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Simulation of threshold switching based on an electric field induced thermal runaway

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***Abstract*—We introduce a new explanation for abrupt threshold switching (TS) based on a Poole-Frenkel like field dependent barrier lowering conduction mechanism. As the barrier lowering induces a thermal runaway the mechanism is named field-triggered thermal runaway (FTTR). The FTTR-type threshold switching has the major characteristics of a hysteresis determined by different switching voltages for the turn-on and the turn-off. In this study, we investigate the influence of a series resistance on the FTTR-type threshold switching. We show that the variation of the memristive resistance is able to lead to a transition of the abrupt TS with a hysteresis into a continuous non-linear TS without a hysteresis effect. The transition between the abrupt and continuous TS occurs suddenly with an increase of the serial resistance, which consequently defines a minimum resistance change for the abrupt TS.**

Keywords—Threshold switching, MIT/IMT, steep slope, Poole Frenkel

I. Introduction

Threshold switching and a corresponding negative differential resistance between a low resistive state ON_{Th} and a high resistive state OFF_{Th} is a widely known feature of metal insulator metal structures, based on NbO_2 and related materials [1, 2]. From the application point of view threshold switching devices are highly interesting as selector device for redox-based resistive memories (ReRAM) in order to overcome the so called sneak path problem [3, 4]. The most common model for the threshold switching is given by the explanation of an insulator to metal transition IMT [5]. However, it has been shown that a Poole Frenkel (PF) barrier lowering in combination with a small Joule heating is able to explain the negative differential resistance [6-8]. In our previous study, we showed that the FTTR is able to explain a full threshold switching I - V curve [6]. The simulation results of the developed model are in great accordance with the measurements results of an NbO_x based MIM structure, as shown in Fig. 1. The FTTR effect stems from a positive feedback loop or self-accelerating process [6]. At the turn-on an electric field is applied, which lowers the barrier into the range of the thermal energy. At this point, the charge carriers overcome the lowered activation energy barrier. This leads to an enhancement in the conductivity, which again results in an increase in current and Joule heating. Due to this heat up the ratio of excited carriers increases again, which is the starting point of the positive feedback loop. Consequently, the threshold switching is a result of a thermal runaway process, which is triggered by the electric field dependent barrier lowering. In our previous study, we showed that the resistance of the memristive part R_M strongly influences the magnitude between the ON_{Th} and OFF_{Th} [6]. However, up to now, it is not clear under which circumstances the FTTR-type threshold switching is observed. In this study, we will show that the abrupt FTTR-type threshold switching is restricted to a special range of serial memory resistances. At a certain value for the memristive resistance R_M a sudden transition occurs that leads to a vanishing of the abrupt threshold switching character and transforms it into a continuously threshold switching without a hysteresis. Nevertheless, also for the continuous TS it is clearly possible to distinguish between a low resistive ON_{Th} and a high resistive OFF_{Th} state. This influence of the memory resistance to the TS defines a minimal possible jump in the current. Furthermore, it gives an important insight for the required conditions of the abrupt TS switching.

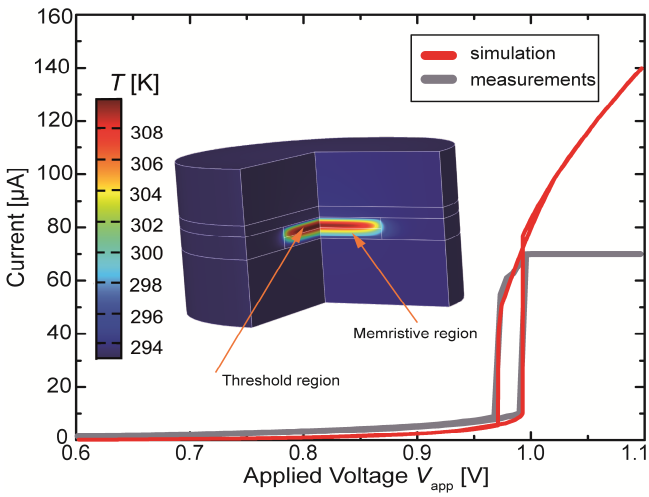

Fig. 1. $I - V$ characteristics of the FTTR type threshold switching (red) model in compairson with measurement (grey) obtained by an 1Th1M ReRAM memory cell. As inset the simulated axial symmetric structure is shown containing the metal electrodes and the insulating area. The filament in the middle is divided into a memristive region and a threshold switching region. The temperature distribution is taken at the onset voltage $V_{Th,ON}$.

