Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Effect of polar interfaces on thin-film ferroelectricity YONG WANG, MANISH NIRANJAN, KAROLINA JANICKA, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, USA, JULIAN VELEV, Department of Physics, University of Puerto Rico, USA, MIKHAIL ZHURAVLEV, Kurnakov Institute for General and Inorganic Chemistry, Moscow, Russia, SITARAM JASWAL, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, USA — Based on first-principles and model calculations we investigate the effect of polar interfaces on the ferroelectric stability of thin-film ferroelectrics [1]. We consider Vacuum/LaO/BaTiO3/LaO, LaO/BaTiO3, and SrRuO3/LaO/BaTiO3/LaO heterostructures as representative systems, where a LaO monolayer at the interface with a TiO2-terminated BaTiO3 produces a polar interface. The polar interfaces create an intrinsic electric field which produces electric polarization in BaTiO3 directed into the interior of the BaTiO3 layer. This creates a ferroelectric dead layer near the interfaces that is non-switchable and thus detrimental to ferroelectricity. The effect is stronger for a larger effective ionic charge at the interface and longer screening length due to a stronger intrinsic electric field that penetrates deeper into the ferroelectric. The predicted mechanism for a ferroelectric dead layer at the interface controls the critical thickness for ferroelectricity in systems with polar interfaces. [1] Y. Wang et al., Phys. Rev. B. 82, 094114 (2010).

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Date submitted: 17 Nov 2010 Electronic form version 1.4