Stochastic Modeling of the Resistive Switching Mechanism in Oxide-Based Memory

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***Abstract*-We have investigated a stochastic model of the resistive switching mechanism in resistive random access memory (RRAM) based on electron hopping. The distribution of electron occupation probabilities analyzed with our approach is in good agreement with previous work. In particular, a low occupation region is formed near the cathode for bipolar behavior or near the anode for unipolar behavior. Our simulation of the temperature dependence of the electron occupation probability near the anode and the cathode shows an amazing stability of the low occupation region. This result indicates high robustness of failure-free RRAM switching from a state with low resistance to a state with high resistance for elevated temperature.**

I. INTRODUCTION

With memories based on charge storage (such as DRAM, flash memory, and others) approaching the physical limits of scalability, research on new memory structures has significantly accelerated. Several concepts as potential replacements of the charge memory were invented and developed. Some of the technologies are already available as prototype (such as carbon nanotube RAM (NRAM), copper bridge RAM (CBRAM)), others as product (phase change RAM (PCRAM), magnetoresistive RAM (MRAM), ferroelectric RAM (FRAM)), while the technologies of spin-torque transfer RAM (STTRAM), racetrack memory, and resistive RAM (RRAM) are under research. A new type of memory must exhibit low operating voltages, low power consumption, high operation speed, long retention time, high endurance, simple structure, and small size [1], [2].

One of the most promising candidates for future universal memory is the RRAM. Resistive switching phenomena are observed in several metal oxides, such as TiO_2 [3], HfO_2 [4], Cu_xO [5], NiO [6], ZnO [7] and perovskite oxides, such as doped $SrTiO_3$ [8], doped $SrZrO_3$ [9], $Pr_{1-x}Ca_xMnO_3$ [10]. This type of memory is characterized by low operating voltage (<2V), fast switching time (<10 ns), high density, excellent scalability, long retention time, and simple structure. On the other hand, RRAM devices have not demonstrated yet sufficient endurance. Unless this problem can be solved, this technology is unlikely to be brought to market in the 2020 timeframe [2].

In the literature a broad spectrum of electronic and/or ionic switching mechanisms for oxide-based memory has been suggested: a model based on trapping of charge carries [11], electrochemical migration of oxygen vacancies [12], [13], electrochemical migration of oxygen ions [14], [15], a unified physical model [16], a domain model [17], a filament anodization model [18], a thermal dissolution model [19], and others. However, a proper fundamental understanding of the switching mechanism is still missing and is thus a high priority task.

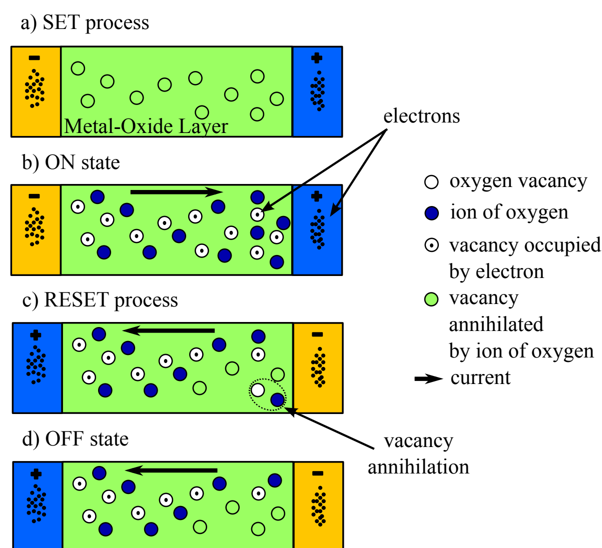

Fig. 1. Schematic illustration of the resistive switching mechanism in bipolar oxide-based memory cell: (a) Schematic illustration of the SET process. (b) Schematic view of the conducting filament in the low resistance state (ON state). (c) Schematic illustration of the RESET process. (d) Schematic view of the conducting filament in the high resistance state (OFF state). Only the oxygen vacancies and ions that impact the resistive switching are shown.

In this work we present a stochastic model of the resistive switching mechanism based on electron hopping between the oxygen vacancies along the conductive filament in an oxide-layer.

