In-situ TEM Study of Charge Compensation in Ferroelectric Thin Films

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Understanding charge compensation phenomena at ferroelectric domain walls and interfaces may lead to novel functionalities for nanoelectronic applications. Charge compensation can be achieved in various ways including dielectric responses such as displacements of valence electrons and/or ion cores, changes in valence states of metals, and stoichiometry variations. Noticeably, charged defects associated with nonstoichiometry, such as oxygen vacancies, are believed to play an important role in providing compensation charges for polar interfaces [1,2]. In order to understand charge compensation phenomena, we have utilized various electron microscopy techniques including off-axis electron holography, electron-beam-induced-current (EBIC), and atomic-resolution imaging/spectroscopy, combined with *in situ* electrical biasing to directly map out electrostatic potential distributions in ferroelectric thin films. In epitaxial $Pb(Zr_{0.2}Ti_{0.8})O_3$ (PZT) thin films grown on the (001) Nb-doped $SrTiO_3$ (Nb-STO) substrate, the EBIC and electron holography data consistently show asymmetric and unidirectional bias fields at the PZT/Nb-STO interface, similar to semiconductor *pn* junctions [3]. In addition, the electronic band bending across the PZT/Nb-STO interface is modulated by polarization charges; when there are the positive polarization charges at the interface, the depletion region on the Nb-STO side becomes wider, compared to the depletion region width with the negative polarization charges at the interface. Finally, we have observed formation of crystallographic shear planes (CSPs) by DC electric poling [4]. Surprisingly, these CSPs are strongly coupled to the charged domain walls (CDWs) in head-to-head configuration; negatively charged CSPs effectively compensate the positively charged CDWs. By atomic imaging and spectroscopy we illustrate that CSPs consist of both conservative and nonconservative segments when coupled to CDWs. The CDW/CSP coupling yields an atomically narrow domain walls, consisting of a single layer of oxygen. The coupled CDW/CSP was immobile even under external biases far exceeding coercive fields. Our TEM study demonstrates a viable way to experimentally study charge compensation phenomena at ferroelectric domain walls and interfaces.

References

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