PFM-tip induced 90° switching in $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin film: Phase-field modeling

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Ferroelectric thin films have been extensively studied in the past few decades due to their multifunctionality and applications in nonvolatile dynamic random access memory, microelectromechanical systems, microelectronic and sensing applications. Among them, $Pb(Zr_xTi_{1-x})O_3$ **(**PZT) thin films are perhaps the most well studied systems due to their large piezoelectric and pyroelectric responses. Under external stimuli, the bending or moving of 90° domain walls, across which the polarization directions change by 90°, will give rise to extra "extrinsic" contributions to the local displacements, thus to the electromechanical responses.

Piezoresponse Force Microscopy (PFM) has emerged as a powerful tool in domain imaging, domain patterning, domain dynamics and domain switching spectroscopy. Many attempts have been made to visualize and even artificially control the prototype ferroelectric domains with PFM. In general, an applied voltage is applied through a conductive tip with the piezoelectric responses of the surface detected by the vibration of a PFM cantilever. Thus, images of ferroelectric domains can be obtained. Moreover, by applying a DC voltage through the tip, the local polarization can be switched at the nanoscale, i.e., "writing" of a ferroelectric domain.

Previously, Chen *et al.* showed in experiments that the 180° switching could be stabilized by the existence of newly-formed surrounding *a*-domains which form to release elastic energy during electric loading. Meanwhile, both experiments and theoretical analysis indicate that the newly-formed less mobile 90° domain wall cannot be fully switched back by a reverse electric field, which could lead to the so called "fatigue behavior". So in both senses, understanding the dynamics of 90° switching during the local 180° switching is of fundamental importance to the future applications of the ferroelectric /ferroelastic thin films.

Herein, we extend the phase-field model with a semi-implicit Fourier transform scheme to investigate the ferroelectric switching in ferroelectric/ ferroelastic PZT epitaxial thin films under applied bias through PFM tip. 90° switching during local 180° switching is observed, in good agreement with experimental observations. The coherency strain and applied bias effects will be discussed. Different switching patterns are observed under different strain and applied bias conditions. With decreasing magnitude of compressive strain, higher ratios of *a*-domains are favored which lowers the voltage bias for 90° switching. Under low to medium bias, 90° switching is favored due to a huge release of elastic energy, while for high applied bias 180° switching dominates with a large electric energy decrease.

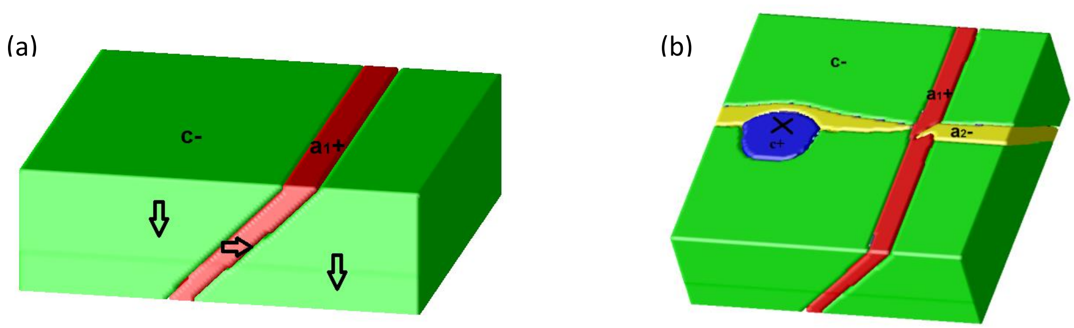

Fig 1(a) Initial *a*/*c* domain configuration, arrows indicate the polarization direction. (b) Equilibrium domain configurations with applied bias of -2.2V at the location indicated by black cross, showing the 90° switching along with the local 180° switching.