II. MODEL DESCRIPTION

We associate the resistive switching behavior in oxide-based memory with the formation and rupture of a conductive filament (CF). The CF is formed by localized oxygen vacancies (V_o) [16] or domains of V_o. The conduction is due to electron hopping between these V_o. Fig. 1 shows schematic illustration of the resistive switching mechanism in bipolar oxide-based memory. Formation and rupture of a CF is due to a redox reaction in the oxide layer under a voltage bias. If a positive voltage is

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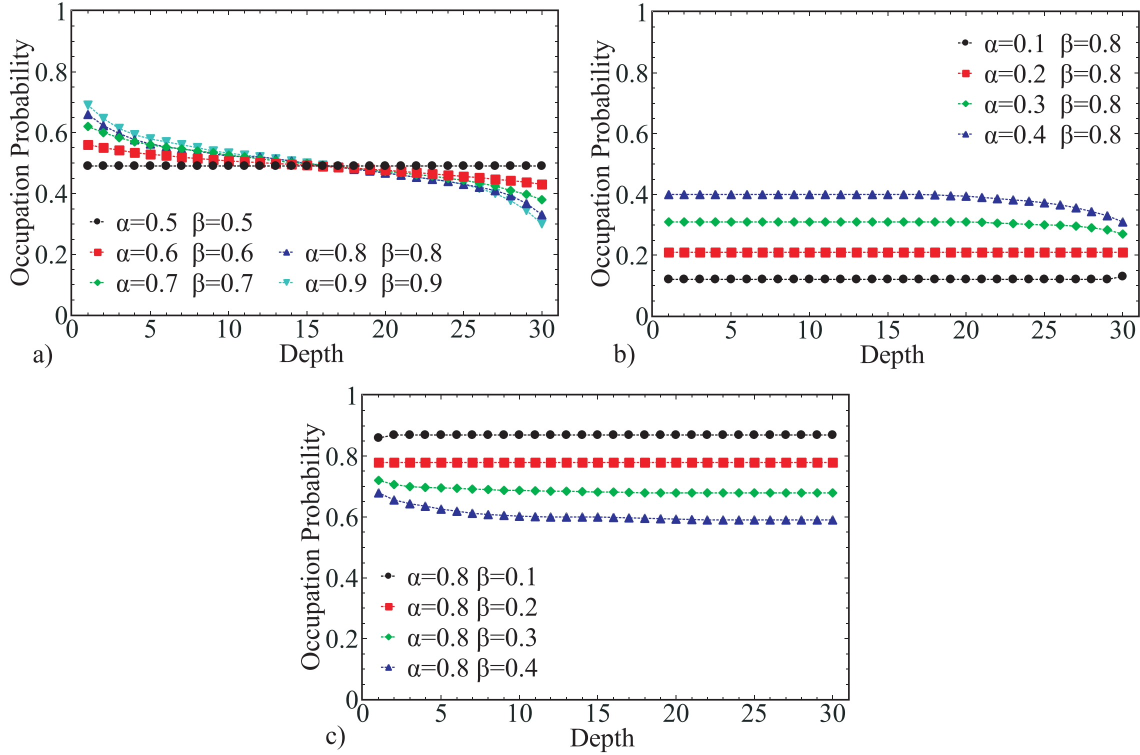

Fig. 2. Calculated distribution of electron occupation probabilities for unidirectional next nearest neighbor hopping between the V_o (the 1st V_o is near the cathode, the last V_o is near the anode): (a) α>0.5 and β>0.5, p_c=0.5; (b) α<0.5 and α<β, p_c=α; (c) β<0.5 and β<α, p_c=1-β.

applied, the formation of a CF begins, when the voltage reaches a critical value sufficient to create V_o by moving oxygen ion (O^{2-}) to an interstitial position. This leads to a sharp increase in the current signifying a transition to a state with low resistance. If a reverse negative voltage is applied, the current increases linearly, until the applied voltage reaches the value at which annihilation of V_o is triggered by means of moving O^{2-} to V_o. The CF is ruptured and so the current decreases. This is the transition to a state with high resistance.

If the CF is formed, the following events can happen:

1) an electron hops into an V_o from an electrode;
2) an electron hops from an V_o to an electrode;
3) an electron hops between two V_o.

In order to model the dependence of transport on the applied voltage and temperature we choose the hopping rates as [20]:

$$\Gamma_{nm} = A_e \cdot \frac{dE}{1-\exp(-dE/T)} \cdot \exp(-R_{nm}/a), \quad (1)$$

Here, dE is the difference between the energies of an electron on sites n and m, R_{nm} is the hopping distance, a is the localization radius. The hopping rates between an electrode (0 or N+1) and an oxygen vacancy m are described as [16]:

$$\Gamma_m^{iC} = \alpha \cdot \Gamma_{0m}, \; \Gamma_m^{oC} = \alpha \cdot \Gamma_{m0}, \quad (2)$$

$$\Gamma_m^{iA} = \beta \cdot \Gamma_{(N+1)m}, \; \Gamma_m^{oA} = \beta \cdot \Gamma_{m(N+1)}, \quad (3)$$

Here, α and β are the coefficient of the boundary conditions on the cathode and anode, respectively, N is the number of sites, A and C stand for cathode and anode, and i and o for hopping on the site and out from the site, respectively.

III. Model verification

To verify the proposed model, we first evaluate the average electron occupations of hopping sites under different conditions. Then we simulate the temperature dependence of the electron occupation probabilities near the anode and the cathode.

