Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Stabilizing ferroelectric polarization of ultrathin BaTiO3 films through interface engineering XIAOHUI LIU, YONG WANG, PAVEL LUKASHEV, J.D. BURTON, EVGENY TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanotechnology, University of Nebraska, Lincoln, NE 68588, UNIVERSITY OF NEBRASKA–LINCOLN TEAM — Ferroelectric tunnel junctions have recently attracted considerable interest due to their potential for device applications [1]. The main challenge for the implementation of these devices is to stabilize ferroelectricity in nanometer- thick films where depolarizing fields and interface effects play an important role. Here, we report results of first- principles calculations of ferroelectric polarization in epitaxial SrRuO3/BaTiO3/SrRuO3 junctions. We show that the ferroelectric polarization is very sensitive to the surface termination of the electrodes and film thickness. In particular, we find that the presence of RuO2/BaO interface is detrimental to ferroelectricity due to the pinning of polar displacements in BaTiO3 in the direction away from the interface making the polarization of ultra-thin films non- switchable. We find that ferroelectricity can be stabilized by adding a thin layer of SrTiO3 at this interface. A phenomenological model is developed to explain the correlation between ferroelectric properties and junction geometry.

[1] E.Y. Tsymbal and H. Kohlstedt, Science 313, 181 (2006).

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Date submitted: 12 Nov 2010 Electronic form version 1.4