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Switching dynamics of TaO$_x$-based threshold switching devices

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Bi-stable volatile switching devices are being used as access devices in solid-state memory arrays and as the active part of compact oscillators. Such structures exhibit two stable states of resistance and switch between them at a critical value of voltage or current. A typical resistance transient under a constant amplitude voltage pulse starts with a slow decrease followed by a rapid drop and leveling off at a low steady state value. This behavior prompted the interpretation of initial delay and fast transition as due to two different processes. Here, we show that the entire transient including incubation time, transition time, and the final resistance values in TaO$_x$-based switching can be explained by one process, namely, Joule heating with the rapid transition due to the thermal runaway. The time, which is required for the device in the conducting state to relax back to the stable high resistance one, is also consistent with the proposed mechanism. Published by AIP Publishing. https://doi.org/10.1063/1.5020070

INTRODUCTION

Resistive random access memory arrays in crossbar architecture need a memory element and an access device (selector) connected in series at every node of an array. The memory element stores information as a value of resistance, while the primary function of the access device is to reduce the sneak path leakage current and allow for selection of one cell for reading and writing operations. 1 This function requires a highly nonlinear $I$-$V$ characteristic of the selector: the leakage current in half selected cell (at $V_{TH}/2$) should be smaller than the current at $V_{TH}$ by at least a factor equal to the array size. In addition, the selector needs to source enough current to switch the memory element, switch faster than the memory, and has better endurance. The best candidate that can meet all of the above requirements appears to be the threshold switch. Such devices inherently have highly nonlinear $I$-$V$ arising from S-type negative differential resistance (S-NDR) part of characteristics. 2 The device initially traces the lower part of the S-curve, referred to as the high resistance OFF-state, and upon reaching the threshold voltage ($V_{TH}$), transitions to a volatile low resistance ON-state with the $R_{OFF}/R_{ON}$ resistance ratio as high as $10^7$.3

Several classes of materials have been used to fabricate threshold switches including amorphous chalcogenides, 4,5 oxides exhibiting a metal-insulator transition, 6,7 and dielectric oxides. 8,9 The name “threshold switch” implies that the transition occurs at a well-defined value of voltage referred to as the “threshold voltage.” This is misleading as a majority of threshold switches can transition to the ON-state in a range of voltages. Specifically, if a constant voltage pulse is applied to a threshold switch, it does not switch instantly. Initially, its resistance decreases slowly with time. After some time, deemed the incubation period, the device rapidly transitions to the conducting ON-state followed by a slower approach to the steady state resistance. 4,10,11 For example, in amorphous chalcogenides, multiple authors reported incubation times as long as 10 $\mu$s, 10,12 while the transition time is shorter than 1 ns. 4,13 The incubation time is a strong function of the applied voltage, increasing at lower bias. At this point, it is not known whether there is a critical value of bias below which the transition to the ON-state does not occur. It could be that for every value of bias, there is a finite incubation time. 14,15

The large difference in incubation and transition times was frequently interpreted as a consequence of two different processes. For example, in the most extensively studied class of threshold switches, i.e., amorphous chalcogenides, the incubation time was associated with nucleation of a conducting crystalline inclusion, while the rapid change was interpreted as due to the growth of the inclusion. 16 The same model was used to explain the dynamics of oxide-based devices. 11,17 The electro-thermal model was one of the first to be proposed to explain threshold switching in chalcogenides but rarely invoked in 1990s and 2000. 18 The model was recently successfully reapplied to both chalcogenides and oxides. 9,19,20

Here, we present the results of the switching dynamics of TiN/TaO$_x$/TiN crossbar devices and their interpretation as due to Joule heating. We show that one mechanism can account for both slow initial change of resistance and the rapid transition without any ad hoc assumptions. The rate of resistance change increases after incubation due to a thermal runaway, which occurs when the device reaches a critical value of conductivity change. The mechanism does not include ion motion or a phase change, relying exclusively on an increase in conductivity with temperature. Also presented are data and interpretation of the recovery of threshold switching, i.e., transition from the ON-state back to the high resistance OFF-state.