For comparison with previous works the calculations are made on a one-dimensional lattice consisting of thirty equivalent, equidistantly positioned hopping sites V_o. All V_o are at the same energy level, if no voltage or temperature is applied. To simplify the calculations we assume that the oxygen vacancy is either empty or occupied by one electron [16].

A. Calculation of electron occupation probability

Following [21], we first allow hopping in one direction and only to/from the closest V_o. Each site i of a one-dimensional lattice of N sites is either occupied by an electron or empty; during a time interval dt, each electron has a probability Γ_{nm} of hopping to its right, provided the target site is empty; moreover, during the time interval dt, an electron may enter the lattice at Site 1 with probability $\alpha \cdot \Gamma_{01}$ (if this site is empty) and an electron at Site N may leave the lattice with probability $\beta \cdot \Gamma_{N(N+1)}$ (if this site is occupied). The occupation probability of a central V_o (p_c) is described, depending on the boundary conditions, as follows: 1) for α>0.5 and β>0.5, p_c=0.5; 2) for α<0.5 and α<β, p_c=α; 3) for β<0.5 and β<α, p_c=1-β. Fig.2 shows simulation

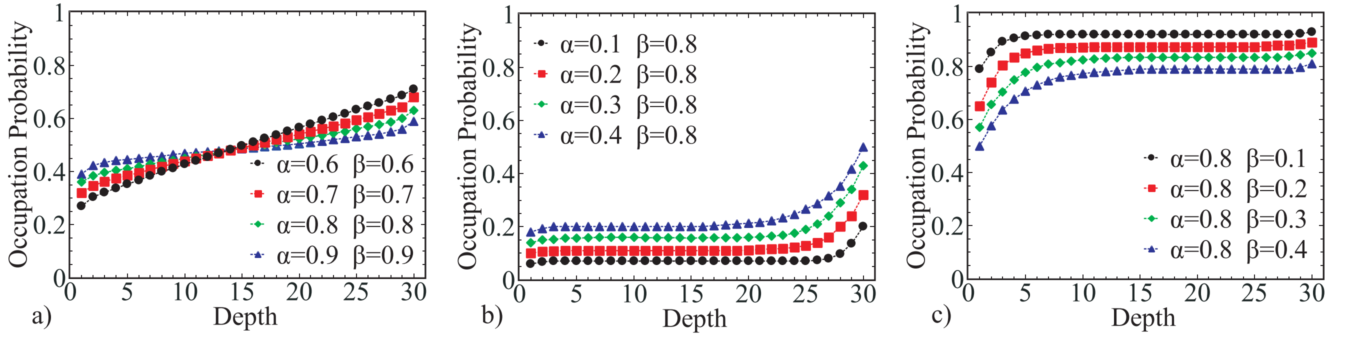

Fig. 3. Calculated distribution of electron occupation probabilities, if unidirectional hopping is allowed not only to/from the closest V_o: (a) α>0,5 and β>0,5; (b) α<0,5 and α<β; (c) β<0,5 and β<α.

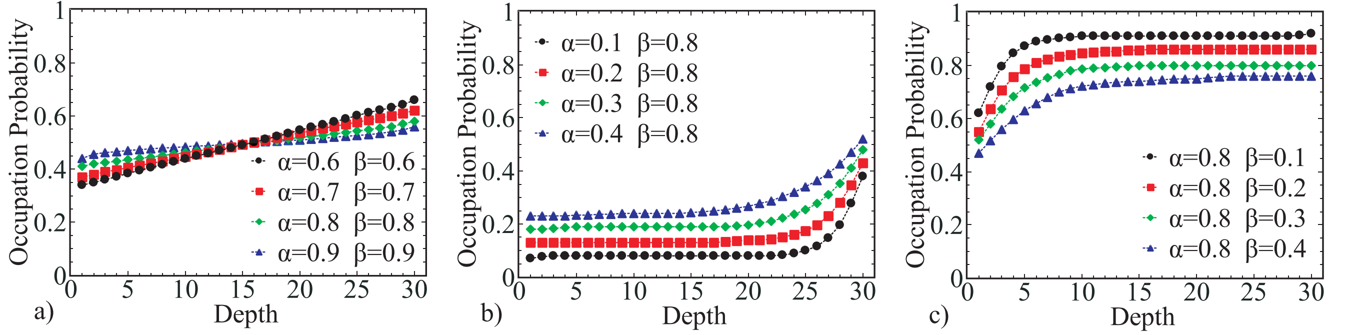

Fig.4. Calculated distribution of electron occupation probabilities for hopping according to (1-3) for T>0: (a) α>0,5 and β>0,5; (b) α<0,5 and α<β; (c) β<0,5 and β<α.

results of the stochastic model, which fully coincide with theoretical calculations [21].

