Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Mixed Ising-Bloch-Néel Character to 180 ° Ferroelectric Domain Walls[1] VENKATRAMAN GOPALAN, Pennsylvania State University, DONGHWA LEE, RAKESH BEHERA, University of Florida, PINGPING WU, Pennsylvania State University, HAIXUAN XU, University of Florida, YULAN LI, Pacific National Laboratory, SIMON PHILLPOT, University of Florida, LONG-QING CHEN, Pennsylvania State University — Ferroelectric 180-degree domain walls are well-known to be predominantly Ising-like. Using density functional theory, and molecular dynamics simulations, the 180 degree domain walls in prototypical ferroelectrics, lead titanate (PbTiO3) and lithium niobate (LiNbO3), are shown to have mixed character: while predominantly Ising-like, they also manifest some Bloch- and Néel-like character. Phase-field calculations show that such mixed wall character can be dramatically enhanced in nanoscale thin film heterostructures such as BaTiO3/SrTiO3, where the internal wall structure can form polarization vortices. Such mixed character walls can be expected to exhibit dynamical wall properties distinct from pure Ising walls.

[1]National Science Foundation

Venkatraman Gopalan
Pennsylvania State University

Date submitted: 24 Nov 2009 Electronic form version 1.4