New developments in a finite-volume electro-thermal solver coupled with the Level Set Method to study crystallization mechanisms in PCM devices

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***Abstract*— A macroscopic model for Ovonic Threshold Switching and an improvement of the analytical models for GST electrical conductivities are introduced in a PCM simulation tool based on a GST thermodynamic model, a local and transient crystallization model coupled to an electro-thermal solver. Simulations on the µtrench structures are used to illustrate the local occurrences of electronic switching and how it opens the way to crystallized domains.**

PCM simulation; Ovonic Threshold Switching; Crystallization

I. INTRODUCTION

Phase Change Memory (PCM) is an emerging technology for non volatile memory devices which relies on reversible and fast switching between the amorphous and crystalline phases of chalcogenide materials, such as $Ge_2Sb_2Te_5$ (GST), that exhibit very different conductivities at room temperature. Recent developments in a PCM simulation tool based on a Finite Volume electro-thermal solver coupled to the Level Set Method [1] are presented. A macroscopic model for Ovonic Threshold Switching (OTS) and an improvement of the analytical models for GST electrical conductivity are introduced. Our objective is to provide an electrical model based on few parameters that reproduce as faithfully as possible the current-voltage measurements for GST. A local and transient crystallization model is coupled to the electro-thermal solver. Simulations on µtrench device are presented to illustrate the local occurrences of electronic switching and how it opens the way to crystallized domains.

II. A MACROSCOPIC MODEL FOR OVONIC THRESHOLD SWITCHING

A. *Presentation of the model*

The electro-thermal solver relies on the coupled system of partial differential equations formed by the current conservation equation and the heat transfer equation:

$$\mathrm{div}\,(-\sigma\ \mathbf{grad}\ V) = 0, \qquad (1)$$

$$\rho\ C_p\ \partial T/\partial t\ = \mathrm{div}\,(k\ \mathbf{grad}\ T) + \ \mathbf{j}^{\,2}/\sigma, \qquad (2)$$

where σ, ρ, C_p and k respectively stand for the materials electrical conductivity, density, heat capacity and thermal conductivity.

OTS is the reversible switching mechanism that takes place in the amorphous GST between an electrical low conductive state (off-state) and a high conductive state (on-state). In the previous version of this solver [1], OTS was only modeled through an electric field exponential dependence of the amorphous GST electrical conductivity. We propose to go further by introducing a discontinuity in the electrical conductivity of the amorphous GST. The macroscopic model used for OTS relies on the introduction of a high conductivity amorphous state. The electrical conductivity in amorphous GST is modelled by an off-state if the local electric field (E) is lower than a threshold electric field (E_{th}) and if the temperature is lower than the melting temperature (T_m) and switches to an on-state if the local electric field becomes higher than E_{th}. Conductivity for the amorphous on-state model is considered the same than in crystalline GST:

$$\sigma_{on} = \ \sigma^0_{cr}(E,T)\ \exp(-E_{cr}/(kT)) \quad (3)\ ,$$

where $\sigma^0_{cr}(E,T)$ is a pre-factor analytic function illustrated by Fig. 1 [2].

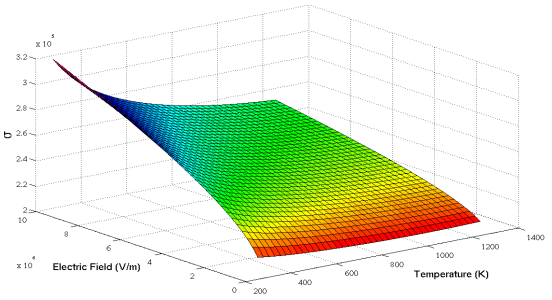

Figure 1. Function $\sigma^0_{cr}(E,T)$.

