Model and simulation of bilayered tantalum-oxide (Pt/Ta$_2$O$_5$/TaO$_x$/Pt) memristor

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Abstract. As a new type of microelectronic device with a special resistance change mechanism, the memristors based on the novel resistive materials have been an emerging hot-spot in the area of electronics. Among tremendous memristors, the bilayered tantalum-oxide (Pt/Ta$_2$O$_5$/TaO$_x$/Pt) devices are believed to one of the typical device structures, its peculiar current-voltage (I-V) feature makes it distinct from other traditional devices, like resistor, capacitor or metal-oxide-semiconductor (MOS) transistor. It has been accepted as an alternative candidate of the traditional silicon-based memories. There have been lots of experimental works in this field, however, the theoretical works about its physical model and simulation are relatively few. In this work, its working principle is illustrated firstly, according to the thermionic emission theory of Schottky barrier in semiconductor physics. Then a quantitative physical model is presented and simulated, the calculated results are compared with the reported data to evaluate the effectiveness of the proposed model. The established physical model is constructed and calculated mathematically by using MATLAB, the computed results are compared with the experimental data to verify the proposed arithmetic model.

1. Introduction

Memristor was first proposed by Chinese professor Cai Shaotang in 1971 [1], it was extended to generalized memristor, also known as memristor system [2]. The typical feature of memristor is its "pinned hysteresis loop" shown by its current - voltage (I-V) curve and its special change to the excitation frequency, that is: with the increase of excitation frequency, the hysteresis loop gradually shrinks to a single value function [2, 3], which made it distinct from the traditional electronic components. It is well believed, the invention of memristor can generate an important supplement to the field of circuits and systems. However, due to the limited microelectronic manufacturing level at that time, and the complementary metal oxide semiconductor (CMOS) technology has just started and has greater development potential, the academic community did not pay attention to the research of memristors. Until 2008, HP lab announced that it had discovered the physical prototype of memristor [4, 5], the concept of memristor returned to the vision of researchers. According to the different electrode and dielectric materials, the memristor shows a variety of different response mechanisms. The specific explanation of the response mechanism has always been one of the hot topics in the research of memristor. A reasonable and accurate description of the resistance variation process is conducive to more stable control of the behavior of memristor and improve the performance of memristor. However, limited by the level of characterization technology, it is difficult to observe the internal physical and
chemical changes of nano scale memristor with high resolution and continuous dynamics. Therefore, the research on the resistance mechanism of memristor has been slow.

At present, the resistance mechanisms of memristors can be classified as 3 kinds, which are: ion migration mechanism, charge trap effect and thermochemical reaction. For the first one, ion migration mechanism is the main mechanism of memristor at present [6]. According to different ion charging, it can be divided into cation migration and anion migration, and its related research is also extensive. The main principle can be summarized as the movement and aggregation of ions under the electric field, the formation of conductive channels by deposition or changing the valence state of local regions, and the transformation of high and low resistance states can be completed. In recent years, the finding of conductive filaments improved the ion migration mechanism [7]. The charge trap effect mainly changes the resistance state of resistive materials through electrons’ capture and release. Researchers have proposed corresponding models to explain its unique response mechanism, such as SCLC (space charge limited current) model [8]. The resistance formed by thermochemical reaction is produced by the change of chemical integrity and redox reaction. The common memristor materials based on thermochemical reaction are NiO, Fe$_2$O$_3$ and so on [6], because the thermochemical reaction is independent of the polarity of bias voltage and these type devices show “non polarity” characteristics, their behavior was explained by the model proposed by Kim [9]. In fact, with the proposal of various new devices, researchers have also found many other unique resistance variation mechanisms [10], which are different from the above three mechanisms, and have also aroused extensive attention and research interest in the academic community. In this work, the resistance process under the ion migration mechanism is modeled and simulated, by using the double-layer tantalum oxide structure (Pt/Ta$_2$O$_5$/TaO$_x$/Pt) as a proof of concept. The response mechanism of the structure by using the semiconductor energy band theory is analyzed to established the corresponding physical model.

2. Basics of memristor’s feature

One of the typical current-voltage (I-V) feature of the bilayered tantalum-oxide memristor is shown in Figure 1 [11]. Commonly, it is believed there are two kinds of states, which are named as high resistance state (HRS) and low resistance state (LRS). When the voltage reaches a certain threshold voltage, the memristor will start the transition from LRS to HRS. This process is named as Reset, and the corresponding threshold voltage is called HRS switching voltage (HSV). Similarly, under a certain negative voltage excitation, the memristor will complete the transition from HRS to LRS, which is defined as Set, and the corresponding threshold voltage is called LRS switching voltage (LSV). As shown in Figure 1, the Set and Reset processes are occurred under the negative and positive voltages respectively, therefore, the I-V feature is bipolar.

