

Multi-Scale Modeling of Phase-Change Memory Materials

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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. There are several performance limitations with the current NVM market leader, Flash memory, particularly with respect to cycles per lost bit (cyclability) and in bit loss per year (retention) [1]. A leading candidate to replace Flash (and other types of) memory is phase change memory (PCM). 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 done by “switching” between the crystal and amorphous phases. Phase change memory is an order of magnitude faster than Flash, and has also proven to be robust in terms of cyclability and retention [1].

Challenges remain, however, in optimizing the implementation of PCM at large scales. Phase change memory devices are peculiar in that while their operation has been demonstrated, little is known about how/why they work as well as they do [2-4]. It is thus difficult to predict how the materials and devices might be improved. Atomic-level analysis can provide the required insight. 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) [4,9]. *The objective of this project is to build a framework for using classical Molecular Dynamics (MD) simulations to model PCM materials, allowing for simulation over the experimental length and time scales.*

Modeling PCM materials using MD simulation requires interatomic potentials to describe the interactions between Ge, Sb, and Te atoms. To parameterize these potentials, we use a multi-variable, non-linear fitting procedure based on the minimization of a sum-of-squares error. The sum-of-squares error is based on the difference between observable quantities and those quantities calculated from the fitted interatomic potentials. These observable quantities include high-level quantum mechanical DFT (Density Functional Theory) calculations as well as experimental data. This part of the project is in collaboration with Dr. Juarez L. F. Da Silva from the Institute of Physics of Sao Carlos (Brazil), who is an expert in quantum-level modeling of PCM materials [2,3].

Once accurate potentials are obtained, we will investigate structural and operational properties of PCM materials and devices, including: (i) The effect of homogeneous vs. heterogeneous nucleation on the speed of the read/write cycle [1], and (ii) The role played by vacancies in the phase change process [7,8]. With the ability to perform large atomistic level simulation, it will be possible to predict material performance subject to structural changes, which can inform novel device design. For example, $\text{Ge}_2\text{Sb}_2\text{Te}_5$ -(N-doped) $\text{Ge}_2\text{Sb}_2\text{Te}_5$ superlattices are being considered to reduce thermal conductivity, thus increasing Joule heating, lowering the power required for switching, and improving device efficiency [5,6]. An understanding of how structural effects reduce thermal conductivity will aid in the design of PCM devices and materials.

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Stuff to Include in Letter

Modeling PCM materials using MD simulation requires interatomic potentials to describe the interactions between Ge, Sb, and Te atoms. Such potentials do not exist. The formulation and validation of interatomic potentials is high risk and not of direct interest to funding agencies. The time scale for interatomic potential development is beyond the short horizon expected from semiconductor industry funding.

Atomistic simulation of PCM materials fits directly into CIT's nanotechnology initiative and is a focus of the Data Storage Systems Center (DSSC). This project is also aligned with ICES's Center for Multiscale Modeling for Engineering Materials (CM²EM) and Center for Nano-enabled Device and Energy Technologies (CNXT), both of which McGaughey is affiliated with. The work will provide a compelling example of multi-scale modeling by demonstrating how high-level (quantum) computational techniques can feed into and drive classical-level methods.