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Properties of Ferroelectric Nanostructures[1]

INNA PONOMAREVA, Physics Department, University of Arkansas

Ferroelectric nanostructures (FENs) such as thin films, nanowires and nanodots are receiving a lot of attention due to their potential for technological applications and to the rich variety of underlying physics. Interestingly, properties of FENs can substantially deviate from their bulk counterpart due to their sensitivity to many factors. Examples of such factors are the electrical boundary conditions (associated with the full, partial or non-existent screening of polarization-induced surface charges) and mechanical boundary conditions (arising from the lattice mismatch between the FEN and its substrate).
Here, we developed and used computational schemes to predict many properties in various FENs, as well as, to provide atomistic insight to their complex phenomena. In particular, we will show the striking following features and reveal their origins:

- The interplay between electrical boundary conditions, mechanical boundary conditions and growth direction results in the appearance of novel dipole patterns and new low-symmetry phases possessing superior dielectric properties in ferroelectric dots, wires and films [1,2].
- FENs can exhibit dielectric anomalies, such as a *negative* dielectric susceptibility [3].
- Nanobubbles can form in ferroelectric films under an external electric field [4].
- An homogeneous electric field can be used to control the chirality of vortex structures in asymmetric ferroelectric dots, via the creation of original intermediate states [5].

[1] I. Ponomareva *et al.*, Phys. Rev. B **7**2, 214118 (2005).
[2] I. Ponomareva and L. Bellaiche, Phys. Rev. B **7**4, 064102 (2006).
[3] I. Ponomareva *et al.*, to be published in Phys. Rev. Lett. (2007).
[4] B.-K. Lai *et al.*, Phys. Rev. Lett. **96**, 137602 (2006).
[5] S. Prosandeev *et al.*, submitted (2007).

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