Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Modeling Micron Size Multi-domain Ferroelectric Switching using a Massively Parallel Time Domain Phase-Field Model KHALID ASHRAF, SAYEEF SALAHUDDIN, UC Berkeley, LABORATORY OF EMERGING AD EXPLORATORY DEVICES TEAM — For the study of devices incorporating multi-domain ferroelectric materials, it is necessary to extend the current capabilities of the phase field model up to the micron scale where experiments are typically performed. Also arbitrary electrical and mechanical boundary conditions need to be incorporated relatively easily. In this work, we report a time domain implementation of the 3D phase field model that can simulate multi-domain ferroelectric switching. This massively parallel implementation enables us to study the switching properties of micron size devices with $\sim 10^9$ degrees of freedom. We used a mixed finite difference and finite element grid, for calculating the nonlocal electrostatic and elastic interactions respectively. All the local and non-local interactions are shown to scale linearly up to thousands of processors. The model can take into account arbitrary electrical and mechanical boundary conditions suitable for the study of devices with arbitrary structures. Using this model, we report the simulation results of ferroelectric switching in devices incorporating the multi-ferroic material $BiFeO_3$. We explain the domain growth mechanism observed in multiple experiments reported recently on various surfaces of $BiFeO_3$.

Khalid Ashraf
UC Berkeley

Date submitted: 28 Nov 2011 Electronic form version 1.4