EXPERIMENTAL PROCEDURES

The devices used in this study were fabricated in a TiN/TaO$_x$/TiN sandwich structure with 30 nm thick electrodes...
and 60 nm thick functional layer. TiN layers were deposited by DC magnetron sputtering with a chamber pressure at 3 mTorr and an argon flow rate of 60 sccm. The TaOx functional layer was reactively sputtered at the same pressure and a flow rate of argon and oxygen at 57 and 3 sccm, respectively. The device structure was 210 × 210 nm laterally and patterned in a ground-signal-ground configuration to allow for fast pulse measurements. Quasi-static I-V characteristics were obtained using an Agilent 4155C Semiconductor Parameter Analyzer. Pulse measurements were carried out by connecting a device in series with an Agilent Infinium DSO80804A oscilloscope and a pulse generator (either Agilent 81110A or Tektronix PSPL10070A). All measurements were obtained with the stage temperature of 300 K.

RESULTS

Quasi-static I-V characteristics of TiN/TaOx/TiN structures were obtained using a circuit consisting of the voltage source, device under test, and a load resistor of 15 kΩ. It should be noted that many threshold switching devices require an electro-formation step (also referred to as “first fire”) before they can be switched. These permanent changes of electrical characteristics are thought to be associated with local breakdown and formation of a small permanent filament. The devices discussed here did not show any such changes and were used in the “as-fabricated” state. Accordingly, the current flow at low voltages is thought of as uniform. The I-V results are shown in Fig. 1 as a black continuous line. Figure 1(a) plots current versus source voltage, while Fig. 1(b) presents the same measurement versus voltage drop across the device. Both curves show a high resistance OFF-state at low voltages, a threshold “snap” denoted by the dashed line, and the stable ON-state at higher source voltages. The transition occurs at 3.9 V across the device and was too fast for the source-meter to register any data in this range. The slope of the dashed line in Fig. 1(b) corresponds to $-1/R_{\text{LOAD}}$, where $R_{\text{LOAD}}$ is the resistance of the load resistor. With further increase in the source voltage, the voltage across the device in the ON-state continued to decrease slightly to 3.2 V with a steep increase in current to $\sim 80 \mu$A. The red curves have been obtained from a finite element simulation that solved coupled charge and heat flow equations. The simulation used experimental values of electrical conductivity as a function of temperature and electric field, which were fitted by a Poole-Frenkel formula with an activation energy of 0.23 eV. Simulation used a simplified layout of the device by assuming a circular rather than a square structure with a radius of 120 nm, resulting in the same resistance OFF-state. Accordingly, the transmitted pulse amplitude is low and close to the noise level resulting in a

FIG. 1. Experimental (black) and simulated (red) quasi-static I-V characteristics measured at 300 K with a 15 kΩ series resistor. (a) The current as a function of source voltage with (b) plotting the same data as a function of voltage drop across the device. The inset in (b) re-plots the I-V on a logarithmic scale to show the fit at low voltage values.
large scatter of resistance values. Nevertheless, one can notice that the initial value of resistance is lower for the pulses with higher amplitudes. This is due to the super-linear dependence of Poole-Frenkel-type conductivity on electric field, a fact reflected in the simulated transients marked by the red lines. The resistance decreases monotonically with time with initial slow change followed by a sharp transition where resistance drops from \( \approx 400 \, \text{k}\Omega \) to a much lower resistance characteristic of the ON-state. The incubation time, which was defined in this experiment as the time required for the resistance to reach 100 k\( \Omega \), decreases sharply with increasing amplitude of the voltage pulse. After the transition, the resistance reaches a steady state value in the ON-state. This value varies from 70 k\( \Omega \) at pulse amplitude of 4.194 V to 50 k\( \Omega \) at 4.9 V. The change is consistent with the \( I-V \) characteristics in Fig. 1(a): the resistance in the circuit decreases with the source voltage.

