

## THERMAL REVERSIBLE BREAKDOWN AND RESISTIVITY SWITCHING IN HAFNIUM DIOXIDE

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### ABSTRACT

We present a model of thermal reversible breakdown via conductive filaments (CFs) in hafnium dioxide ( $\text{HfO}_2$ ). These CFs appear as a result of electrical pretreatment of a metal/ $\text{HfO}_2$ /metal (semiconductor) nanostructure (MIM(S)). The model is based on an assumption that the thermal reversible breakdown of a CF is due to Joule heating displaying an exponential dependence of conductivity on temperature. The corresponding current-voltage characteristic and temperature of a CF in its middle and at the interface with an electrode are calculated taking into account the heat conduction equation and boundary conditions with heat dissipation via electrodes. It is found that the current-voltage characteristic of a CF has three specific regions. The initial and final regions have turned out to be linear with respect to the current and display different slopes, while the middle region is characterized by S-shaped or ultralinear dependences which are affected by the ambient temperature and nanostructure parameters. The switching potential from high resistivity state (HRS) to the low resistivity state (LRS) was shown to decrease with the ambient temperature and with worsened heat dissipation conditions.

**Key words:** hafnium dioxide, thermal reversible breakdown, conductive filament, s-shaped, current-voltage characteristic

### INTRODUCTION

$\text{HfO}_2$  nanostructures are currently considered to be very promising for different applications including gate oxides in Si transistors and emerging nonvolatile memory cells such as resistive random access memory (RRAM). For RRAM development a clear understanding of switching mechanisms from a HRS to a LRS is demanding. Several models were proposed to explain the switching effect [1-3], however, they did not cover comprehensively experimental observations. It is experimentally shown by means of high resolution transmission electron microscopy that formation of CFs with diameters of 30-50 nm in  $\text{HfO}_2$  occurred by an electrical pretreatment [2]. According to experimental data [3,4] current-voltage characteristics of MIM(S) nanostruc-

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tures with  $\text{HfO}_2$  are characterized by a current jump at a specific set voltage ( $V_{set}$ ) indicating that only the current-voltage characteristic of a CF displays the S-shaped or ultralinear behavior. In order to provide an interpretation of such behavior we have developed a model of thermal switching breakdown due to of the Joule heating of CFs.

### MODEL

We have assumed a CF to be formed along the  $z$  axis from  $z=-L/2$  to  $z=+L/2$  in a  $\text{HfO}_2$  layer of MIM(S) nanostructure. The heat release and voltage drop at contacts are not taken into consideration because heat removal is expected to be uniformed and to follow the Newton law. Temperature distribution in the CF can be written as [5]

$$\kappa_d \frac{d^2 T}{dz^2} + jF = 0, \quad (1)$$

$$\frac{dT}{dz} \Big|_{z=0} = 0, \quad \kappa_d \frac{dT}{dz} \Big|_{z=L/2} = \frac{\lambda(T_b - T_0)}{1 + \lambda\delta / \kappa_c}, \quad (2)$$

where  $\kappa_c$  is the heat conduction of a contact,  $\kappa_d$  is the heat conduction of a CF,  $\lambda$  is the coefficient of external heat removal,  $\delta$  is the thickness of contacts,  $T_0$  is the ambient temperature,  $T_b$  is the temperature at the interface between the CF and the electrode. The current density and the voltage drop on the CF can be defined in a drift approximation

$$j = \sigma_0 F \exp(-\Delta E / k_B T), \quad V = 2 \int_0^{L/2} F(z) dz, \quad (3)$$

where  $F$  is the electric field strength in the CF,  $\sigma_0$  is the conductivity in the CF at  $T_0$ ,  $\Delta E$  is the trap energy in the CF,  $k_B$  is the Boltzmann constant.

By solving (1)-(3), the current-voltage characteristic of the CF can be calculated in the parametric form

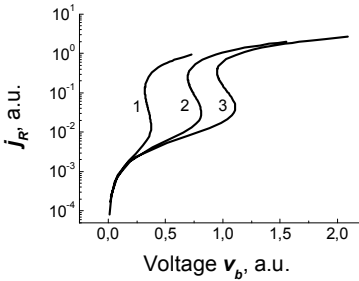
$$j_R = \int_{t_b}^{t_m} \left( \int_t^{t_m} \exp(1/t) dt \right)^{-1/2} dt, \quad \frac{v_b^2}{2} = \int_{t_b}^{t_m} \exp(1/t) dt, \quad (4)$$

where  $v_b = (V/2) \sqrt{(\sigma_0 k_B / \kappa_d \Delta E)}$ ,  $j_R = (\sqrt{2}/4) j_L [k_B / (\kappa_d \Delta E \sigma_0)]^{1/2}$ ,  $t_b = t_0 + (jV/W_b)$ ,  $W_b = (4\gamma \kappa_d \Delta E) / (k_B L)$ ,  $\gamma = \lambda L / (2\kappa_d [1 + (\lambda\delta / \kappa_c)])$ ,  $t_{(0,m)} = k_B T_{(0,m)} / \Delta E$ ,  $T_m$  is the temperature in the middle of the CF at  $z=0$ .

