Case Study Summary-Jason Marshall: Multi-Scale Modeling of Ferroelectrics: Qausicontinuum Method and Interatomic Potentials

Jason Larkin ME 24-623

This case study reviewed multi-scale modeling of ferroelectrics, a class of materials which can sustain a spontaneous net electric polarization. Ferrorelectricity is the electric field analog of ferromagnetism, which is the permanent magnetic moment of a material. Both of these phenomena can be controlled with external fields (electric and magnetic), and many phenomena are closely linked to the ability to electrically polarize a material. For example, the phenomenon of piezoelectricity is nothing more than the induced electric polarization of a material under an applied strain/stress. At the heart of the phenomena is the change in a material's polarization density, which under mechanical load or applied electric field can be manipulated. There are a wide range of applications for ferroelectric materials, one notable application being the fine motor control (piezoelectrics) used in scanning tunneling and atomic force microscopes.

The first paper reviewed [1] involved the fitting of interatomic potentials to the material $PbTiO_3$. The potential forms include a Buckingham potential for all inter-species interactions, and a core-shell model for each species to model to polarizability of each atom. The core-shell model is a 4th order model. With these choices of potentials, there were 20 total parameters to fit. This fitting was done to first-principle calculations of effective charges, phonon calculations, and total structural energies using the minimization of a sum of squares. This mode is able to capture the thermal expansion effects on both the lattice structure and the spontaneous de-polarization of the material at finite temperature. However, the system is unstable in the cubic phase above 800K, which is an example of a typical limitation of interatomic potentials. The author's admit that this is a first generation potential, so it would be interesting to see if they have published any further results or other potentials.

The second part of this case study reviewed Quasi-continuum (QC) methods [2]. These methods combine atomistic modeling with continuum (finite element/difference) methods. The idea is to model "important" regions of the material in an atomistic way. These areas are typically things like material cracks or fractures, where a complete atomistic description is necessary to capture the physics of the phenomena. The most important part of a QC simulation is how the atomistic and continuum regimes of the simulation communicate with each other. One of the simplest methods is to "coarse-grain" a finite element/difference mesh over the atomistic domain, which allows the continuum to sample the atomistic regime. However, there are a number of ways to bridge the two regimes, and the reviewer notes that the best QC methods are usually problem dependent The use of QC for studying ferroelectrics was not discussed in the case study, which would have been an interesting topic. The case study was quite interesting and well done, although I would have liked to have seen a discussion of QC methods for studying ferroelectrics.

[1] Sepliarsky and Cohen. *Development of a shell model potential for molecular dynamics for PbTiO3 by fitting first principles results.* Fundamental Physics of Ferroelectrics, 2002, American Institute of Physics.

[2] Miller and Tadmor. *The Quasicontinuum Method: Overview, applications and current directions.* Journal of Computer-Aided Materials Design, 9: 203-239, 2002