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The model used for the off-state is:

$$\sigma_{am} = (A/E)\exp(-E_{am}/(kT))\sinh(BqE/kT) \quad (4),$$

where the term sinh(BqE/kT), similar to that used by Ielmini [3], is derived from the Poole-Frenkel (PF) model. By using PF model, we use a largely shared physical model in the literature of a traps limited conduction regime in the off-state amorphous state. Once the material has locally switched to the on-state, our model includes a possible recovery of the off-state; if the density of current is locally lower than a holding current density (J_{hold}) to maintain the material in on-state, the conductivity is locally turned back to off-state. Our OTS model relies on two parameters E_{th} and J_{hold}. Constant values inspired from literature [4, 5] are used for these parameters ($E_{th} = 3x10^7$ V/M and $J_{hold} = 10^9$ A/m^2).

B. Introduction of the amorphous on-state in the algorithm

In each cell of the PCM mesh, the phase has one of the following values: crystalline, melted, amorphous off-state or amorphous on-state. The complex evolution of the interface between crystalline and amorphous phase during nucleation and growth is implemented using the Level Set Method [1]. The phase is evaluated from the level set function, the temperature and a field that indicates if electronic switching has locally occurred or not. Splitting of the amorphous phase in two electrical states (low and high conductive) does not modify the interface separating crystal and amorphous phases so the level set implementation is not modified.

III. CALIBRATION OF THE ON-STATE AND OFF-STATE ELECTRCIAL CONDUCTIVITY MODELS

The on-state (respectively off-state) electrical conductivity is calibrated for GST using a low field pulse (Vmax 0.4 V) which is applied to a 100 nm GST based PCM plug type initially in a crystalline state (respectively previously amorphized by a stair-case up procedure) at 25 °C, 50 °C and 80 °C.

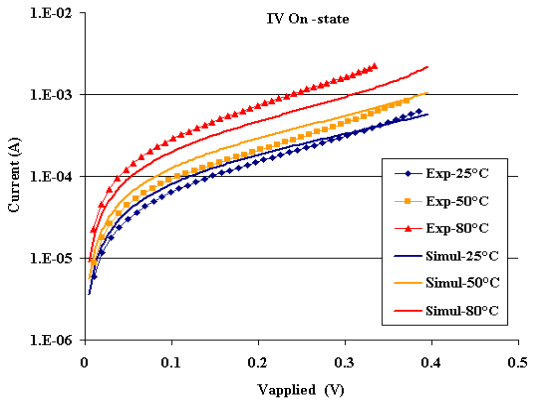

Figure 2. IV on-state with $E_{cr} = 0.149$ eV.

As plotted in Fig. 2 and Fig. 3, a set of parameters corresponding to good agreement between the low field IV simulated and experimental curves has been found. The deviation from the experimental curve that we observe in the simulation at 80 °C in amorphous off-state might be minimized by taking into account a probability of emission contribution to conductivity as reported in [6].

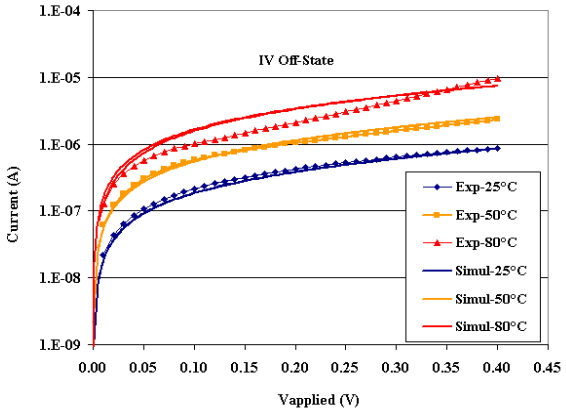

Figure 3. IV off-state with $E_{am} = 0.39$ eV, $A = 3.6\ 10^{13}$ A/m^2 and $B = 3.6\ 10^{-9}$ m.

Current-voltage curves obtained by simulation and by electrical characterization for a 100 nm GST µtrench device are plotted in Fig. 4. The device is first partially amorphized. In this particular simulation the device is switched to the steady on-state and the intercept of the extrapolated linear part of the on-state with the V-axis defines the holding voltage (V_h) [5]. The threshold voltage given by the simulation is slightly overestimated in comparison with the experimental threshold voltage (V_{th}) and this work must be completed by more extensive comparison; nevertheless, the simulated curve reproduces qualitatively the experimental curve and this result illustrates the ability of our model to reproduce correctly the complete current-voltage characteristic of an amorphous switch.

