Ab-initio Modeling of CBRAM Cells: from Ballistic Transport Properties to Electro-Thermal Effects

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We present atomistic simulations of conductive bridging random access memory (CBRAM) cells from first-principles combining density-functional theory and the Non-equilibrium Green’s Function formalism. Realistic device structures with an atomic-scale filament connecting two metallic contacts have been constructed. Their transport properties have been studied in the ballistic limit and in the presence of electron-phonon scattering, showing good agreement with experimental data. It has been found that the relocation of few atoms is sufficient to change the resistance of the CBRAM by 6 orders of magnitude, that the electron trajectories strongly depend on the filament morphology, and that self-heating does not affect the device performance at currents below 1 \( \mu \)A.
I. INTRODUCTION

The $I$-$V$ characteristics and non-volatile storage capability of conductive bridging random access memories (CBRAM) strongly depend on the atomic properties of the underlying nano-filaments that form between two metallic plates through a dielectric layer. Due to the extremely narrow dimensions of these filaments, high current densities are expected, with potentially significant self-heating effects. To design better performing CBRAM cells it is therefore critical to precisely understand the interplay between electron transport and atom positions as well as their influence on temperature.

Device simulations can address this issue and give insight into the functionality of CBRAMs, provided that the following two modeling challenges are resolved. First, tools that can handle realistically extended structures rely on classical physics, they do not capture the atomic granularity of filaments, and they require several material parameters as inputs. Secondly, quantum mechanical solvers based on \textit{ab-initio} methods do not suffer from these limitations, but they are restricted to systems made of a couple hundred atoms, either with ballistic transport or simple scattering approaches.

Advanced physical models that combine density-functional theory (DFT) and the Non-equilibrium Green's Function (NEGF) formalism have been developed here to eliminate these bottlenecks and demonstrate the first atomistic quantum transport calculations of realistic CBRAMs, as depicted in Fig. 1. For that purpose, structures with up to 4500 atoms have been carefully constructed and simulated in the ballistic limit and with coupled electron-phonon transport. These breakthroughs have been the key to obtain results in good agreement with experiments, to identify possible electron trajectories through the studied device, to shed light on the nano-filament dissolution process, to assess the power dissipated in the cell, and to determine the lattice temperature of each atom.

II. APPROACH

Since the goal of this paper is not to simulate the growth of metallic nano-filaments, but to study the transport properties of CBRAM cells, the first modeling step consists in creating practical device structures made up of two copper contacts separated by a slab of amorphous silicon dioxide (a-SiO$_2$). This layer has been generated by a melt-and-quench
approach using classical force-field molecular dynamics routines from the ATK tool and a 
\(\beta\)-cristobalite SiO\(_2\) crystal of 1080 atoms as starting point. The final configuration has been 
relaxed with DFT using the CP2K package before attaching Cu contacts to the a-SiO\(_2\) and 
inserting a conical nano-filament by replacing the silicon and oxygen atoms with Cu. The 
resulting structure has been further relaxed and annealed for several ps with DFT. Two 
examples composed of about 4500 atoms are reported in Fig. 2.

As next step, the Hamiltonian \(H\) and overlap \(S\) matrices of the produced CBRAMs 
have been prepared by CP2K using contracted Gaussian-type orbitals as basis set, PBE 
exchange-correlation functional, and GTH pseudopotentials. These matrices have then 
been loaded into a quantum mechanical device simulator to compute the ballistic transport 
characteristics of the corresponding structures. While double-zeta valence polarized (DZVP) 
basis sets are known to be more accurate than single-zeta valence (SZV) or 3SP ones, 
they induce much larger computational burden. In Fig. 3(a-b) it is however shown that 
for the considered cells, the electron transmission function as calculated with a SZV+3SP 
combination agrees well with the one from DZVP, thus justifying the usage of the lighter 
basis set.

