Track 1: Fundamentals of Heat and Mass Transfer

1-3 Phase Change Phenomena and Heat Transfer

Abstract

**Development of a Shell Model for Ferroelectric Phase Change Material GeTe**

There is a pressing demand for higher density non-volatile memory (NVM) for electronics and computing applications ranging from personal MP3 players to high-performance supercomputers. A leading candidate to replace Flash (and other types of) memory is phase change (PC) memory. Phase change memory devices use Ge-Sb-Te (GST) compounds that exhibit several order of magnitude contrasts in both optical and electronic properties between their crystal and amorphous phases. Reading or writing binary information in these devices is a thermally driven process which “switches” (by melting) between the crystal and amorphous phases. Challenges remain, however, in optimizing the implementation of PC memory at large scales. Previous atomistic simulations of PCM materials have used computationally expensive quantum mechanics-based methods, restricting the simulations to tens of Angstroms and hundreds of picoseconds (several orders of magnitude less than the experimental scales). Thus, this study is concerned with the classical Molecular Dynamics (MD) simulation of PC materials.

With only two atoms per unit cell, GeTe is one of the simplest PC materials. It is also the simplest ferroelectric crystal. Ferroelectric crystals have applications in a number of technologies. Their pyroelectric properties are used in thermal and infrared sensors. Their high dielectric constants make them candidates to replace SiO2 in metal-oxide-semiconductor devices. Many ferroelectrics (such as GeTe) are also piezoelectrics, which find numerous applications as electro-mechanical transducers.

We present a first-generation set of inter-atomic potentials capable of describing GeTe’s elastic, ferroelectric, dielectric, and piezoelectric properties. Density Functional Theory (DFT) calculations provide the observables necessary to fit the inter-atomic potential parameters. This parameterization process is a multi-variable, non-linear fitting procedure based on the minimization of a sum-of-squares error. A core-shell model is used to describe the spontaneous polarization and the piezoelectric properties of the crystal. The results of the model are compared against the DFT calculations used to fit the potentials and also experimental data. *These potentials are then used in classical MD simulations to study PCM materials over the experimental length and time scales. The results will provide input to device-level models and insight to experimentalists designing new materials and devices.* (maybe too much?)