A Stochastic Model of Bipolar Resistive Switching in Metal-Oxide-Based Memory

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Abstract — A stochastic model of the resistive switching mechanism in bipolar metal-oxide-based resistive random access memory (RRAM) is presented. The distribution of electron occupation probabilities obtained is in agreement with previous work. In particular, a low occupation region is formed near the cathode. Our simulations of the temperature dependence of the electron occupation probability near the anode and the cathode demonstrate a high robustness of the low occupation region. This result indicates that a decrease of the switching time with increasing temperature cannot be explained only by reduced occupations of the vacancies in the low occupation region, but is related to an increase of the mobility of the oxide ions. A hysteresis cycle of a RRAM simulated with our stochastic model is in good agreement with experimental results.

I. INTRODUCTION

With flash memories rapidly approaching the physical limits of scalability, research on new nonvolatile memory concepts has significantly accelerated. Several new memory concepts as potential substitutes of the flash memory were invented and developed: a technology of phase change RAM (PCRAM), spin transfer torque RAM (STTRAM), carbon nanotube RAM (NRAM), copper bridge RAM (CBRAM), racetrack memory, and resistive RAM (RRAM). A new type of nonvolatile memory must exhibit low operating voltages, low power consumption, high operation speed, long retention time, high endurance, simple structure, and small size [1].

One of the most promising candidates for future universal memory is the resistive random access memory (RRAM). It is based on new materials, such as metal oxides [2-4] and perovskite oxides [5]. This type of memory is characterized by high density, excellent scalability, low operating voltages (<2V), fast switching times (<10ns), and long retention time.

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 carriers [6], electrochemical migration of oxygen vacancies [7, 8], electrochemical migration of oxygen ions [9, 10], a unified physical model [11, 12], a domain model [13], a filament anodization model [14], a thermal dissolution model [15], and others. Unfortunately, a proper fundamental understanding of the switching mechanism is still missing.

In this work we present a stochastic model of the bipolar 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 ($V_o$) [11, 12] or domains of $V_o$ (Fig. 1). Formation and rupture of a CF is due to a redox reaction in the oxide layer under a voltage bias. The conduction is due to electron hopping between these $V_o$.

For modeling the resistive switching in bipolar oxide-based memory by Monte Carlo techniques, we describe the dynamics of oxygen ions ($O^-$) and electrons in an oxide layer as follows:

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In order to model the dependences of transport on the applied voltage and temperature we choose the hopping rates for electrons as [16]:

\[ \Gamma_{nm} = A_e \cdot \frac{dE}{1 - \exp(-dE/T)} \cdot \exp(-R_{nm}/a) \]  

(1)

Here, \( A_e \) is a coefficient, \( dE = E_n - E_m \) is the difference between the energies of an electron positioned at 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 [12]:

\[ \Gamma_{0m}^{\alpha} = \alpha \cdot \Gamma_{0m}, \quad \Gamma_{0m}^{\beta} = \beta \cdot \Gamma_{0m} \]  

(2)

\[ \Gamma_{(N+1)m}^{\alpha} = \alpha \cdot \Gamma_{(N+1)m}, \quad \Gamma_{(N+1)m}^{\beta} = \beta \cdot \Gamma_{(N+1)m} \]  

(3)

Here, \( \alpha \) and \( \beta \) are the coefficients 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.

The current generated by hopping is calculated as:

\[ I = q_e \cdot \sum dx \sum m \left( \frac{1}{\sum \Gamma_m} \right) \]  

(4)

III. MODEL VERIFICATION

All calculations are made on one or/and two-dimensional lattices, the distances between two nearest neighboring \( V_o \) in all directions are equal. All \( V_o \) are at the same energy level, if no voltage or temperature is applied. Despite the fact that in the binary metal oxides, oxygen vacancies can have three different charge states with charge 0, +1, +2, to simplify the calculations, we assume that the oxygen vacancy is either empty or occupied by one electron.

A. Calculation of electron occupation probability

To verify the proposed model, we first evaluate the average electron occupations of hopping sites under different conditions. For comparison with previous works all calculations in this subsection are made on a one-dimension lattice consisting of thirty equivalent, equidistantly positioned hopping sites \( V_o \).

Following [17], we first allow hopping in one direction and only to/from the closest \( V_o \). The occupation probability of central oxygen vacancies, \( p_{c0} \), is described, depending on the boundary conditions as follows: 1) for \( \alpha=0.5 \) and \( \beta=0.5 \), \( p_{c0}=0.5 \); 2) for \( \alpha=0.5 \) and \( \alpha=\beta \), \( p_{c0}=\alpha \); 3) for \( \beta=0.5 \) and \( \beta=\alpha \), \( p_{c0}=1-\beta \). Fig.2 shows simulation results of our stochastic model, which are fully consistent with theoretical predictions [17].
To move from a model system [17] to a more realistic structure, 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, where hopping (1-3) is allowed in both directions (Fig. 4). Note that for \( \alpha > 0.5 \) and \( \beta > 0.5 \) (Fig. 3a and Fig. 4a) we still have \( p_e = 0.5 \) in the center, while for other values \( \alpha, \beta \) we observe a decrease in \( p_e \) for \( \alpha < \beta \) and an increase in \( p_e \) for \( \beta < \alpha \).

