Design of ReRAM Cell Structure by Metal Buffer and Contact Engineering via First-Principles Transport Calculation

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ABSTRACT

We performed first principles simulation of ReRAM cell, which consists of HfO_2 conductor and TiN electrodes. To analyze the transport mechanism of low/high resistive (ON/OFF) states, we examined several model structures of HfO_x filaments. We found that the oxidized contact effect by scavenged oxygen affects transport mechanism. Inelastic current by electron-phonon scattering was evaluated based on the first principles nonequilibrium Green's function theory (NEGF)[1] to argue transport mechanism. Then we proposed *insertion of thin metal buffer layer* to control the oxidized contact effects.

INTRODUCTION

Resistive random access memory (ReRAM) is one of the most promising next-generation memory technologies. In order for fast switching and electric power saving, distinct ON/OFF-*IV* in low *V* are desired for sub 10 nm scale device. In the present study, we show that the oxidized contact effect by ON/OFF redox process controls the conductive channel wavefunctions directly and its impact to distinct ON/OFF *IV* and inelastic processes via first-principles approach.

RERAM CELL MODEL

We first analyzed $TiN/HfO_x/TiN$ (Fig. 1) ReRAM cell. We define the minimum cell (unit "bin") of $TiN/HfO_2/TiN$, and extended the ReRAM cell to 2x2 bins supercell structure. By moving O ions from each bin to TiN surface, we made some conductive filament models in the cell. In Fig. 2, our first-principles ballistic *IV* is presented, where four bins have equivalent ON states ($HfO_{1.33}$) in the cell. Although the bulk $HfO_{1.33}$ has metallic character, ON/OFF *IV* distinction is not clear because of very low ballistic *I*. By filtered electron density analysis, we found that the conductive channel is terminated partially by TiN-O interaction (Fig. 3). When the ON state filament is modeled by two bins of $HfO_{0.89}$ and two OFF bins (i.e., locally V_O density is concentrated), the ballistic current increased rapidly. However, our inelastic transport calculations showed that temperature dependence of resistance is still semiconductor-like due to the oxidized contact.

To focus on the oxidized contact effect, we examined insertion of thin metal buffer layer ($\mathbf{M_B}$). In Fig. 4, *IV* of the cell consisting of four $HfO_{1.33}$ bins with $\mathbf{M_B}$=Hf, is presented. The conducting site energies were rigorously calculated by *complex energies* based on NEGF and effective MPSH.[2] They tell us which energy levels are conductive channels quantitatively (Fig. 5)

CONCLUSION

Our simulation suggests that avoiding localization of conducting wavefunctions at the oxidized interface is critical to obtain distinct ON/OFF *IV* and its temperature dependence. We suggest the following guiding principles to design thin buffer material in ReRAM cell: the oxidized contact effect can be suppressed when "free" $\mathbf{M_B}$O compound has sufficiently delocalized LUMO+1 (or slightly higher energy MOs) .

REFERENCES

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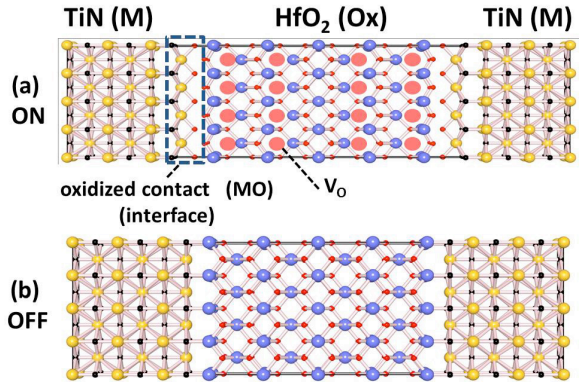

Figure 1. The models of the ReRAM cell, /TiN/HfO_2/TiN for ON (a) and OFF states (b). HfO_2 insulator of OFF state was set to stoichiometric and cubic HfO_2. Vacancies V_O's are created in each bin of HfO_2 insulator to represent ON and the relating O ions are scavenged at the TiN electrodes. Large blue, yellow, and thin red circles represent Hf, Ti, and V_O, respectively. Small red and black circles are O and N atoms. The cell consits of four bins (mínimum unit cells)

