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 a wide range of electronics and computing applications (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 (order 100 nm) capable with current 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) materials 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. The read/write process can be completed in less than 100 ns, an order of magnitude faster than flash memory [1]. PCM devices have also proven to be robust in terms of cyclability and retention [1].

There are still challenges, 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 and why they work as well as they do [2,3,4]. 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 mechanical-based methods, restricting the simulations to *10s* of Angstroms and *100s* of picoseconds (several orders of magnitude less than 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 time and length scales.* The results will inform both materials design and experiment at the nanoscale.

New interatomic potentials, which describe the interaction between atoms, are needed to model PCM materials using MD simulation. The formulation and validation of interatomic potentials is high risk and not of direct interest to funding agencies. The time scale for this development is also beyond the short horizon expected from semiconductor industry funding.

**Approach and Methodology**

We will 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 the operation and structure of PCM materials over experimental time and length scales, the results of which will provide input to device–level models and to experimentalists. This project will also provide a compelling example of multi-scale modeling, by demonstrating how higher-level (quantum) computational techniques can feed classical-level methods.

Density Functional Theory (DFT) calculations will first be used to measure the energy surfaces of PCM materials. These energy surfaces will then be used, along with experimental data, to parameterize the interatomic potentials required for MD simulations. 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]. These interatomic potentials will then be validated against both experimental data and higher-level quantum simulations [2,3,4,9]. The results of preliminary DFT calculations are currently being used to fit a set of potentials for Ge-Te. While many PCM devices use Ge-Te, it is also an important building block in Ge-Sb-Te alloys. Thus, the development of interatomic potentials for Ge-Te will be valuable for paramaterizing more complicated PCM alloys, which will begin in the next few months. Parameterizing and validating these interatomic potentials will constitute the focus of this project over the funding year.

Once accurate potentials are obtained, we will investigate the following operational and structural properties of PCM devices. The role of heterogeneous nucleation on the speed of the read/write cycle will be investigated [1]. In many PCM materials, vacancies play a significant role in the material’s performance [7,8]. With classical MD, the roles of these vacancies can be explored. With an atomistic level simulation, one can begin to predict performance subject to structural changes, which can inform novel device design. For example, the role of superlattice design on the thermal conductivity of PCM can be explored as a means to lower the power required in switching, improving the efficiency of devices [5,6].

**Relationship to CIT/ICES Strategic Focus**

Atomistic simulation of PCM materials fits directly into CIT’s nanotechnology initiative and is of interest to 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.

**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 has developed a first-generation interatomic potential for Ge-Te that correctly predicts the structure of the crystal, amorphous, and liquid phases. The methodology developed to produce the interatomic potentials for Ge-Te will be of great use when developing potentials for more complex Ge-Sb-Te alloys, which should begin in the next few months. Jason also initiated a 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 compounds. With these potentials in hand, the team will be competitive for funding from NSF’s Thermal Transport Processes (ENG-CBET) and Electronics, Photonics & Device Technologies (ENG-ECCS) programs, SRC’s Device Sciences – Modeling and Simulation program (a call will open in Spring 2011), and CMU’s DSSC. The team will collaborate with CMU’s Jim Bain (ECE, DSSC), who does experimental work on PCM materials and devices and Jon Malen (ME), who thermally characterizes micro- and nanoscale materials and devices. Together, they will apply for funding from NSF’s Interdisciplinary Research (IDR) program.

**References**

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While much research is being done experimentally here in the U.S. (and particularly here at CMU), the majority of PCM materials simulations are being done internationally. This project presents an opportunity to…**(more)**