Finally, to go beyond ballistic transport and account for electro-thermal effects, the 
dynamical matrix (DM) of the systems in Fig. 2 has also been calculated using the frozen-
phonon approach of ATK and the reactive force-field (reaxFF) parameters of Ref. 11. With 
the DM, the phonon transmission function can be evaluated, as indicated in Fig. 3(c). More 
importantly, if the derivatives of \(H\) and \(S\) are also built with CP2K, all necessary quantities 
are available to solve the electron and phonon Green’s Functions and to self-consistently 
couple them via scattering self-energies. This has been done here to gain access to the 
lattice temperature distribution inside atomic-scale CBRAM cells.

III. RESULTS

First, the ballistic current flowing through the CBRAM in Fig. 2(b) has been computed 
and is displayed in Fig. 4(a) in the form of the conductance \(G\). The obtained low resistance 
state (LRS) value \(G = 0.32\ G_0\) (\(G_0\): conductance quantum), falls exactly in the same range 
as the one measured from the experimental device in Fig. 1. This is a strong indication that 
the technique used to generate the atomic systems gives rise to realistic filament geometries.

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Since CBRAMs usually operate between a low and high resistance state (HRS), we have tried to establish how many Cu atoms should move away from the filament tip to enable a LRS→HRS transition. Starting from the structure in Fig. 2(b), the far most right filament atoms have been removed one-by-one and the conductance at each step simulated. The results in Fig. 4(a) reveal that 20 atoms must be relocated and a gap of 1.5 nm created to go from the LRS to the HRS. Furthermore, the conductance of the decreasing nano-filament exhibits several plateaus, in qualitative agreement with experiments (see inset of Fig. 4(a)), suggesting that the removal of some atoms is more critical than others. This is confirmed by the current map reported in Fig. 4(b): it can be clearly seen that electrons follow curly paths and avoid certain filament regions. As a consequence, the presence or absence of atoms carrying little current does not affect the overall device conductance.

The \( I-V \) characteristics of the investigated CBRAM can be found in Fig. 5(a) for the LRS up to \( V=0.2 \) V, both in the ballistic limit and with coupled electron-phonon transport, assuming a linear potential drop between the contacts. The ballistic resistance/conductance is obviously not constant and changes as a function of the applied voltage, contrary to the one obtained in the presence of electron-phonon interactions. Turning on scattering decreases the low voltage \( G \) from 0.32 to 0.22 \( G_0 \). It can therefore be estimated that the simulated device operates at about 70\% of its ballistic limit. Note that \( G=0.22 G_0 \) is still in the experimental range (see Fig. 1).

By coupling electron and phonon transport, the power dissipated inside the CBRAM can be accurately determined from the difference in thermal energy current between the left and right contacts. An effective lattice temperature can also be derived for each atom from the non-equilibrium phonon population. Collecting these data requires that the electrical and energy currents are conserved, which has been verified in the present case. The dissipated power \( P_{\text{diss}} \) and maximum average temperature \( T_{\text{max,avg}} \) are plotted in Fig. 5(b) as a function of the current \( I_0 \): both quantities behave as predicted by simpler physical models, i.e. they increase quadratically with the current. Up to a current \( I_0=1 \) µA, \( P_{\text{diss}} \) and \( T_{\text{max,avg}} \) do not exceed 10 nW and 305 K, respectively, so that self-heating is almost negligible. Past this point, the situation rapidly deteriorates as \( I_0 \) increases.

The simulated dissipated power obeys a \( P_{\text{diss}}=\alpha \cdot R \cdot I_0^2 \) rule with the CBRAM LRS resistance \( R=58 \) kΩ. The pre-factor \( \alpha=0.16 \) indicates that only 16\% of the injected electrical power is converted into heat inside the simulation domain, the rest being wasted in the right
contact and having a limited impact on the nano-filament dynamics. The reason behind \(\alpha < 1\) can be inferred from the spectral current distribution in Fig. 5(c). At the applied voltage \(V = 0.2\) V, electrons should undergo an energy relaxation of 200 meV corresponding to the Fermi level difference. However, the distance between both electrodes is too short for electrons to emit enough phonons and dissipate the expected energy.

