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A multiscale study of the structure, chemistry and ferroelectric properties of epitaxial sol-gel $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ films for nanomechanical switching

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Polarization switching phenomena in ferroelectrics are complex processes entangled to electronic, chemical and (micro)(nano)structural properties, and intrinsic and extrinsic defects. These phenomena become critical in the framework of ferroelectric nanostructures, *e.g.* integrated thin films, where interface and surface effects dominate against volume-related properties.

Here, we explore the mechanical and electrical polarization switching of ferroelectric thin films of the prototypical tetragonal ferroelectric $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ (PZT). Using different parameters for sol-gel derived processing and rapid thermal annealing crystallization, we gain control over the electrical properties, chemistry and nanostructure of epitaxial PZT thin films of different thicknesses. The ferroelectric properties determined from microcapacitors indicate that polarization switching under electric field is compatible with out-of-plane *c*-oriented tetragonal PZT, depicting bulk-like remnant polarization values for films thicker than 100 nm. In capacitors based on films less than 100 nm thick as well as in those undergoing different crystallization processes, a decrease of the measured remnant polarization and the appearance of a leakage current are observed.

Piezoresponse force microscopy was used to understand the nanoscale nature of the ferroelectric properties and the polarization switching under different stimuli of these films and environment. Through application of voltage and/or stress using the atomic force microscope tip, and under different electrical boundary conditions, we studied nucleation and switching phenomena in as-grown and in electrically and stress-induced patterned ferroelectric domains. Coercive electric fields and threshold forces required for polarization switching are not only dependent on the conditions of poling, but also on the structure, chemical and electronic properties, and concentration of defects, which we analyzed at different scales using X-ray diffraction and photoemission spectroscopy, scanning electron transmission microscopy, electron energy loss spectroscopy, and Rutherford backscattering and secondary ion mass spectrometry. Phase field simulations of PZT films depicting nanoscale defects support the experimental evidence of the significant contribution of the strain gradient leading to nanomechanical switching.

Our results on polarization switching in epitaxial sol-gel derived PZT films will be discussed in the framework of integrated ferroelectric thin films and nanoscale ferroelectric switching for nanomechanical applications in stress sensors.