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 — Ultrathin-film 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 $\text{BaTiO}_3$ in epitaxial $\text{SrRuO}_3/\text{BaTiO}_3/\text{SrRuO}_3$ 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