II. Simulation Model

The simulation model is implemented in a two dimensional axial symmetric configuration, as shown in the inset of Fig. 1. The geometry consists of a top electrode of 25 nm Pt and 5 nm Ti. The bottom electrode consists of a 30 nm thick Pt layer. The insulating layer has a total layer thickness l_{layer} of 10 nm. The threshold switching occurs in a filamentary region consisting of two parts: a resistive region and the actual threshold switching region [6]. Consequently, a filamentary geometry is embedded in the middle of the layer with a radius of 30 nm. The filament consists of a threshold switching NbO_2 region and a memristive switching Nb_2O_{5-x} region, which is modelled as a static ohmic resistance. The filament surrounding material is treated as Nb_2O_5. A detailed overview about the geometry and the electrode material parameters is given in [6]. For the simulation, model the coupled heat equation

$$\rho_m C_p \frac{\partial T}{\partial t} - \nabla \kappa \nabla T = \frac{J^2}{\sigma} \tag{1}$$

and the current continuity equation

$$\nabla J = \nabla \sigma \nabla V = 0, \tag{2}$$

which are solved self-consistently by Newton-Raphson iteration steps. In equation (1) and (2) T defines the local temperature, V the local potential, σ the local electric conductivity, J the current density, κ the thermal conductivity, ρ_m the density of mass, and C_p the heat capacity. The thickness of the threshold region l_{Th} and the thickness of the memristive region l_M are 5 nm in accordance with a total layer thickness of 10 nm. The conductivity of the memristive region is adjusted to

$$\sigma_M = \frac{1}{R_M} \frac{l_M}{\pi r_{fill}^2} , \tag{3}$$

which results in a certain total resistance R_M for the memory region. The conductivity for the FTTR-type threshold switching is described using the intrinsic conductivity with an additional PF term due to the inherent polaron hopping conduction mechanism [6, 9]. As a result, the conductivity in the threshold region is given by

$$\sigma_{Th} = \sigma_0 \exp\left(\frac{\Delta W_A - \beta\sqrt{E}}{k_B T}\right) \tag{4}$$

with

$$\beta = \sqrt{\frac{e^3}{\pi \varepsilon_0 \varepsilon_r}} . \tag{5}$$

In equation (4) and (5) ΔW_A is the electron hopping activation energy, E the electric field, ε_r the high frequency dielectric constant, σ_0 the conductivity pre-factor, e the elementary charge, ε_0 the electric field constant and k_B the Boltzmann constant. The temperature boundary conditions are Dirichlet boundary conditions with a constant temperature of 293.15 K except for the top electrode, where the heat flux is set to zero. For the potential a zero current flux condition is used at the radial boundary. For the bottom and top electrodes Dirichlet boundary conditions are applied. The bottom electrode potential is forced to a ground potential of 0 V. At the top electrode a time-dependent triangular voltage sweep is applied with an amplitude of 2 V and a total duration of 35 ms. The modelling parameters are listed in Table 1. For the simulations the software package COMSOL™ is used.