The relationship between \(T_{\text{max,avg}}\) and the electrical current \(I_0\) can be fitted with the following quadratic function
\[
T_{\text{max,avg}} = T_0 + R_{\text{th}} \cdot R \cdot I_0^2,
\]
where \(T_0 = 300\) K is the room temperature. A thermal resistance \(R_{\text{th}} = 68\) K/\(\mu\)W can be extracted from the simulation data. In the fitting procedure, it is crucial to consider the average temperature, and not individual values because large variations may occur between the coldest and hottest atoms situated in the same segment of length \(dx = 0.2\) nm along the \(x\) direction, as can be observed in Fig. 6(a). In particular, the lattice temperature of the Cu atoms forming the nano-filament tends to be much higher than that of the left and right contacts and of the SiO\(_2\) matrix. With this respect, Fig. 6(b) distinctly shows that a local hot spot is situated in the middle and second half of the filament, where the hottest atoms have temperatures up to 40 K larger than the average of their immediate surrounding. At high current densities these particles might acquire enough energy to change site, alter the filament geometry, and destroy its conductivity in the process. As a side note, it should be emphasized that classical simulation approaches using the same relation as above to model \(T_{\text{max,avg}}\) cannot properly describe the large, atomic-scale temperature variations of Fig. 6(b) and might underestimate the influence of self-heating.

IV. CONCLUSION

We have studied the electrical and thermal properties of a realistic conductive bridging random access memory cell from first-principles with a state-of-the-art solver based on DFT and NEGF. By coupling electron and phonon transport we could enlighten the mechanisms that limit the performance of such nano-devices. As possible design improvement, it appears that bringing closer to each other the two metallic electrodes that surround the central dielectric layer, although technologically not evident, would reduce the nano-filament length and thus prevent electrons from emitting enough phonons to significantly contribute to self-heating.
ACKNOWLEDGMENT

This work was supported by the Werner Siemens Stiftung, by SNF under Grant No. PP00P2_159314, by ETH Research Grant ETH-35 15-2, and by a grant from the Swiss National Supercomputing Centre (CSCS) under Project s714.

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FIG. 1. (a) Scanning electron microscope view of a Cu-SiO$_2$-Pt conductive bridging random access memory (CBRAM) cell that was fabricated on a silicon-on-insulator wafer with a 220 nm thick silicon layer and a 3 µm-thick buried oxide. A 3D atomic point contact was created in the middle via local oxidation of silicon to precisely control the location of the forming metallic nano-filament. The Cu and Pt contacts were deposited using a sequence of e-beam lithography, e-beam evaporation, and lift-off processes. (b) Illustration of the central active region of the CBRAM structure. The separation between the Cu and Pt layers can be made as thin as 15 nm and is filled with SiO$_2$. The device is put in series with a resistance to limit the current magnitude. A DC voltage is applied to the Cu contact, while the Pt one remains grounded. This bias triggers the growth of a Cu nano-filament through the SiO$_2$ matrix, starting from the Pt side. (c) Extracted conductance $G$ vs. voltage $V$ (as a function of the conductance quantum $G_0$) for the Cu-SiO$_2$-Pt CBRAM in (a) and (b). 30 set/reset hysteretic cycles of a single device are reported. The two red dots refer to the low and high resistance states of the structures shown in Fig. 2.
FIG. 2. Schematic view of the 3-D atomic structures considered in this work. Contrary to the experimental device, they are composed of two 4.25 nm long, $<111>$-oriented copper metallic plates (instead of platinum on the left) surrounding a 3.5 nm long SiO$_2$ matrix through which a Cu nano-filament growths and dissolves upon application of an external voltage $V$. The cross section along the $y$ and $z$ axes (assumed periodic) measures 2.34×2.38 nm$^2$, respectively. Each structure is composed of roughly 4500 atoms, where the large gray spheres represent Cu atoms, the small orange ones either Si or O. (a) Incomplete nano-filament with a gap $\Delta L=1$ nm between its end and the active Cu plate. (b) Full, cone-shaped nano-filament made of 96 Cu atoms.

