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.