To move from the model systems [21] to more realistic systems, we calculated the distribution of electron occupations for a chain, where hopping is allowed not only to/from the nearest V_o (Fig. 3), and for systems with T>0, where hopping (1-3) is allowed in both directions (Fig. 4). Note that for α>0.5and β>0.5 (Fig. 3a and Fig. 4a) we still have p_c=0.5 in the center, while for other values α, β we observe a decrease in p_c for α<β and an increase in p_c for β<α.

We have calibrated the model in a manner to reproduce the results reported in [16], for V=0.4 V to V=1.6 V. Fig. 5(a) shows a case, where the hopping rate between the electrodes and V_o is larger than the rate between the two V_o (i.e. α, β > 1). In this case the low occupation region is formed near the anode (unipolar behavior).

Fig. 5(b) shows a case, where the hopping rate between the two V_o is larger than the rate between the electrodes and V_o (i.e. α, β < 1). In this case the low occupation region is formed near the cathode (bipolar behavior).

In practice, the values of the coefficients of the boundary conditions are determined by the condition of separation of physical environments, i.e. by the materials from which the electrode and the oxide-layer are made. A dependence of resistive switching on the electrode material was recently reported in research for ZrO_2 [22] and TiO_2 [23].

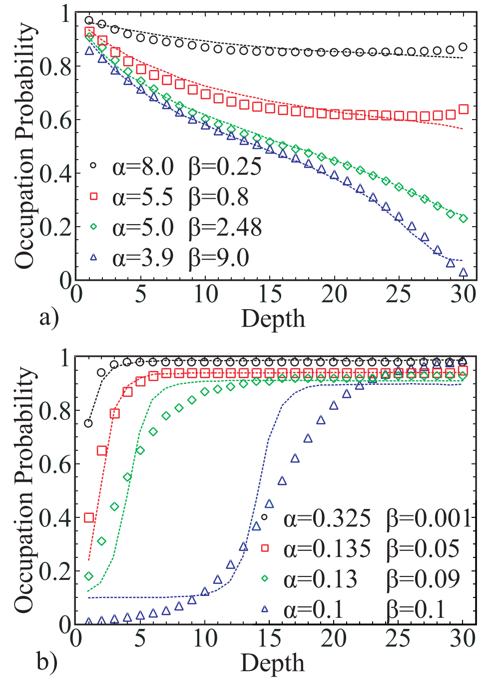

Fig. 5. Calculated distribution of electron occupation probabilities under different biasing voltages. Lines are from [16], symbols are obtained from our stochastic model.

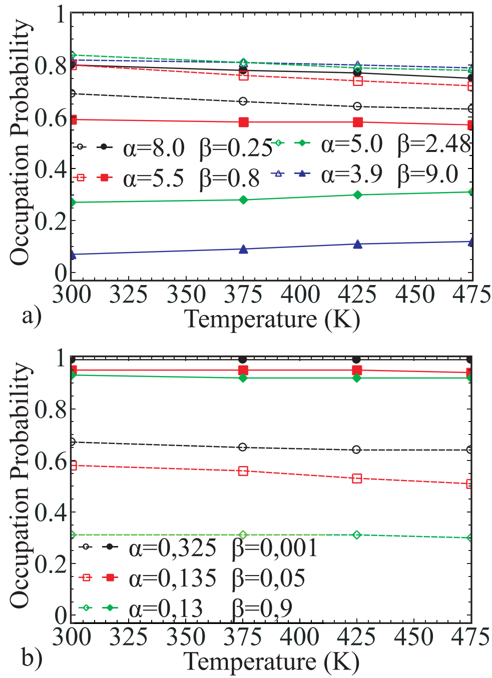

Fig. 6. Temperature dependence of electron occupation probability near the anode (filled symbols) and the cathode (open symbols).

B. Modeling of temperature dependence

Following [16] the rupture of the CF is possible only in the low occupation region. In order to simulate failures in switching from a state with low resistance to a state with high resistance for an elevated temperature, we calculated the dependence of the electron occupation distribution near the anode and the cathode for a system with α, β > 1 (Fig. 6a) and α, β < 1 (Fig. 6b). In both types of systems the change is marginal amounting to less than 10% for a temperature increase from 25° *C* to 200° *C*. This result indicates high robustness of failure-free RRAM switching from a state with low resistance to a state with high resistance for elevated temperature.

IV. Conclusion

In this work we have investigated a stochastic model of the resistive switching mechanism. The distribution of electron occupation probabilities calculated with our stochastic approach is in excellent agreement with previous work. Our calculations of the temperature variation of electron occupation probabilities near the anode and the cathode indicate high robustness of failure-free RRAM switching from a state with low resistance to a state with high resistance, when the temperature is elevated from 25° *C* to 200° *C*. The proposed stochastic model can be used for better understanding the degradation mechanisms for performance optimization of RRAM devices.

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