Unusual polarization patterns in flat epitaxial ferroelectric nanoparticles

IVAN NAUMOV, ALEXANDR BRATKOVSKY, Hewlett-Packard Laboratories — We investigate the effects of a lattice misfit strain on a ground state and polarization patterns in flat perovskite nanoparticles (nanoislands of BaTiO$_3$ and PbZr$_{0.5}$Ti$_{0.5}$O$_3$) with the use of an ab-initio derived effective Hamiltonian. We show that the strain strongly controls the balance between the depolarizing field and the polarization anisotropy in determining the equilibrium polarization patterns. Compressive strain favors 180° stripe/tweed domains while a tensile strain leads to in-plane vortex formation, with the unusual intermediate phase (s) where both ordering motifs coexist [1]. The results may allow to explain contradictions in recent experimental data for ferroelectric nanoparticles. [1] Ivan Naumov and Alexander M. Bratkovsky, Phys. Rev. Lett. 101, 107601 (2008).