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Ferrolectric nanodots and nanowires under different electrical and mechanical boundary conditions[1] INNA PONOMAREVA, IVAN NAUMOV, LAURENT BELLAICHE, University of Arkansas — Intense effort has been recently made in synthesizing, characterizing and/or simulating ferroelectric nanostructures (FENs), because of their technological and fundamental promise. Among the different possible classes of FENs, thin films are, by far, the ones that have been the most investigated. However what is crucially missing nowadays is to gain a deep knowledge of 0D-like and 1D-like FEN and understand how their properties depend on mechanical and electrical boundary conditions. We report results on ferroelectric nanodots and infinite wires of $Pb(Zr_{0.4}Ti_{0.6})O_3$ alloy under different boundary conditions investigated via Monte-Carlo simulations using an atomistic first-principle-based effective Hamiltonian[1]. It was found that these nanosystems all exhibit a spontaneous polarization that points along a non-periodic direction, for situations close to short circuit electrical boundary conditions and independently of the epitaxial strain. On the other hand, unusual dipole patterns arise in these systems when they experience a large-enough depolarizing field. The dependency of these patterns on the nanostructure's dimensionality is revealed and explained. [1] L. Bellaiche *et al*, Phys. Rev. Lett. **8**, 5427 (2000).

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