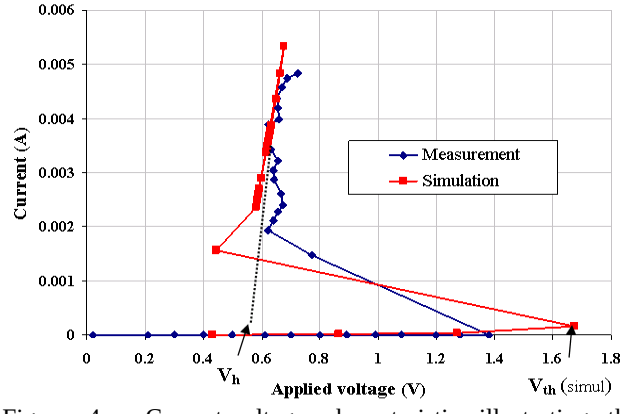

Figure 4. Current-voltage characteristic illustrating the amorphous switch.

Once the electrical conductivities in the on-state and in the off-state have been calibrated, the work must go on with the calibration of the thermal properties of GST and of the properties of crystallization model. This work is being carried out for GST. With the values actually used, the reset-set and set-reset transitions obtained by simulation are in qualitative agreement with those obtained by electric characterization as illustrated by Fig. 5 where the low field resistance is plotted versus applied courant for both simulation and electrical characterization. The curve plotted in Fig. 5 is obtained by applying 50 ns programming pulses to a plug type PCM device with a 100 nm GST layer initially amorphized. The first part of the curve is the SET-RESET transition (from Current = 0 to 0.015) and the second part is the SET-RESET transition.

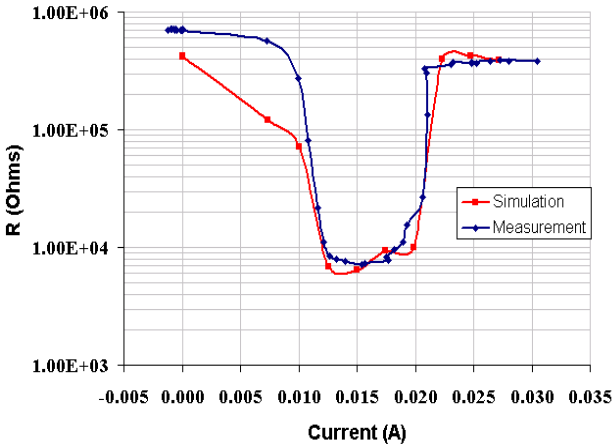

Figure 5. RESET-SET and SET-RESET transitions.

The RESET-SET curve correctly reproduces the current at which the recrystallization of the device is maximal. The simulated SET-RESET curve is in very good agreement with the simulated one. The slight difference observed in the RESET-SET transition between simulated and measured resistances comes from the parameters of our crystallization model not fitted at low temperature on our particular GST. By evidence, overestimating even slightly crystalline growth speed can lead to overestimated final recrystallized volume.

IV. COMPARISON WITH OUR PREVIOUS ELECTRICAL CONDUCTIVITY MODELS

In the previous version of our software presented in [1], crystalline and amorphous GST conductivities were given by the following expressions:

$$\sigma_{cr} = \sigma^0_{cr} \exp(-E_{cr} / (kT)), \quad (5)$$

$$\sigma_{am} = \sigma^0_{am} \exp(-E_{am}/(kT)) \exp(E/E_0) \quad (6),$$

$\sigma_{cr}(T)$ given by (5) approaches the constant value σ^0_{cr} when the temperature gets higher than the melting temperature. On the contrary, our model assumes a linear behavior of the on state electrical conductivity in the range of temperature that we get in our devices during programming pulses. This difference is illustrated in Fig. 6, where the values of electrical conductivity given by $\sigma_{cr}(T)$ (blue curve) and given by $\sigma_{on}(T,E)$ (red curve) are plotted versus temperature for a fixed electric field (E = 0).