The second transmissometry experiment was carried out without the load resistor. The load in this case was only the internal resistance of the oscilloscope and pulse generator. The use of ground-signal-ground waveguides and high frequency cables and probes eliminated signal distortions allowing for collection of high frequency data. Three examples of transients are shown in Fig. 2(b). They exhibit very similar behavior to the ones shown in Fig. 2(a) with the difference being a significantly lower value of resistance in the ON-state. This is to be expected as lower load gives a much steeper load line in Fig. 1(b), which intersects the intrinsic device characteristics at much higher current. The consequence of higher current, however, was a higher temperature within the device, which allowed for permanent change of resistance. This is the common failure mechanism for threshold switching devices both in oxides and in chalcogenides.\(^{23,24}\) The failure occurred at the end of the transients without affecting the measurement of the incubation time. As the device resistance at steady state does not correspond to the ON-state of the threshold switch, the experimental transient plots in Fig. 2(b) were terminated immediately after the transition. Each of the transients shown in Fig. 2(b) was collected on a different as-fabricated device. It should also be noted that the incubation time for devices with a 100 \( \Omega \) series load was defined as the time required to reach 10 k\( \Omega \). A different resistance level was used here in order to account for the highest applied biases, where resistance values at the beginning of the pulse were already below 100 k\( \Omega \) and thus would result in an effective incubation time of 0 s. The difference in resistance levels defining incubation time for the two experiments has not affected the values of incubation time because the transition to the ON-state is quite rapid compared to the length of the pulse.

Figure 2(c) shows incubation times (\( \tau_{\text{INC}} \)) as a function of source voltage. Blue diamonds correspond to experimental data extracted from Fig. 2(a), black squares denote data from Fig. 2(b), and the red dashed line presents results of the electro-thermal simulation. The incubation time decreases monotonically with increasing voltage. The rise time of the pulse generator used in this experiment was 65 ps which allowed for recording switching times as short as 400 ps (significantly faster than the previous report on TaO\(_x\)).\(^{11}\) Incubation times do not appear to saturate at high voltages, indicating that switching could be even faster although at the expense of increasing overvoltage. This is in agreement with the thermo-electric model, which always allows for faster heating with increased power dissipation.

The reason for two other features of the resistance transients is less obvious. These are (i) large difference of resistance change rates as a function of time and (ii) very rapid increase in incubation time at low voltages. Both have the
same origin: the positive feedback loop between current and temperature. At the beginning of the pulse, the current is determined by the conductivity of the functional layer and the electric field. After time $\Delta t$, the current increases due to Joule heating, affecting the value of conductivity. This feedback can be represented as a geometric series of $I_n$

$$I = I_0 + \Delta I_1 + \cdots = a_0 V + \sigma \left[ \Delta T \frac{\partial \ln \sigma}{\partial T} \right]_{\text{Stage}} + \cdots \quad (1)$$

The common factor in the square brackets corresponds to the relative conductivity increase. The series converges at low values of voltage corresponding to small values of the factor but will diverge when it exceeds unity. Its value increases with time at a given pulse voltage (as the temperature rises) and also increases with the pulse amplitude (faster heating of the device). The runaway process is illustrated in Fig. 3(a) where a simulated device with a 100 $\Omega$ load was subjected to 10 $\mu$s voltage pulses of varying magnitude. The temperature in the middle of the functional layer is shown as a function of time. Each response starts at the stage temperature (300 K). The rate of temperature change increases with the source voltage and initially decreases with time ($\partial^2 T/T^2 < 0$). Whenever the temperature exceeds 400 K ($\Delta T \sim 100$ K), the current diverges, increasing the rate of temperature change.

The plot is terminated at 500 K because experimental values of $\sigma(T)$ are not well known at high temperatures. It is also clear that at low pulse amplitudes, the temperature will saturate before reaching the critical value and the device will never transition to the ON-state. This effect is responsible for the incubation time diverging to infinity below the critical value of applied voltage in agreement with data in Fig. 3(a). It is important to note here that with changing stage temperature, the temperature at the onset of the runaway will also change. It is the $\Delta T$ rather than the absolute temperature that decides the runaway. The temperature versus time plot displayed in Fig. 3(a) similar to the resistance versus time plot displayed in Figs. 2(a) and 2(b): the resistance change closely follows the temperature change. The rapid increase in temperature causes the resistance drop. If the critical $\Delta T$ is not reached, both the resistance and temperature asymptotically approach a constant value.