![Figure 1. The typical I-V feature curve.](image-url)
The understanding for the electronic feature was believed to be caused by the anion transfer mechanism, which is sketched in Figure 2 [7, 12]. In the layer of TaO_x, there are lots of negatively charged oxygen vacancies (VO). The resistance changing process of double-layer tantalum oxide structured memristor is believed to be controlled by anion migration mechanism. Under the external electric field, these negatively charged ions can be migrated in the direction opposite to the electric field. So, this process can also be regarded as the movement of positively charged ions along the direction of the electric field. That is to say, these charges can be moved to the layer of Ta_2O_5 when the negative voltage (V) is applied between the top electrode (TE) and the bottom electrode (BE). In the view point of semiconductor, VOs in tantalum oxide can be regarded as doped impurities in the n-type semiconductor, in the VOs aggregated region they can provide electrons in conductive energy band, bring about the conductive changes. In Figure 2 (a) to (c), BE is grounded, TE is connected to the negative voltage (V). When the applied V is low, due to the Schottky barrier at the interface of TaO_x and Ta_2O_5 layers, the resistance is high, Ta_2O_5 layer can be equivalent to an off-state resistance (ROFF in Figure 2 (a)). With the increasing absolute value of V, the positively charged VO will gradually migrate from TaO_x layer to Ta_2O_5 layer, and diffuse along the diffusion channel. Thus, VO aggregated "filaments" are gradually formed. These "filaments" have the ability of local conductivity, are called as conductive filaments (CF). When CF extends to TE, the heavy doped region of VOs can be formed, the Schottky barrier at the interface between TE and Ta_2O_5 will disappear and change to an ohmic contact, in this state Ta_2O_5 layer can be equivalent to an on-state resistance (RON in Figure 2 (c)) with lower resistance.

3. Methods

3.1. CF growing model

Mott and Gurney rigid point-ion model is used to describe this CF growing model [13]. Assuming that the total thickness of the Ta_2O_5 is D, when VOs begin to diffuse, the local region will be changed from insulate to conductive. Therefore, the thickness of the effective insulating region (named as w) in the Ta_2O_5 layer will be altered gradually. The direction of external electric field (E) affects the migration direction of oxygen ions, and then changes the value of w. The relation of E and w can be expressed as Eq. (1):

\[
\frac{dw}{dt} = v_{TE} - v_{BE} = a \cdot c \cdot \exp \left( -\frac{U}{KT} \right) \cdot \left\{ \exp \left( \frac{qAE}{2KT} \right) - \exp \left( -\frac{qAE}{2KT} \right) \right\} \\
\approx a \cdot c \cdot \exp \left( -\frac{U}{KT} \right) \cdot \sinh \frac{E}{E_0} 
\]  

(1)
In which, $E_0 = \frac{2KT}{qa}$, $a$ is the effective transition distance and $q$ is the electron charge.

### 3.2. Energy band model

The carriers’ movements from TaO$_x$ to Ta$_2$O$_5$ and at the contacts of metal and semiconductors are the main issues to determine the memristor’s electronic feature. According to the energy band between metal and semiconductor as shown in Fig. 3, the relation of current ($I$) and voltage ($V$) can be described by the Eq. 2 [4].

$$I = A \cdot A^* \cdot T_0^2 \cdot \exp \left( - \frac{\Phi_{Bn}}{kT} \right) \cdot \left\{ \exp \left( \frac{V_S}{kT} \right) - 1 \right\}$$

(2)

In which, $A$ represents the area of contact, $A^*$ is the Richardson constant, $\Phi_{Bn0}$ represents the Schottky barrier height, $V_T$ is the thermal voltage (26 mV at the room temperature), $V_S$ represents the applied voltage at the interface of the metal and semiconductor, which can be determined by the Eq. (3).

$$V_S = V - I \cdot (R_I + R_S)$$

(3)

![Figure 3. Energy band model.](image)

### 4. Results and discussions

#### 4.1. Simulation result

To verify the accuracy of the presented method, we choose the data published by Hur groups’ works [14, 15]. The simulated responding curves are plotted with their measured data in the same coordinate, as shown in Figure 4. It could be found that the simulated results are well fitted with the measured ones in the range of -2 - 1 V which corresponds to the Set process. It demonstrates the proposed method can successfully simulate the current voltage relationship under states of HRS and LRS, as well as the setting process.

However, there are still deviations when the voltage exceeds HSV (> 1 V, in Figure 4). The simulated curves are lower than the measured data [5, 6], it is deduced to be caused by the residual oxygen vacancies, as shown by Figure 2 (b). These accumulated charges can promote the conduction behavior under high electric field. But this issue is not considered the classical current voltage behavior under Schottky barrier, i.e., the Eq. (2).
4.2. Modified simulation

To solve the mismatch problem between the model and the experimental data after HSV, an additional current source Iextra is assumed, as expressed by the Eq. (4), in which the meanings of Rs and D are provided in Figure 2, the value of Itotal is the sum of the previous data in Figure 4 and Iextra, C1 and C2 are used as the adaptive parameters.

$$I_{\text{extra}} = c_1 \cdot \exp(c_2 \cdot \frac{V - I_{\text{total}} \cdot R_s}{a}) \quad (4)$$

The purpose of introducing Iextra is to affect the current when the voltage is over the process of RESET, and almost zero when the device is under the state of LRS. The modified simulations are conducted and presented in Figure 5. It could be found the modified results are matched with the experimental data in the whole working processes.

5. Summary

In this work, we described the electronic behavior of the double-layer tantalum oxide memristor firstly, then proposed an arithmetic method to simulate its I-V characteristic curves. Based on this theoretical work, calculations were conducted by using MATLAB. The comparisons with the reported data in Ref. 14, 15 demonstrated the accuracy of the proposed model and the practicable of the method for simulating the double-layer tantalum oxide memristor.
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