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 capable with current lithographic techniques **[cite]**. 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) **[cite]**.

A leading candidate to replace flash (and other types of) memory is phase change memory (PCM) **[cite]**. 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 **[cite]**. PCM devices have also proven to be robust in terms of cyclability and retention **[cite]**.

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 **[cite]**. 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 hundreds of atoms and hundreds of picoseconds. *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 various aspects of PCM materials over experimental time and length scales. The results of the MD simulations will provide input to device–level models of PCM devices. This project will provide a compelling example of multi-scale modeling, by demonstrating how higher-level (quantum) computational techniques can feed classical-level methods, allowing for larger scale analysis.

Density Functional Theory (DFT) calculations will first be used to supply the quantum mechanical data to parameterize the interatomic 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. The results of preliminary DFT calculations are currently being used to fit a Ge-Te potential.

Once accurate potentials are obtained, we will investigate a number of interesting properties of PCM devices. For example, the role of heterogeneous nucleation on the speed of the read/write cycle. In many PCM materials, vacancies play a significant role in the material’s performance **[cite]**. With classical MD, the roles of these vacancies can be explored. With an atomistic level simulation, one can begin to predict the performance of PCM materials under a variety of operational conditions, which can inform novel device design.

**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 … 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.

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)**