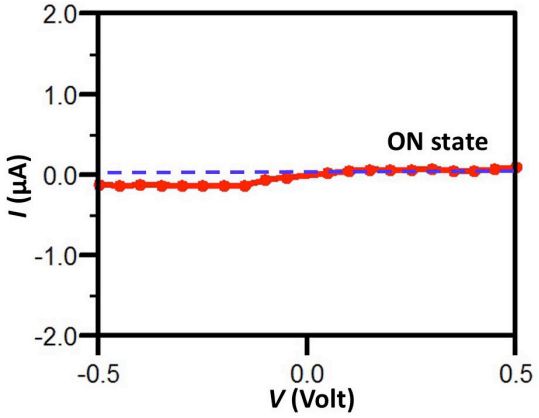

Figure 2. First principles *IV* characteristics of ON state (red line and diamonds) of TiN/HfO_2/TiN cell for the model in Fig. 1. As reference, plot of zero current profile is inserted in the figure as blue dot line.

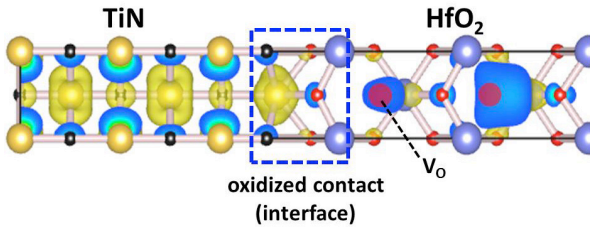

Figure 3. The electron density filtered by energy range $[E_F - 0.5\text{eV}, E_F + 0.5\text{eV}]$ for ON state of TiN/HfO_2/TiN. V_O's make conduction pathway as expected. However, Electron density is close to 0 at the interface of the TiN and HfO_2, and electric transport pathway is disconnected.

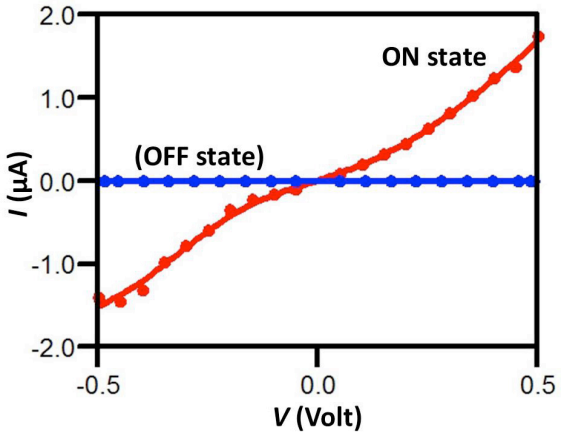

Figure 4. First principles *IV* characteristics of ON (red line and diamonds) and OFF states (blue line and diamonds) of TiN/Hf/HfO_2/Hf/TiN cell. Electric current per the unit cell of ON state is much larger (*ca* 730 %) than that of "without $\mathbf{M_B}$" given in Fig. 2 while the leak current of OFF state is sufficiently

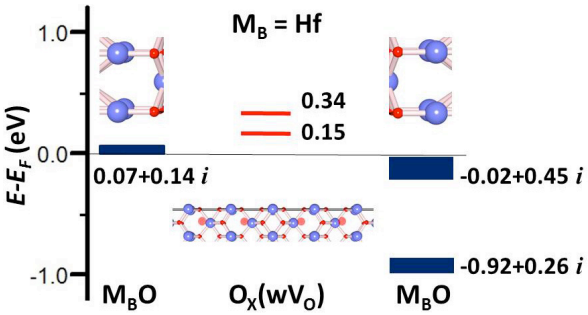

Figure 5. The complex site energy diagram of ON state of TiN/Hf/HfO_2/Hf/TiN calculated by effective MPSH, where bias 0.2 Volt is applied. (Positive bias is set to the direction from the left to right electrode.) The thickness of the bar of the left and right oxidized contact sites ($\mathbf{M_B}$O) represents electronic coupling strength with TiN bulk electrode, i.e., imaginary part of site energy.