THE EFFECTS OF SURFACE AND INTERFACE COMPENSATION ON THE POLARIZATION IN FERROELECTRIC $PbTiO_3$ ULTRATHIN FILMS

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INTRODUCTION

It has recently become possible to synthesize, to characterize experimentally, and to simulate from first principles ultrathin ferroelectric films that display remarkable properties stemming from strong surface and interface effects.

RESULTS

Inspired by these developments, we investigate the effects of electrical boundary conditions on the polarization of such films. A [001]-oriented $PbTiO_3$ film (space group *P4mm*) on conducting $SrRuO_3$ substrate is employed as a model system. The vanishing of external electric fields under 3-dimensional periodic boundary conditions is enforced by using a dipole-corrected density-functional theory based computational approach. The results are analyzed by extracting the lattice parameter, layer rumpling and charges, and the nanosmoothed electrostatic-potential profiles across the films.

CONCLUSIONS

We find that stoichiometric $PbTiO_3$ films remain non-polar up to the thickness of 7 unit cells, with surface relaxation effects extending for about 3 unit cells into the film.

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