A dependence of incubation time on stage temperature is shown in Fig. 3(b). The tested devices shown here are the devices with the functional layer deposited with 4.5 sccm oxygen flow as discussed in our previous publication. Similarly, the devices were tested with 100 $\Omega$ series resistor and the incubation time was defined as the time required for the resistance to reach 10 k$\Omega$. There is a clear trend: as the stage temperature increases, the incubation time versus voltage curve shifts to lower voltages. Its shape remains very similar. This trend continues until the stage temperature is large enough to where the device becomes so conductive that threshold switching is suppressed altogether, as was seen at high temperatures in our previous work. Figure 3(b) also indicates that for the same source voltage, a longer incubation time is required as the stage temperature is lowered. This is a consequence of the device resistance increasing with the drop of temperature resulting in lower dissipated power at any given voltage.

The rapid increase in incubation time at low voltages appears to be a “fingerprint” of the thermal runaway process and can be used to differentiate between different proposed models. In particular, in a previous report on dynamics of threshold switching in TaO$_x$, we have modeled the incubation as due to the nucleation of a conductive phase. However, the nucleation model predicts a finite incubation time even at zero bias and cannot replicate as steep increase in the incubation time as observed experimentally. It also should be pointed out that most publications on amorphous chalcogenide devices have reported a different behavior. Some authors observed large scatter of incubation times at low over-voltages, while others reported switching at voltages significantly below the threshold and exceedingly long times. This behavior could indicate a different operating mechanism in these materials.

An important remaining question is the recovery time for threshold switching devices: how long would a device stay in the ON-state after a voltage pulse is terminated? This question has been addressed in detail in amorphous chalcogenides in a series of double pulse studies. We conducted a similar experiment on TaO$_x$. A sequence of two pulses with the same amplitude (4.4 V) and the same length (5 $\mu$s) was applied to a device with a series resistor of 15 k$\Omega$.

![FIG. 3. (a) Simulation of the TaO$_x$ temperature as a function of time for varying source voltages with a 100 $\Omega$ load resistance. (b) Experimental (points) and simulated (solid lines) incubation times as a function of source voltage and stage temperature.](image-url)
The only variable was the length of the delay between the two pulses. Each test was carried out on the same device, which retained its original characteristics throughout the experiment. The device shown in Fig. 4 was nominally the same as in Figs. 1 and 2 but with \( V_{TH} \) of 4 V, slightly higher than one in Fig. 1. Figure 4(a) shows a resistance transient corresponding to two pulses separated by 300 ns delay time. The beginning and end of each pulse are marked by vertical red dashed lines. Both transients closely resemble transients in Fig. 2 where each starts with a gradual drop, steep decrease, and eventual saturation in the ON-state. There are two noticeable differences between the two responses. The initial resistance of the second transient is lower than that of the first one and the incubation time (marked by blue dashed line) is shorter (~1 \( \mu \text{s} \) versus 1.5 \( \mu \text{s} \)). The qualitative interpretation is straightforward: the delay of 300 ns allowed for some temperature drop after termination of the first pulse but the temperature remained higher than 300 K. This caused the initial resistance during the second pulse to be lower and it took less time for the temperature to reach critical \( \Delta T \), thus reducing the incubation time. The temperature versus time was modeled by the same electro-thermal model and the extracted incubation times are shown as a function of delay by the red dashed curve in Fig. 4(b). The experimental points are shown as black squares. The agreement confirms the origin of recovery as associated with cooling of the device. The device transitioned to the OFF state (recovered) after the delay time of less than 100 ns. The full recovery time corresponding to the same incubation time was approximately 0.8 \( \mu \text{s} \). Both times are expected to get shorter with decreasing device size and with decreasing thermal resistance. In the case of the structures used, the thermal resistance was determined primarily by the thermal oxide layer.

CONCLUSIONS

Threshold switching in TaOx-based devices was interpreted as due to a positive feedback loop between conductivity and device self-heating leading to a thermal runaway. A finite element electro-thermal model was able to reproduce the quasi-static I-V and transient R-t responses and, in particular, the slow-fast-slow dynamics of the threshold switching process. It can also account for the divergence of the switching time to infinity at a well-defined threshold voltage. This model provides a template for engineering selector devices that meet all necessary access device requirements.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{(a) Resistance response of a device to 2 applied voltage pulses of 4.4 V each with a delay of 300 ns. (b) Incubation times for the 2nd pulse as a function of delay time between the two applied voltage pulses. The black points are experimental and the red dashed line represents simulated values.}
\end{figure}