We have calibrated our model in a manner to reproduce the results reported in [12], for \( V = 0.4 \text{ V} \) to \( V = 1.6 \text{ V} \). Fig. 5a shows a case, when the hopping rate between the electrodes and \( V_o \) is larger than the rate between two \( V_o \) (i.e. \( \alpha, \beta > 1 \)). In this case the low occupation region is formed near the anode (unipolar behavior).

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

Note that when \( V = 0 \text{ V} \), the probability of occupation of all vacancies becomes equal to 0.5 regardless of the voltage applied before. This result indicates that, after the voltage is turned off, the probability of a CF rupture should increase substantially due to a decrease of the occupation probability of the vacancies from 1 to 0.5. But in practice we do not observe this, so to associate a CF rupture only with the formation of the low occupation region is wrong.

### B. Modeling of temperature dependence

With the model calibrated to [12] we simulated the temperature dependence of the site occupations in the low occupation region. The results shown in Fig. 6a and Fig. 6b indicate high robustness of the low occupation region demonstrating changes of less than 10%, when the temperature is elevated from 25°C to 200°C. At the same time this result indicates that the measured decrease of switching time with increasing temperature reported in [12] stems from the increased mobility of oxide ions, rather than from reduced occupations of \( V_o \) in the low occupation region.

### C. Modeling of the RESET process

Results obtained from simulations of the temperature dependence of the site occupations in the low occupation region demonstrate a necessity to include the dynamics of oxygen ions.

To describe the motion of ions we have chosen the ion rates similar to (1):

\[
\Gamma_{\alpha} = A \left( \frac{dE}{1 - \exp(-dE/T)} \right)
\]

Here we assume that \( O^- \) can only move to the nearest interstitial. A distance-dependent term is thus included in \( A \). \( dE \) includes the formation energy for the \( m \)-th \( V_o \) annihilation energy of the \( m \)-th \( V_o \), when \( O^- \) is moving to an interstitial or back to \( V_o \), respectively.

To verify the model, we simulated the reset \( I-V \) characteristics for a single-CF device [12]. For the simulations we have used a one-dimensional lattice consisting of thirty equivalent, equidistantly positioned hopping sites \( V_o \). Near each \( V_o \) an oxygen ion is placed. Fig. 7 shows the simulation results of the stochastic model, which are in perfect agreement with measurements from [12].
is the transition to a state with high resistance. When a reverse negative voltage is applied, the current decreases (Fig. 8 Segment 4). This rupture of the CF is determined by the dynamics of oxygen ions and not only by the formation of the low occupation region. The proposed stochastic model can be used for performance optimization of RRAM devices.

**D. Modeling of the hysteresis cycle**

All calculations of RRAM I-V characteristics are now performed on a two-dimensional lattice ($2 \times 30$). We have investigated the $I-V$ hysteresis by applying a saw-tooth like voltage $V$. We have assumed that the coefficients of the boundary conditions are constant and equal to 0.1. The simulated RRAM switching hysteresis cycle is shown in Fig.8. The cycle is in good agreement with the experimental one from [4] shown in the inset of Fig.8.

The interpretation of the RRAM hysteresis cycle obtained from the stochastic model is as follows. If a positive voltage is applied, the formation of a CF begins, when the voltage reaches a critical value sufficient to create $V_o$ by moving $O^-$ to an interstitial position. This leads to a sharp increase in the current (Fig. 8 Segment 1) signifying a transition to a state with low resistance. When a reverse negative voltage is applied, the current increases linearly (Fig. 8 Segment 3), until the applied voltage reaches the value at which annihilation of $V_o$ is triggered by means of moving $O^+$ to $V_o$. The CF is ruptured and so the current decreases (Fig. 8 Segment 4). This is the transition to a state with high resistance.

Interestingly, for parameters different from those in Fig.8 ($\alpha=0.135$, $\beta=0.05$ and $\alpha=0.13$, $\beta=0.09$) we still see a hysteresis cycle (Fig. 9), although the region of low occupation which, according to [12], is responsible for the rupture of the CF is almost absent. This result supports the observation that the ion dynamics is critical in describing the RRAM switching mechanism.

**IV. CONCLUSION**

In this work we have presented a stochastic model of the bipolar resistive switching mechanism. The distribution of the electron occupation probabilities calculated with the model is in excellent agreement with previous work. The simulated RRAM switching hysteresis cycle is in good agreement with the experimental result. We have shown that the process of rupture of the CF is determined by the dynamics of oxygen ions and not only by the formation of the low occupation region. The proposed stochastic model can be used for performance optimization of RRAM devices.

**REFERENCES**