FIG. 3. (a) Energy-resolved electron transmission function $T(E)$ through the incomplete nano-filament from Fig. 2(a) with $\Delta L=1$ nm and 9 atoms missing (87 instead of 96 Cu atoms). The reported data were computed with a Hamiltonian matrix created by CP2K and expressed in either a double-zeta valence polarized (DZVP, solid blue line) basis set or a combination of 3SP for the Si and O atoms and single-zeta valence (SZV) for the Cu ones (dashed red line). Note that the Fermi level energy was shifted to $E=0$. (b) Same as (a), but for the complete nano-filament from Fig. 2(b). (c) Phonon transmission function through the same structure as in (b) with the dynamical matrix obtained from a reactive force field (reaxFF) model with the parameters from Ref. 11.
FIG. 4. (a) Ballistic conductance $G$ extracted from the CBRAM cell in Fig. 2(b) as a function of the number of Cu atoms removed from the filament extremity. By gradually expelling the far most right filament atom, a gap of length $\Delta L$, as sketched in Fig. 2(a), opens up and leads to a step-like reduction of $G$, as in experiments (see inset: zoom in of the area of filament removal in Fig. 1(c)). About 20 atoms must be removed to go from the LRS ($G=0.32 G_0$) to the HRS ($G=4e-7 G_0$). (b) Ballistic current map through the same CBRAM as before under the application of an external voltage $V=1$ mV. The blue and red lines illustrate the electron trajectories, as computed from quantum transport, while the gray dots refer to Cu atoms, the orange ones, to Si and O.
FIG. 5. (a) Current vs. voltage characteristics of the CBRAM cell in Fig. 2(b) in the LRS. The current in the ballistic limit (blue curve with circles) and as obtained with coupled electro-thermal transport (red curve with triangles) are reported, together with the corresponding conductance values. (b) Power dissipated inside the same structure as before ($P_{\text{diss}}$, left y-axis) and average maximum lattice temperature ($T_{\text{max}}$, right y-axis) as a function of the electrical current $I_0$. The simulated power (black squares) follows a $P_{\text{diss}}=\alpha \cdot R \cdot I_0^2$ relationship (solid blue curve), where $\alpha=0.16$ is the amount of power dissipated inside the simulation domain (the rest is wasted in the contacts) and $R=58$ kΩ is the LRS device resistance. The simulated temperature (black triangles, see Fig. 6(a) for the exact definition) exhibits a similar quadratic behavior $T_{\text{max}}=T_0+R_{\text{th}} \cdot R \cdot I_0^2$ (dashed red curve), with $T_0=300$ K and $R_{\text{th}}=68$ K/μW as the fitted thermal resistance. (c) Spectral current (current as a function of position and energy) for the device in (a) and (b), in the presence of electron-phonon scattering ($V=0.2$ V). Red indicates high current concentrations, green no current. The left and right contact Fermi levels ($E_{FL}$ and $E_{FR}$) are indicated.
FIG. 6. (a) Atomically resolved lattice temperature as a function of the $x$-coordinate of each atom for the device from Fig. 2(b) at $V=0.1$ (blue symbols) and 0.2 V (red symbols). The Cu atoms forming the central nano-filament are marked with larger circles. The thin black lines show the average lattice temperatures, as computed by averaging the temperature of all atoms present in a segment of length $dx=0.2$ nm along the $x$-axis. Their maximum, $T_{\text{max,avg}}$, are indicated and reported in Fig. 5(b). (b) Same as (a), but with the color of the atoms directly representing their lattice temperature at $V=0.2$ V.