Abstract Submitted for the MAR12 Meeting of The American Physical Society

Exploring and alleviating detrimental interface dipole effects in ultra-thin all-oxide metal-ferroelectric-metal heterostructures XIAOHUI LIU, YONG WANG, PAVEL LUKASHEV, J.D. BURTON, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska-Lincoln — Ultrathinfilm metal-ferroelectric-metal heterostructures present an exciting prospect for switchable nanoelectronic memories and devices such as ferroelectric tunnel junctions. The main challenge is to realize ferroelectricity in ultrathin-films where detrimental interface effects become increasingly more pronounced as ferroelectric film thicknesses approach the nanoscale. We studied the ferroelectric polarization of BaTiO₃ in epitaxial SrRuO₃/BaTiO₃/SrRuO₃ junctions by first-principles density functional theory and phenomenological modeling. The calculations show that the presence of a RuO_2/BaO termination sequence at the $SrRuO_3/BaTiO_3$ interface leads to a pinned interface dipole and is therefore detrimental to the stability of ferroelectricity, leading to the disappearance of switchable polarization under a certain thickness. Here, we propose to alleviate this behavior by depositing a thin layer of $SrTiO_3$ at this interface to suppress the RuO_2/BaO interface termination sequence, thereby eliminating the associated unfavorable pinned interface dipole. By doing this we find, and experiments confirm, that a switchable ferroelectric state can be stabilized in much thinner heterostructures.

> Xiaohui Liu Department of Physics and Astronomy, University of Nebraska-Lincoln

Date submitted: 03 Jan 2012

Electronic form version 1.4