Stochastic Simulation of Forming, SET and RESET Process for Transition Metal Oxide-based Resistive Switching Memory

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Abstract—**a stochastic method based on the percolation theory and resistor network model, is developed to self-consistently simulate the microscopic process of the oxygen vacancies and interstitial oxygen ions in transition metal oxide-based resistive switching devices under the external electric field. The method can simulate the evolution of the oxygen vacancies' distribution and conductive filaments' geometry under the critical switching factors and the correlated electrical properties such as resistance. The simulated electrical characteristics were experimentally identified, indicating the validity of developed simulation methodology.**

Keywords- stochastic simulation, resistive switching, oxygen vacancies' distribution, conductive filaments' geometry

I. INTRODUCTION

Transition metal oxide (TMO)-based resistive switching memory (RRAM) has been extensively studied as one of the most promising candidates for next generation of Non-Volatile Memory devices due to its excellent memory and scalability performance [1-2]. It has been commonly accepted that resistive switching is due to formation and rupture of conductive filaments (CFs) and the switching characteristics are strongly correlated with the geometry of CFs as a direct result of generation and recombination of oxygen vacancies (V_O) in the switching oxide layer [3-6]. Understanding the physical evolution of CFs' geometry and the correlation with RRAM switching characteristics are imperative. In this paper, a stochastic method is presented to self-consistently simulate the microscopic process of the generation and recombination of V_O and the transport of interstitial oxygen ions (O^{2-}) under the external electric field. By using the resistor network based on the percolation theory [7-9], the simulation program is developed to simulate the evolution of CFs' geometry during the whole switching process with the various operation conditions.

II. PHYSICAL MODEL AND SIMULATION METHOD

Fig.1 shows various physics processes of V_O and O^{2-} considered in this work. Under the external bias, V_O generation (process ①) is modeled as a random process with the probability [10-11]:

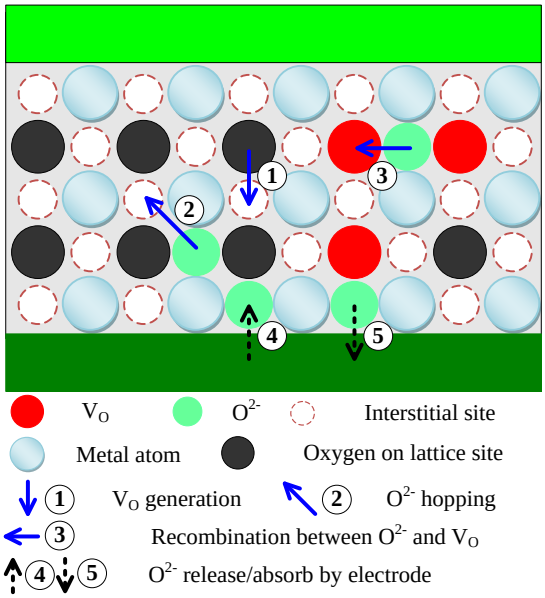

Fig.1 Schematic structure (two electrodes and the sandwiched switching oxide layer) used in this work and the physics processes have taken into consideration in our simulation. The electrode act as O^{2-} reservoir which can release and absorb O^{2-}.

$$P_a = f \exp(-\frac{E_a - \Delta\varphi_1}{k_B T_{loc}}) \quad (1)$$

where f is the vibration frequency of oxygen, E_a is the active energy of V_O, T_{loc} is the local temperature and $\Delta\varphi_1$ is the barrier decrease of E_a due to the local electric field. When O^{2-} is locating at the neighbor of V_O, the recombination process ③ occurs with the lifetime t_0. The transport of O^{2-} includes three physics processes: hopping through interstitial sites (process②), release/absorb by the electrode (processes ④⑤). Under the external bias, the hopping probability of O^{2-} to the neighbored interstitial sites is [12]:

$$P_h = f \exp(-\frac{E_h - \Delta\varphi_2}{k_B T_{loc}}) \quad (2)$$

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where $\Delta\varphi_2$ is barrier decrease of E_h due to the local electric field, E_h is the hopping barrier of O^{2-}.The processes ④⑤ are the same as the process ② except the barrier change to E_i [12]. Stochastic method is used to simulate the above microscopic physical processes.

