**Project Title:**

Large-Scale Molecular Dynamics Modeling of Phase-Change Memory Materials

**Research Team:**

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(John Malen’s Group) **(more)**

**Project Description**

Over a wide range of computing applications (from personal MP3 players to high-performance supercomputers), there is a growing need for higher density (more GBytes/m2 or m3) non-volatile memory (NVM). Progress in the semiconductor industry, in terms of both computational speed and memory, has been dominated by the famous Moore’s Law principle, which is a generation by generation improvement of computational power. This principle leads to an effective doubling of computing power (in either speed or memory density) every few years. However, sustaining this exponential increase in memory density with the current NVM market leader (Flash memory) presents the same challenges that the semiconductor industry faces in general **[cite]**. This includes, primarily, the lower limits of feature sizes capable with current lithographic techniques, limiting the memory density of Flash devices **[cite]**. In addition to this, there are also general issues with Flash memory’s write/erase performance, in terms of both number of cycles per lost bit (cyclability) and in bit loss per year (retention) **[cite]**.

One of the leading candidates to replace Flash memory, and possibly a number of memories across a range of computing platforms, is Phase Change Memory (PCM) **[cite]**. PCM devices are based on a variety of materials which exhibit several order of magnitude contrasts in both optical and electronic properties between crystal and amorphous phases. Reading or writing binary information in these devices is done by “switching” between the crystal and amorphous phases. The entire read/write process can be done in less than 100 ns, which is at least an order of magnitude faster than Flash memory **[cite]**. PCM devices have also proven to be robust in terms of cycalbility and retention **[cite]**.

However, there are still a number of challenges in implementing PCM. PCM devices are peculiar in that the implementation has been proven, but very little is known about how and why these devices work as well as they do, particularly at the atomic scale **[cite]**. Thus, it is difficult to predict how these materials might be improved and/or optimized. This presents the need for an atomistic level description and analysis of these devices so that methods of device improvement can be identified. Currently, atomistic simulations of PCM materials are limited by computationally expensive quantum mechanical based methods. This project will utilize high-level ab-initio (quantum) calculations to perform classical Molecular Dynamics (MD) simulations of PCM materials, which will allow the simulation of these materials over experimental time and length scales.

**Approach and Methodology**

This project will use input data from high-level quantum mechanical calculations to parameterize a set of classical MD force-field potentials describing various PCM materials. These classical MD potentials will then be used in classical MD simulations to study various aspects of PCM materials over experimental time and length scales. This project will provide a compelling example of the way higher-level (quantum) computational techniques can feed classical-level methods, allowing for larger scale analysis. **(this section might be too specific, and I can re-word things to get rid of things like “classical MD force-field potentials”, etc.)**

Current computational power limits the ability of quantum methods in simulating PCM materials over experimental length and time scales. For example, one can perform a quantum MD simulation on a system of PCM containing less than 103 atoms for 100’s of ps **(too specific?)**, taking an entire month’s worth of computation time on a supercomputer. However, experimental length and timescales approach 100’s of nm and 100 ns, respectively. Thus, to probe interesting properties of Phase-Change materials at experimental conditions one must use a more cost-efficient simulation scheme. This is where classical MD will be used. The most important parts of classical MD simulations are the force-field potentials, and this will constitute the focus of this project over the funding year.

Density Functional Theory (DFT) calculations will be used to supply the quantum mechanical data to parameterize the force-field potentials. This part of the project is being done with the help of Dr. Juarez L. F. Da Silva at the Institute of Physics of Sao Carlos. Dr. DaSilva has worked on PCM materials for several years, specifically on the crystal structure of various PCM alloys, and his expertise will aid greatly in this part of the project. The majority of these DFT calculations have already been performed and testing has begun on the MD potentials. International collaboration…**(more)**.

Once appropriate potentials are obtained, the expertise of the Nanoscale Transport Phenomena Laboratory (NTPL) group will allow the project to investigate a number of interesting properties of PCM devices. For example, the role of heterogeneous nucleation on the speed of the read/write cycle can be examined **(too specific?)**. 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 **(too specific?)**. 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.

This project will also work closely with experimentalists working at Carnegie Mellon. The goal of performing classical MD simulations is to access experimental length and time scales for PCM. These simulations will work best when they can be informed and compared against actual experiments. There are two groups…**(more)** 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)**

**Relationship to CIT/ICES Strategic Focus**

This project’s focus falls under both CIT and ICES strategic focuses. Atomistic-level simulation (both quantum and classical) of PCM materials falls under the general focus of CIT’s nanotechnology initiative, in terms of both length scale and PCM materials as a data storage system. PCM materials could have an enormous impact over a wide range of computing memory applications. This project will show how atomistic-level simulations can inform both materials design and experiment at the nanoscale.

This project also presents an interesting example of how high-performance, multi-scale computing can play an important role in research. This part of the project fits in with ICES research initiative at the Center for Multiscale Modeling for Engineering Materials. This project will utilize quantum mechanical calculations to feed much faster, classical simulations. This will allow the simulation of large time (>100ns) and length (100’s of nm) scales. This project also presents an interesting example of the way different simulation schemes (quantum and classical) can work together. Bridging these two domains (quantum and classical) will require the understanding of a wide range of topics, including statistical mechanics, thermodynamics, quantum chemistry, and materials science.

**Present and Future Funding**

**Didn’t leave much room for this…will have to cut some above**