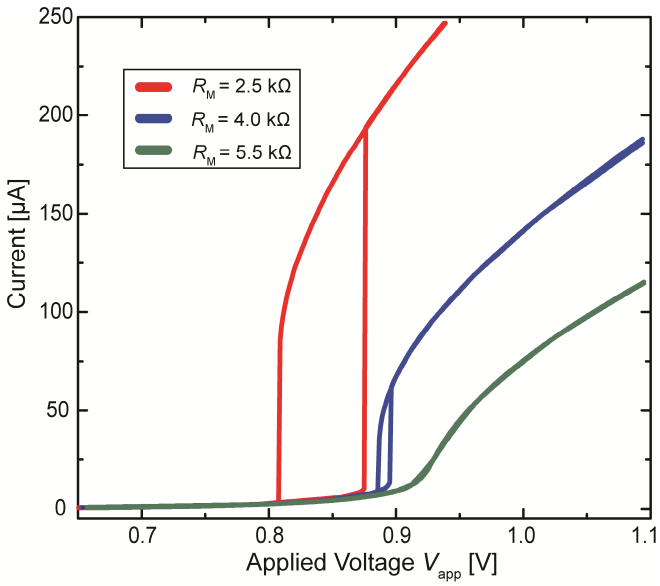

Fig. 2. *I–V* characteristics of the simulated FTTR type threshold switching using different memristive resistances. The red *I-V* curve with the lowest memory resistance shows a significant higher resistance jump and a greater hysteresis. With increasing resistance of the memristive part the resistance jump and the hysteresist decreases until the abrupt threshold switching vanishes (green curve).

TABLE I. MATERIAL CONSTANTS [6]

Parameter	**Value [Unit]**
σ_0	9.99 10^6 [S m^{-1}]
ΔW_A	0.66 [eV]
ε_r	9.5
κ	0.12 [W m^{-1} K^{-1}]

III. Simulation Results

The important aspect for this study is the stable ON_{Th} state, which determines the end of the thermal runaway. At the triggering point of the thermal runaway most voltage drops across the TS area due to the much lower conductivity in comparison to the memristive conductivity σ_M. According to equation (4) the conductivity in the TS region increases with the start of the thermal runaway effect. At some certain point the conductivity of the threshold region reaches the conductivity of the memory region, given by equation (3). This results in a stable ON_{Th} state, where the thermal runaway finishes. As shown in Fig. 2 different ON_{Th} states are accessible by the variation of the serial resistance R_M.

A. Variation of the resistance R_M

The resistance of the memristive region is varied and therefore the memrisitive conductivity defined by equation (3) is modified. The resulting *I-V* curves are shown in Fig. 2. By increasing R_M the hysteresis shrinks and vanishes finally for $R_M > 5.5$ kΩ. In addition, the switching magnitude decreases with increasing R_M. Fig. 3(a) contains the average electric field and temperature in the threshold region for the applied voltage sweep. As outlined before the thermal runaway mechanism is limited by the memristive serial resistance R_M. The reason is that the current increase and temperature increase is limited as soon as the conduction of TS region becomes similar to this of the memristive region. This acts like an interruption of the positive feedback loop of the FTTR and results in the stable ON_{Th} state. Consequently, the interruption of the positive feedback loop occurs at higher temperatures and a lower electric field in case of a reduction of the value R_M, as shown in Fig. 3(a). This is a consequence of a positive feedback loop, which is interrupted at higher currents. Hence, it is possible to adjust the FTTR-type threshold switching using an internal or as well an external serial resistance. Another important result is the transition of the abrupt TS into a continuously non-linear TS behaviour as shown in Fig. 2 and Fig 3. This continuous TS is characterized by the missing abrupt jump in the resistance and the vanishing of the hysteresis. Regardless of the missing abrupt switching the given continuous TS curve can still be splitted into an OFF_{Th} state and an ON_{Th} state, by the point of increasing current at the maximal electric field, as shown in Fig. 3(a). The electric field shown in Fig 3(a) clearly shows that a continuous kind of threshold switching occurs at the same turn-on electric field $E_{Th,ON}$. Consequently, the abrupt and the continuous TS occurs at the same turn-on voltage. Interestingly, the turn-off and turn-on electric fields become equal as soon as the abrupt TS transforms into a continuous TS ($E_{Th,OFF} = E_{Th,ON}$). The average temperature during TS shown in Fig. 3(a) exhibits similar to the *I - V* characteristics a transition from a hysteric behaviour to a continuous temperature increase for increasing R_M. Nevertheless, after the turn-on the temperature increase is significantly higher. Further important information can be extracted by the radial temperature distribution illustrated in Fig. 3(b). It shows that for the abrupt TS occurring for $R_M = 2.5$ kΩ a sudden temperature increase is observed. At $V_{Th,ON}$ the OFF_{Th} temperature distribution and the

