The Effects of Surface and Interface Compensation on the Polarization in Ferroelectric $PbTiO_3$ Ultrathin Films*

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We present studies of the effects of electrical boundary conditions on the polarization in ultrathin ferroelectric 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 the nanosmoothed electrostatic-potential profiles across the film. We find that stoichiometric $PbTiO_3$ films remain non-polar up to thickness of 7 unit cells, with surface relaxation effects extending for about 3 unit cells into the film.

(*) Work supported under contract No. DE-AC02-06CH11357 between UChicago Argonne, LLC and the Department of Energy