Fig. 1.

Atomic structures of 180^o domain boundary are shown in Fig. 2. Annular bright-field (ABF) scanning transmission electron microscopy (STEM) shows all atomic columns including oxygen column simultaneously. Atomic displacement, responsible for spontaneous polarization, is clearly shown for both domains in the insets and becomes smaller within the domain wall, of which width is around 8 unit cells.

This research supported by the U.S. Department of Energy, Basic Energy Sciences, by the Materials Sciences and Engineering Division and through use of the Center for Functional Nanomaterials, Brookhaven National Lab.

References

[1] M. Tanaka and G. Honjo, "Electron optical studies of barium titanate single crystal films", Journal of the Physical Society of Japan **9**, 954 (1964).

FIG. 1. TEM images showing ferroelectric domain switching process. All images were taken on the same area with different external bias conditions (a) 0 V, (b) 5 V, and (c) 10 V. Distinct contrast due to violation of Friedel's law allows to identify two ferroelectric domains with antiparallel polarization directions each other. Yellow arrows indicate the direction of polarization.

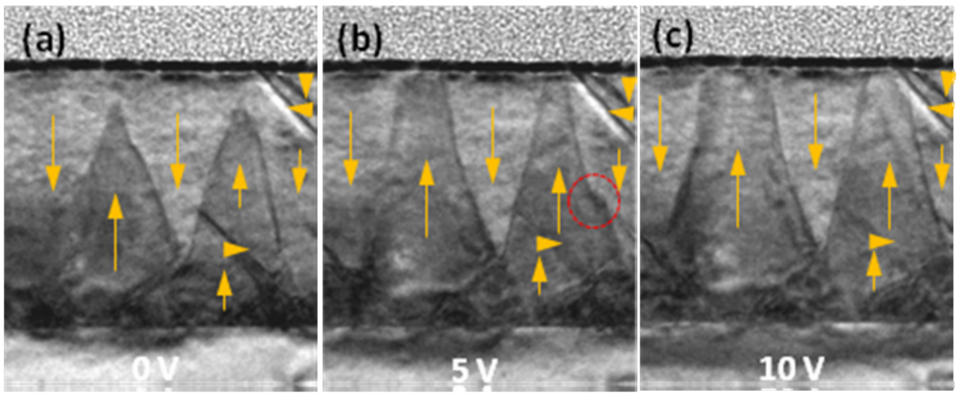

FIG. 2. An ABF-STEM image taken around 180^o domain boundary along [010] directoin. The insets show an enlarged unit cell. Domain boundary is highlighted. Dark, intermediate, and dim spots correspond to Pb^{2+}, Zr/Ti^{4+}, and O^{2-}, respectively.