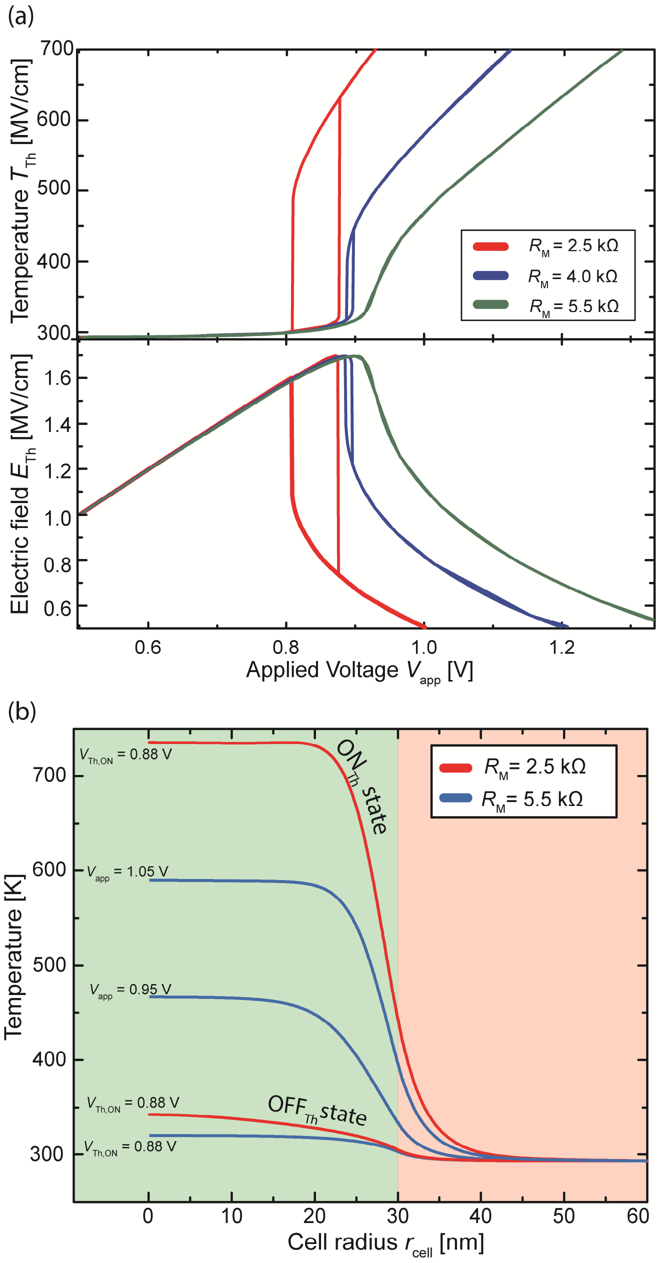

Fig. 3. (a) Average temperature and electric field in the threshold switching region for three different memristive resistances. (b) Radial temperature calculations in the axial center of the threshold region for the case of an abrupt FTTR-type threshold switching (red) at the onset voltage $V_{Th,ON}$ for the OFF_{Th} and ON_{Th} state. For the resistance of 5.5 kΩ (blue) with an contionus *I - V* curve several radial temperature distributions are shown.

