Abstract Submitted
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Ferromagnetic-like closure domains in ferroelectric ultrathin films: First principles simulation[1] JAVIER JUNQUERA, PABLO AGUADO-PUENTE, Dep. CITIMAC, Universidad de Cantabria, Avda. de los Castros s/n, E-39005, Santander, Spain — We simulate from first-principles the energetic, structural, and electronic properties of ferroelectric domains in ultrathin capacitors made of a few unit cells of $BaTiO_3$ between two metallic $SrRuO_3$ electrodes in short circuit. The domains are stabilized down to two unit cells, adopting the form of a domain of closure, common in ferromagnets but only recently detected experimentally in ferroelectric 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 $SrTiO_3$ than in metallic $SrRuO_3$. 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.

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