Multi-Scale Quantum Simulations of Conductive Bridging RAM

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INTRODUCTION

With shrinking sizes of transistors, scaling of memory devices has achieved great success these years. The conductive bridging RAM (CBRAM) as one of the emerging memory technologies has advantages over the flash memory on high scalability, low power consumption, high resistance ratio and long retention[1].

The basic cell of CBRAM is composed of a channel electrolyte between two metal electrodes. Under biases, atoms from the anode will turn into ions by oxidation reaction and diffuse through the solid electrolyte to the cathode. At cathode ions gain electrons and turn into atoms. The atoms start to form metallic conductive filaments from cathode. Devices will switch from high resistance to low resistance when the filaments keep growing and finally reach anode.

The conductance changes with respect to morphologies of conducting filaments are important for evaluating performance and reliability. Tunneling through electrolyte is potentially harmful for achieving high resistance ratio. Quantum simulations are important in predicting conductance changes in the switching processes.

METHODS

The electrochemical process modeling requires application of different physical models in different scales. The filament formation is simulated by molecular dynamics (MD) with the ReaxFF reactive force field [2-4]. Quantum transport is simulated with non-equilibrium Green's function [5].

The atom positions and the Mulliken charges calculated from charge equilibrium calculation under external electrochemical potentials are taken from the MD simulations. The charges are used to calculate the electrostatic potential with Poisson equation. The atomic charge density is assumed to have a Gaussian distribution centered at atom. Empirical Tight Binding Hamiltonian is constructed for an atomic configuration. The simulation flow is shown in Fig.1.

The device is partitioned into slabs based on coupling with the Breadth-first search method[6]. Such slab structure is suitable for transmission coefficient calculation with the recursive Green's function (RGF) technique. Because the charge self-consistent calculation is not required at this stage, only forward RGF is performed. The self energy is calculated with the Sancho-Rubio method[7].

The calculation is performed at Conte supercomputer. Each compute node is equipped with two 8-core Intel Xeon-E5 processors and two 60-core Xeon Phi coprocessors. The calculation is paralleled at each node with 2 MPI ranks and 8 OMP threads. The computationally heavy matrix operations have been offloaded to Xeon Phi coprocessors to gain maximum performance which gives speed up 3.2×. It takes roughly 800 seconds to finish 1 energy point on 1 MPI rank.

RESULTS

In this work, silicon oxide is considered as electrolyte sandwiched between electrodes made from Cu. Cu is parameterized with sp^3d^5 orbitals based on the environmental dependent empirical tight binding (ETB) model[8] with coupling up to 2nd nearest neighbor. The model has been optimized to match *ab-initio* bandstructure calculations of several ultra-thin nanowire unit cells.

SiO_2 parameterization is done with two crystalline forms (α-quartz and β-cristobalite) and used for the amorphous system as shown in Fig. 2. Interactions between Cu and O atoms are strong and favored in the interface relaxation. The Cu-O interaction is parameterized from Cu_2O.

The simulated structures contain 6651 atoms with a cross section of 4nm×4nm. The separation

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of two electrodes in the initial structure is 1.5nm as shown in Fig.3a. The filaments generated at different stages (t=0, 250, 500, 1000 ps in Fig. 3 a-d) from MD are taken as inputs for the ETB calculations for ballistic conductance. The time step for MD simulations is 0.5fs.

With the generated structures, current through the devices are calculated at V_d=-1V. Figure 4 shows the calculated current at different times at V_d=-1V and the transmission coefficient at t=0ps and 250ps. It is shown as soon as the Cu atoms start to form clusters inside SiO_2, the current increases. Current ratio of $I(t_0=0ps)/I(t_1=250ps)$ = 195 is obtained. When more filaments are constructed, the resistance is lowered and the current will keep increasing.

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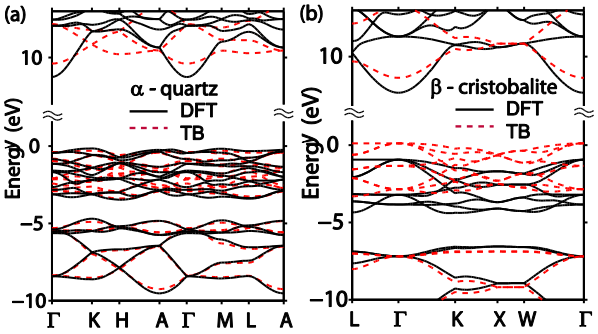

Figure 2 Bandstructure of (a) α-quartz and (b) β-cristobalite calculated with LDA and tight-binding.

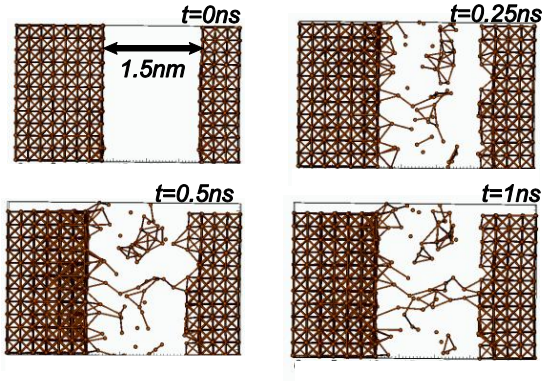

Figure 3 Diffusion of Cu atoms in SiO_2 at t=0, 250, 500, 1000ps. Si and O atoms are not plotted for better visibility. (a) Distance between electrodes is 1.5nm in initial structure. (b) Clusters are formed in SiO_2. Two electrodes are not connected by filaments. (c) Two electrodes are connected by Cu filaments. The connectivity is plotted based on a coupling radius of 0.39nm. (d) More filaments are formed.

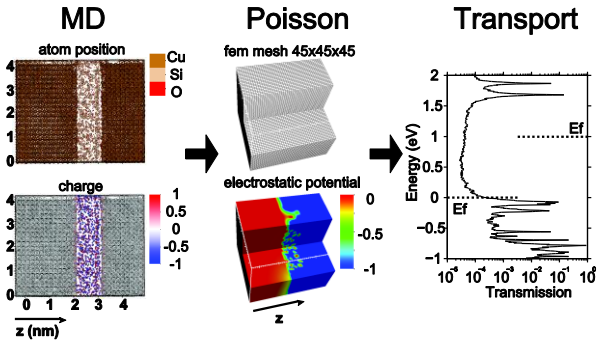

Figure 1 Simulation flow. Structures and charge profiles are generated by MD simulations. The electrostatic potential is calculated based on atomic charges. Current is calculated by NEGF and conductance is extracted.

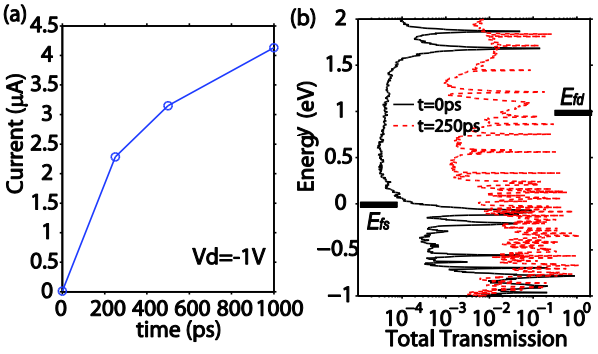

Figure 4 (a) Current for structures at Fig.3 at V_d=-1V. (b) Total transmission at t=0ps and t=250ps.

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