In order to simulate the above mentioned microscopic processes self-consistently and efficiently, a resistor network based on the percolation theory [7-9] is introduced. In this model, a resistor is between two oxygen sites or the oxygen site and electrode. The IV-characteristic between two V_O is liner and can be described as:

$$I = U / R_1 \tag{3}$$

while the resistance between V_O and lattice oxygen or two lattice oxygen is modeled as:

$$I = \sinh(\alpha U) / R_2 \tag{4}$$

where α is a fitter coefficient. For the simplification, we assume that the IV characteristics of electrode with V_O or lattice oxygen are the same as what they are between V_O and V_O or lattice oxygen, respectively. The potential and current can be solved by the Kirchhoff law and the local temperature can be given by the Fourier heat-flow equation:

$$C\frac{\partial T}{\partial t} = \nabla(k \cdot \nabla T) + Q \tag{5}$$

where C is the specific heat per unit volume of TMO, k is thermal conductivity of TMO and Q is the Joule heat power density. All physical quantity is updated after every microscopic physical process based on the (1) ~ (5). Then the microscopic process can be simulated self-consistently. Fig.2 shows the simulation flowcharts. The parameters are summarized in Table I.

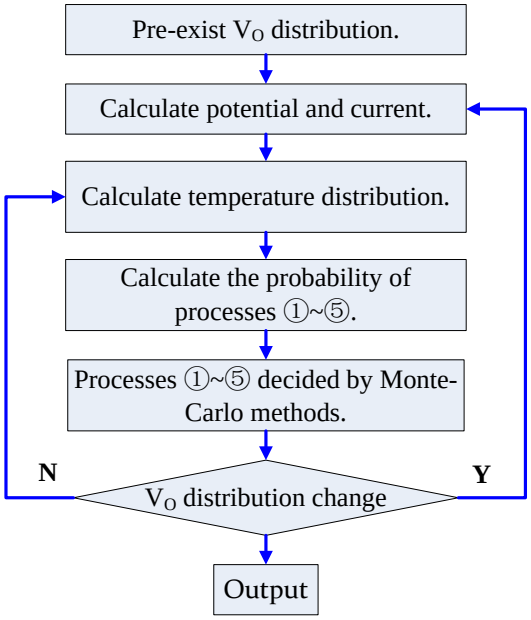

Fig.2 Simulation algorithm flow. Note that the temperature was calculated at every time step for including the effect of local temperature increase.

Table I typical parameters in this work.

Parameter	***Value***
vibration frequency: **f**	10^{13} Hz[10]
activation energy of ①: $\mathbf{E_a}$	1.2 eV[10]
hopping barrier of ②:$\mathbf{E_h}$	1.0 eV[12]
hopping barrier of ④⑤:$\mathbf{E_i}$	1.2 eV[12]
life time of ③: $\mathbf{t_0}$	10^{-6} s
$\mathbf{R_1}$	10^4 Ω
$\mathbf{R_2}$	5×10^{10} Ω
α	30
thermal conductivity of TMO**: k**	5 W/m·K[16]
specific heat per unit volume of TMO: **C**	6×10^6 J/m^3 · K[17]
length of TMO**: l**	50 nm
thickness of TMO**: d**	10 nm
distance of two oxygen sites**: h**	0.5 nm

