Materials Science and Technology Division

Materials Theory Seminar

"Modeling of Ferroic Materials and Devices Using Phase Field Approach"

Samrat Choudhury
The Pennsylvania State University

Wednesday, January 17, 2007
11:00 a.m.
Bldg. 3025M, Third Floor Conference Room

Abstract:
Phenomenological thermodynamic approach used to describe behavior of ferroelectric materials, assumes that the material to be a perfect crystal consisting of a single ferroelectric domain. It is well known that a ferroelectric is generally inhomogeneous and contains domains and domain walls, as well as defects such as surfaces, grain boundaries, dislocations and dipolar defects. Moreover, with a single domain assumption, the ferroelectric properties like coercive field predicted from thermodynamic approach is typically one or more orders of magnitude higher compared to those measured experimentally. A three-dimensional (3-D) phase-field model has been developed for predicting the domain structures and ferroelectric properties in presence of inhomogenities in the form of bulk and thin films. The model takes into account realistic grain structures as well as various energetic contributions, including elastic energy, electrostatic energy, and domain wall energy. It is observed that grain boundary acts a source of nucleation of new domains during polarization switching in ferroelectric polycrystals and the switching between neighboring grains are correlated. Further, it will be shown that the switching behavior in epitaxial thin films is strongly dependent on the type and density of interfacial dislocations. Starting with thermodynamic approach assuming a single domain it will be demonstrated in a systematic manner that possibility of incorporating heterogeneities in phase field approach helps to predict accurately ferroelectric properties like coercive field and remnant polarization. Effect of substrate constraint in epitaxial thin films on ferroelectric transition temperature, phase stability and ferroelectric properties will also be presented.

The model has also been adapted to study the domain structure and switching behavior of other ferroic materials and devices such as thin films patterned into islands, ferroelectric superlattice as well as multi-ferroic materials and preliminary results will be presented. The possibility of modifying the current phase field model to describe the phenomenon of writing of stable ferroelectric domains in thin films using a point charge analogous to an AFM tip will be discussed.

Host: Malcolm Stocks