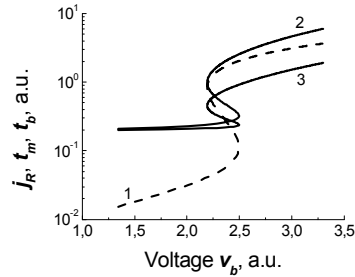
We have defined the function  $t_m(jV/W_b)$  at different values of  $\gamma$  and  $t_0$  parameters and, as a consequence, find the current-voltage characteristics and dependencies of temperature in the middle of a CF and at the interface with electrodes on voltage drop.

## RESULTS AND DISCUSSION

We have found three specific regions in the current-voltage characteristic of a CF. The first region at a small voltage drop is characterized by a linear dependence of current density with a small slope. The slope is found to be slightly dependent of temperature  $t_0$  and independent of the parameter of heat removal  $\gamma$ . The second region is a transition state which displays the nonlinear current voltage characteristic depending on  $t_0$  and  $\gamma$ . This region is S-shaped with the following transformation to nonlinear transition area with increasing  $t_0$ . Finally the third region shows the linear current-voltage characteristic with a high slope and obeys the Ohm law. The shape of the current-voltage characteristic is only defined by  $t_0$  and  $\gamma$ . At  $t_0 \leq 0.3$  between the linear regions the S-shaped region appears while at  $t_0 > 0.35$  there is a nonlinear area. The current-voltage characteristic shifts along the voltage drop axis with increasing the heat removal parameter  $\gamma$  and the formation the S-shaped regions occurs at larger voltage drops as shown in *Fig. 1*.



**Fig. 1** – current-voltage characteristics of the CF at  $t_0 = 0.2$ :  $\gamma = 0.1$  (1);  $\gamma = 0.5$  (2);  $\gamma = 1.0$  (3).



**Fig. 2** – current-voltage characteristics of the CF (1), temperatures  $t_m$  (2) and  $t_b$  (3) at  $t_0 = 0.2$ ,  $\gamma = 10$ .

The  $T_m$  and  $T_b$  dependences on the voltage drop are also characterized by three regions, as it is shown in *Fig. 2*. We have also found that the influence of parameters of a nanostructure on this dependence is analogous to the one described above for the current-voltage characteristic. A notable difference can be traced for temperature only at the boundary of a CF. At  $\gamma \leq 1$  the temperature corresponds to that in the middle of the CF. Whereas, with increasing  $\gamma$  the difference has turned out to be valuable leading to compression of the  $T_b(v_b)$  dependence with respect to the temperature axis. Thus, with increasing of the heat removal the temperature of the CF at the boundary decreases significantly with respect to the temperature in the middle of the CF.

The potential, at which a sharp jump in the current occurs (the switching potential from HRS to LRS,  $V_{set}$ ), decreases proportionally to increasing of the

ambient temperature  $T_0$  according to experimental data [4] for the Pt/HfO<sub>2</sub>/TiN nanostructure. The potential  $V_{set}$  also decreases proportionally to the parameter  $\gamma$  because of the worsened conditions of heat removal.

### **CONCLUSION**

We have developed the model of conductive filament thermal reversible breakdown involving mechanisms of switching between high and low resistivity states in HfO<sub>2</sub> MIM(S) nanostructures. The current-voltage characteristics and dependencies of the filament temperature on the voltage drop, ambient temperature and heat removal parameters are also calculated. We have defined conditions of an appearance of the S-shaped current-voltage characteristic of the conductive filament with a nonlinear transition area. We have also found out that decreasing in the ambient temperature leads to magnification of the transition S-shaped region of the current-voltage characteristic while degeneration of this transition region occurs with an increasing temperature. An increase in the heat removal shifts the current-voltage characteristic to the area of larger voltage drops and decreases the temperature at the filament/electrode interface with respect to the temperature at the middle of the conductive filament.

### *Acknowledgements*

The work is supported by the Agreement on Cooperation between Belarusian State University of Informatics and Radioelectronics and Nanyang Technological University.

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