Large-Scale Molecular Modeling of Phase-Change Memory Materials

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Project Description

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. Progress in increasing memory density has followed the Moore's Law principle, with an effective doubling every few years. Sustaining this exponential increase in memory density with Flash memory, the current NVM market leader, is challenging due to the limits of feature sizes (~100 nm) capable with lithographic techniques [1]. Additionally, there are concerns with Flash memory's write/erase performance, 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. This process is thermally driven, so that understanding heat transfer mechanisms in PCM materials is critical to understanding their behavior and how it can be modified. The read/write process can be completed in less than 100 ns, an order of magnitude faster than Flash memory [1]. Phase change memory devices have 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.* The results will inform both materials design and experiment at the nanoscale.

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.

Approach and Methodology

We will first use high-level quantum mechanical calculations to parameterize a set of interatomic potentials for describing Ge-Sb-Te PCM materials. These potentials will then be used in classical MD simulations to study PCM materials over the experimental length and time scales. These two tasks are elaborated below. The results will provide input to device-level models and insight to experimentalists designing new materials and devices.

Density Functional Theory (DFT) calculations will first be used to map the energy surfaces of Ge-Sb-Te compounds. These energy surfaces will then be used, along with experimental data such as elastic constants and structural properties, to parameterize the interatomic potentials required for MD simulations. This parameterization process is 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 (DFT energies, experimental data) and those quantities calculated from the fitted interatomic potentials. This procedure is challenging due to the large number of fitted parameters required to formulate accurate potentials. 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]. The interatomic potentials will be validated against additional experimental data and quantum-level simulations [2-4,9].

We are currently using DFT calculations to parameterize a set of potentials for Ge-Te, which is used in many PCM devices and is a building block for Ge-Sb-Te compounds. Our first-generation potentials correctly predict the

structure of the crystal, amorphous, and liquid phases of Ge-Te. The methodology developed to generate the Ge-Te potentials will be of great use when developing potentials for the more complex Ge-Sb-Te compounds.

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, $Ge_2Sb_2Te_5$-(N-doped)$Ge_2Sb_2Te_5$ 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. The computational tools required for this part of the project (parallel MD codes, thermal transport/phonon analysis tools, etc.) are in place and ready to use in McGaughey's research group. All that is needed are the interatomic potentials.

Relationship to CIT/ICES Strategic Focus

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 (CM^2EM) 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.

Present and Future Funding

Preliminary funding for this project was through the PITA grant "Multi-scale modeling of phase change materials," with Jason Larkin as the supported graduate student. Jason initiated the collaboration with Dr. Juarez Da Silva from the Sao Paulo Institute of Physics, which been fruitful to date. He does not have support in place for the 2010-2011 academic year.

The Dowd fellowship will enable the team to complete the development of interatomic potentials for a wide range of Ge-Sb-Te materials. With these interatomic potentials in hand, the team will be competitive for funding from

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