III. RESULTS AND DISCUSSIONS

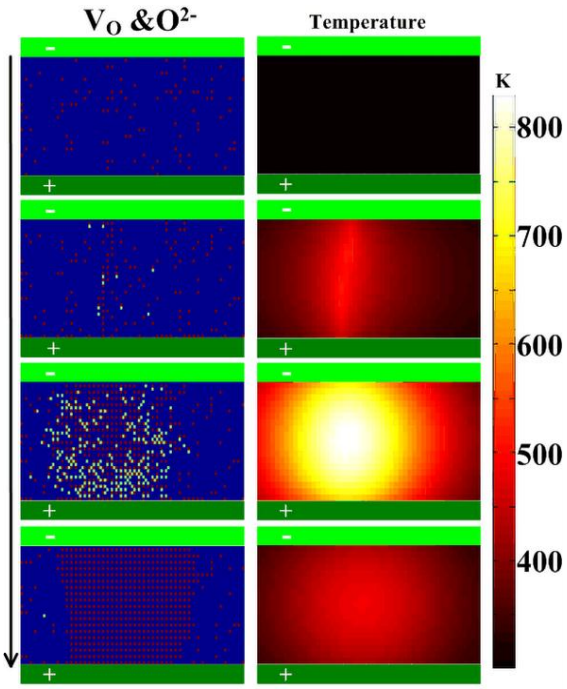

Fig.3 The evolution of Vo and O^{2-} distribution and the corresponding local temperature profile during the Forming process. The red and green dots represent the Vo and O^{2-}, respectively. It can find that the local temperature near to CF is higher which promote the CF to become strong.

The switching process of TMO RRAM including Forming/SET and RESET is simulated. Fig.3 shows the

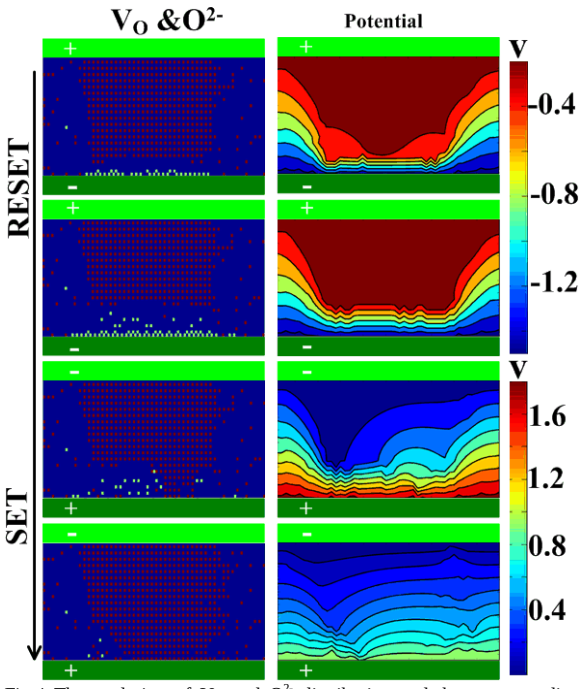

Fig.4 The evolution of Vo and O^{2-} distribution and the corresponding potential profile during a RESET-SET cycle. The initial state of the RESET process is the end state of Forming process which shows in Fig.3.

evolution of V_O and O^{2-} distribution and the corresponding local temperature profile during the Forming process. It can find that a fine filament firstly connect the two electrodes which results in high local temperature, and then the filament quickly become stronger assist by the high local temperature under the external voltage. Meanwhile the O^{2-} hops to the electrode/TMO interface and is absorbed by the active electrode. The resistance of device switching to low resistance state (LRS) due to the formation of CF. Fig.4 shows the evolution of V_O and O^{2-} distribution and the potential distribution during a RESET-SET cycle. O^{2-} is released by the electrode (④) assist by the local electric field and the increase of local temperature, and then recombines with V_O (③), which leads to the rupture of CF and the device switching to high resistance state (HRS) during the RESET process. While V_O forms (①) in the rupture region and CF connect the electrodes again, meanwhile O^{2-} hops to the electrode (②) and is absorbed by the electrode (⑤) in the SET process.

