Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

One-dimensional polydomains in Ferroelectric thin films MATIAS NUNEZ, North Carolina State University, MARCO BUONGIORNO NARDELLI, North Carolina State Sniversity — The local nature of the interface in metal/ferroelectric oxide junctions can drastically affect the polarization in the ferroelectric film. As the thickness of the film is reduced, the intensity of the depolarization field increases and the system will reduce its electrostatic energy in two ways, either by forming lateral 180° domains [1], or by reducing the ionic polarization while remaining in a monodomain state. Using DFT, maximally localized Wannier functions [2] and the layer polarization concept [3], we studied the ferroelectricity in thin layers of $BaTiO_3$ sandwiched between metal. Our results suggest that the structures associated with this spatial scale are more complex than previously thought, and we show how a pattern of the local polarization provides another way to minimize the internal energy below certain critical thickness. This pattern is characterized by the appearance of *one-dimensional polydomains*, consecutive dipoles with opposed orientations in the direction perpendicular to the ferroelectric thin film/metal interface.

[1] V.Nagarajan *et al*, J. Appl. Phys. **100**, 051609 (2006).
[2] N. Marzari, and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997); A. Calzolari *et al.*, Phys. Rev. B **69**, 035108 (2004).
[3] X. Wu *et al*, Phys. Rev. Lett. **97**, 107602 (2006).

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Date submitted: 27 Nov 2007 Electronic form version 1.4