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Onset of ferrielectricity and the hidden nature of nanoscale polarization in ferroelectric thin films MATIAS NUNEZ, MARCO BUONGIORNO NARDELLI, North Carolina State University — Using calculations from first principles we have elucidated the nanoscale organization and local polarization in ferroelectric thin films between metallic contacts. We discovered a ferrielectric pattern of polarization in what was originally thought to be a simple ferroelectric domain. Applying the layer polarization concept (Wu et al., Phys. Rev. Lett. 97, 107602 (2006)), we analyzed the polarization profile for different film thicknesses. The results (M. Nunez and M. B. Nardelli, Phys. Rev. Letters, to be published) unveil a peculiar spatial pattern where individual atomic layers acquire uncompensated opposing dipoles in what was originally thought to be a simple ferroelectric domain. This ferrielectric behavior arises as consequence of the complex energetic competition between the interface effects, the depolarization field, and the mutual interaction of the layer dipoles. Morover, as the thickness of the film is varied, we show that the system undergoes a ferroelectric-to-ferrielectric phase transition at a critical thickness. These results are interpreted using a simple classical model where the interface effects are explicitly taken into account. We propose a method in order to carefully tune the spatial polarization pattern of the film (M. Nunez and M. B. Nardelli, Appl. Phys. Lett. 92, 1 (2008)).

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