The correlated macroscopically electric properties are also investigated in our simulation. Fig.5 plots the simulated I-V curve during the RESET and SET process corresponding to Fig.4, which coincides to the measurement curve [13-14]. Abrupt SET and gradual RESET are reproduced. Current compliance is used to avoid the irretrievable breakdown of the device during the SET process. The SET voltage is the voltage when the current increase abruptly and exceed the current compliance during the SET process. And the RESET voltage is the voltage when the current reach the maximum value during the RESET process. Fig.6 shows the simulated statistical distribution of the RESET and SET voltage. It can

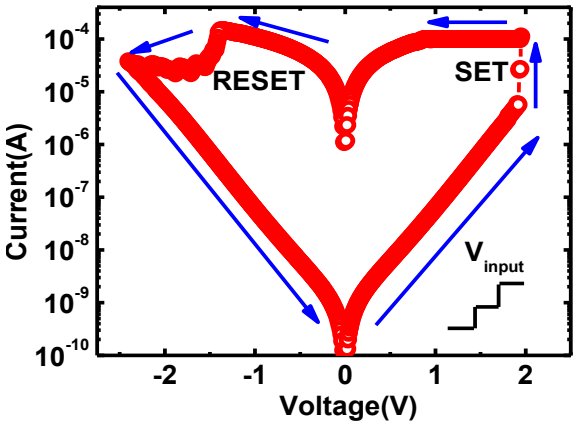

Fig.5 Simulated I-V curve for RESET&SET process. The sweep rate is 10V/s. Abrupt SET and gradual RESET are reproduced.

find the uniformity of RESET voltage is better. The simulated result is well consistent with the experimental data [15]. The statistical distribution of HRS and LRS is also shown in the Fig.7. It can find that the uniformity of LRS is better than the HRS, which is also consistent with the measurement data [1-2]. The variability of HRS and LRS originates from the random V_O generation/recombination and O^{2-} hopping processes [5].

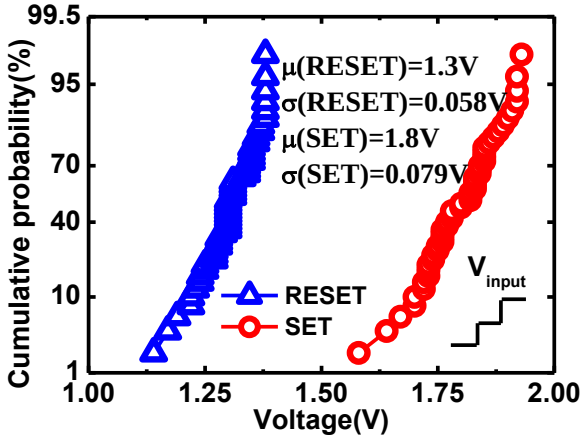

Fig.6 The statistical distribution of RESET and SET voltage obtained by simulated 50 cycles in one device.

IV. Conclusion

We present a stochastic method to self-consistently simulate the microscopic process of the generation and recombination of V_O and the hopping of O^{2-} under the external electric field to simulate the resistive switching process including Forming/SET and RESET both macroscopically and microscopically. The well agreement between the simulated results and the reported experimental data indicates that this new method can be a powerful tool for design and optimization RRAM.

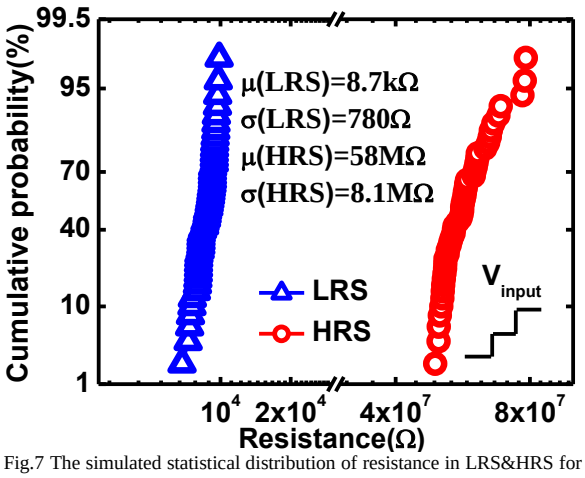

Fig.7 The simulated statistical distribution of resistance in LRS&HRS for 50 DC sweep cycles. The read voltage is 0.5V.

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