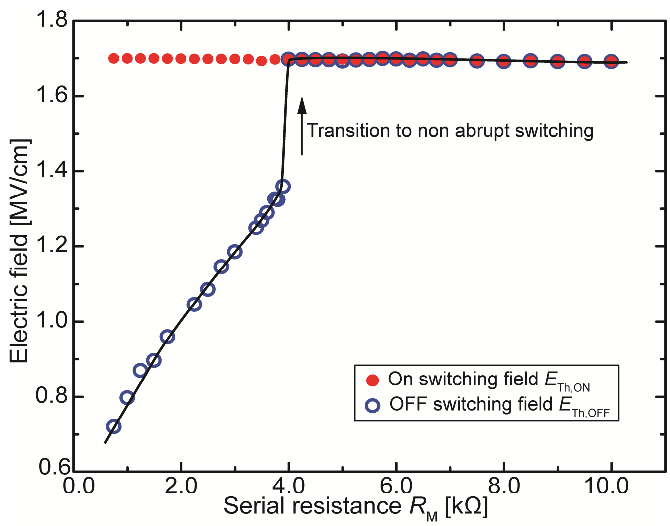

Fig. 4 The switching electric fields are determined by the average electric field in the TS region. The electric field for the turn-on $E_{Th,ON}$ is determined by the point where the electric field is reduced with increasing applied voltage, which equals the maximum of the averaged electric field. The turn-off electric field $E_{Th,OFF}$ is determined at the point of increasing electric field after the turn-on.

ON_{Th} distribution is given. For the ON_{Th} a wide plateau of constant temperature appears. In contrast, the OFF_{Th} temperature profile exhibits a local hot spot in the middle of the filament. For the continuous TS (@ $R_M = 5.5$ kΩ) the temperature does not increase suddenly. Temperature levels in between the two states of the abrupt TS are achieved. A detailed analysis of the different single temperature distributions of the continuous TS shows that during the temperature increase the plateau of the constant temperature is slightly broadening.

IV. Discussion

We have applied a systematic variation of the memristive resistance R_M, which acts like a serial resistance for the FTTR type threshold switching. In this study, we could show that the threshold switching is highly sensitive to the memristive resistance. The main reason for the increasing hysteresis and resistance switching for a decrease R_M is already explained in our previous study [6]. However, the vanishing of the abrupt TS is a new aspect, which needs to be discussed further. Only a slight increase of the R_M leads to a continuous increase in the current rather than an abrupt jump. The plot of the electric field in Fig. 3(a) shows that the turn-on voltages $V_{Th,ON}$ and the turn-on electric fields $E_{Th,ON}$ are very similar for both types of threshold switching. In case of an continuous threshold switching we find that $E_{Th,ON} = E_{Th,OFF}$, which is the same as $V_{Th,ON} = V_{Th,OFF}$. The dependence of both switching fields on R_M is shown in Fig. 4. It confirms that $E_{Th,ON}$ is almost R_M-independent and stays at the same level. In contrast, $E_{Th,OFF}$ depends strongly on R_M. The reason is that for a higher R_M a lower temperature is achieved in the ON_{Th} state, as shown in Fig. 3(a). Considering that, a critical ratio between thermal energy and reduced activation energy is required for the turn-off. This leads to the conclusion that the barrier lowering needs to be stronger for lower temperatures. Consequently, $E_{Th,OFF}$ increases with increasing R_M due to the lower temperature in the ON_{Th} state. At the R_M at which $E_{Th,OFF}$ equals $E_{Th,ON}$ a transition from the abrupt TS to the continuous TS is observed. As shown in Fig. 4 this transition occurs abruptly at an $R_M \approx 4$ kΩ. Consequently, a minimum resistance jump exists for the abrupt TS. The resistance for the ON_{Th} is determined by the memristive resistance $R_M \approx 4$ kΩ. The resistance of the high resistive OFF_{Th} state is given by the nearly constant resistance at the turn on electric field $R(E_{Th,ON})$. The shown difference between an abrupt TS and continuous TS may also explain the experimental results given in [10]. There, a threshold switching and a non-linear continuous *I-V* curve is observed for different layer thicknesses.

V. Conclusion

We investigated the threshold switching based on a novel FTTR threshold model. This threshold switching is based on a combination of a PF barrier lowering and Joule heating. In our investigation we performed an analysis on an increasing serial resistance, which comes from a memristive switching layer R_M. It shows that an increase has a significant influence on the threshold switching. At a certain R_M the abrupt switching transforms into a continuously threshold switching, where the steep slope and hysteresis vanishes and transforms into a non-linear $I - V$ curve. Our analysis reveal that the transition between both switching modes occurs suddenly at a certain resistance value. This leads to a minimum resistance change for the abrupt threshold switching. Our simulation results imply that other parameters like the layer thickness, activation energy or thermal conductivity could also define a minimum resistance change. Additionally, different conduction mechanisms of the series resistance have potentially a big impact on the threshold switching properties.

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