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Peculiar ordering in flat ferroelectric nanoparticles driven by lattice misfit IVAN NAUMOV, ALEX BRATKOVSKY, Hewlett-Packard Laboratories — Flat *free-standing* ferroelectric (FE) nanopartilcles tend to have a vortex-like polarization ordering with the in-plane polarization that curls around an out-of-plane vortex core axis. The question is, if such a structure is still a ground state in presence of noticeable misfit strains induced by a substrate, and whether the 180° stripe domains may form, similarly to the case of ultra thin FE films? Here we perform an *ab initio* based study of disk- shaped $Pb(Zr_{1-x}Ti_x)O_3$ and $BaTiO_3$ nanoparticles that have the vortex ground state when no stress is applied. Our study leads to the following findings for the disks having circular and square footprint: (i) under strong enough compressive strains the curling state is no longer stable and yields to a multi-domain structure with an out-of-plane polarization, and different possible in-plane domains: triangle, stripe-like, or "bubble" in shape, (ii) each separate domain, regardless of its shape, runs through the entire thickness of a disk, and (iii) the 180° stripes occur only under special conditions depending on the shape and chemical composition of the nanostructures. Further, we discovered that starting with the vortex state and then increasing the compressive strains may lead to a metastable bi- or multi-domain phase different from the ground state obtained by gradual cooling at a fixed strain. This leads to a novel hysteretic behavior as a function of the misfit strain.

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