

MAR09-2008-004259

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

First-principles modeling of closure domains in ferroelectric ultrathin films¹

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Capacitors based on ferroelectric perovskites are potentially attractive for nanoelectronic devices. However, in many cases their use depends on the stability of a ferroelectric state with an out-of-plane polarization. The interplay between mechanical and electrical boundary conditions, and the local chemistry at the surface or interface might give rise to exotic patterns of the polarization, especially in the thin film regime. The screening of the interfacial polarization charges by real metallic electrodes has been extensively discussed in the literature. We have carried out first-principles computations on two other screening mechanisms in ultrathin capacitors made of a few unit cells of BaTiO₃ with metallic SrRuO₃ electrodes. First, the simulation of the energetic, structural, and electronic properties of ferroelectric domains in short circuit. ² The domains are stabilized down to two unit cells, adopting the form of a domain of closure, common in ferromagnetic thin films. The domains are closed by the in-plane relaxation of the atoms in the first SrO layer of the electrode, that behaves more like SrO in highly polarizable SrTiO₃ than in metallic SrRuO₃. Even if small, these lateral displacements are essential to stabilize the domains, and might provide some hints to explain why some systems break into domains while others remain in a monodomain configuration. An analysis of the electrostatic potential reveals preferential points of pinning for charged defects at the ferroelectric-electrode interface, possibly playing a major role in films fatigue. The closure domain structure, predicted also by other phenomenological and effective Hamiltonian models, is more general than expected. Second, the possibility of screening by a surface state or metallization of the first few layers of the ferroelectric without a top electrode is also explored.

¹Work done in collaboration with P. Aguado-Puente, and supported by MEC under Project No. FIS2006-02261

²P. Aguado-Puente and J. Junquera, Phys. Rev. Lett. **100**, 177601 (2008).