Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Boundary conditions on ferroelectricity in ultrathin $SrTiO_3$ films on silicon[1] ALEXIE KOLPAK, FRED WALKER, JAMES REINER, CHARLES AHN, SOHRAB ISMAIL-BEIGI, Yale University, CRISP COLLABORATION — The properties of $SrTiO_3$ films expitaxially grown on Si(001) are strongly influenced by the electronic structure of the interface. Using density functional theory, we demonstrate the presence of an intrinsic interface dipole, the direction of which is independent of the particular combination of Sr, Ti, O, and Si atoms at the interface, and therefore independent of growth conditions. As a result of this intrinsic dipole, a local, positive polarization is induced in the $SrTiO_3$ interfacial region, fixing the electrostatic boundary conditions at the interface and preventing the formation of a negatively polarized state with a single domain. We suggest ways in which this constraint on the ferroelectric behavior can be overcome by interfacial cation doping, allowing for the integration of ferroelectricity with traditional silicon-based devices.

[1]Supported primarily by NSF MRSEC DMR 0520495.

Alexie Kolpak
Yale University

Date submitted: 21 Nov 2008 Electronic form version 1.4