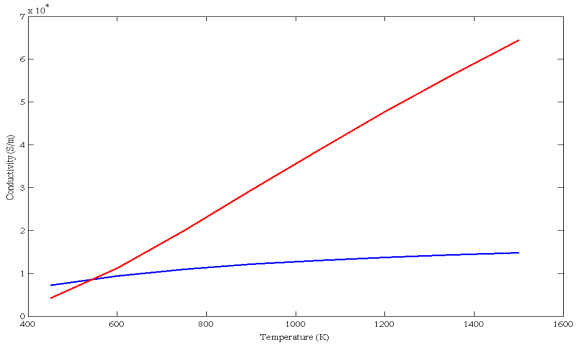

Figure 6. Curves $\sigma_{on}(T)$ red and $\sigma_{cr}(T)$ blue.

Chalcogenide alloys even in their low resistivity state show a non-ohmic behavior characterized by an increase of the electrical conductivity with increasing electric field. The model σ_{cr} defined by (5) can not mimic a non-ohmic behavior at low voltages due to the absence of dependency on the electric field. On the contrary, our model with an electric field dependent pre-factor $\sigma^0_{cr}(E,T)$ can mimic a non-ohmic behavior at low voltages.

V. SIMULATION RESULTS ON THE MICROTRENCH DEVICE

A µtrench device with a 100 nm GST layer corresponding to a device fabricated in LETI is studied. The simulated structure represented in Fig. 8 is a half structure obtained from the schematic µtrench structure depicted in Fig.7.

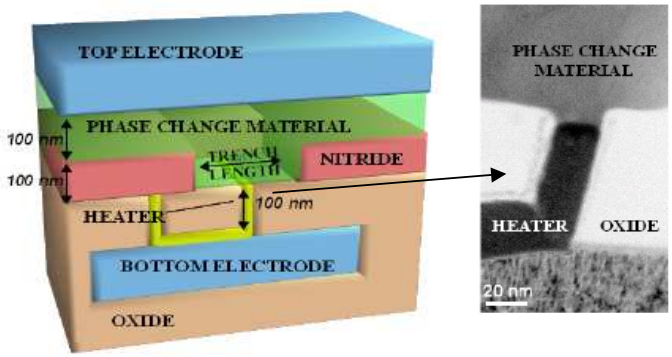

Figure 7. Left: simplified schematic of µtrench structure. Right: TEM image of the interface between heater and phase change material.

Two-dimensional Cartesian coordinates are used and half of the domain is simulated using its symmetry. The mesh is refined in the PCM domain in the PCM domain in order to obtain a cell size of 2 nm compatible with the critical size of nuclei in our crystallization model.

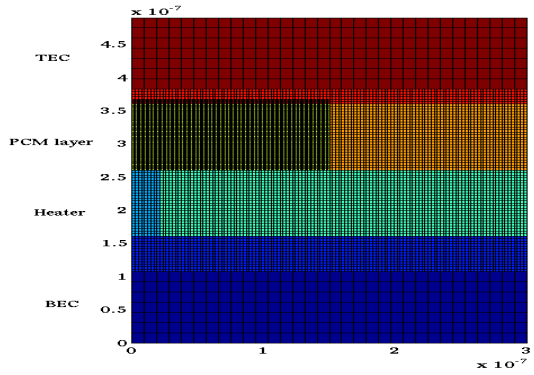

Figure 8: Schematic half structure of the µtrench with the mesh size reported. The material for Top Electrode (TEC), Bottom Electrode (BEC) and Heater are respectively Copper, Al-Cu alloy and Tungsten Silicide. The PCM trench is encapsulated in nitride.

A 100 ns set pulse of 3 V is applied and the simulation starts from a GST domain partially amorphous as illustrated by Fig.9a. An external resistance of 10^3 Ω is coupled to the device. The formation of a filament of amorphous high conductive GST occurs in the area where electric field gets higher that E_{th} as illustrated by Fig. 9b, Fig. 9c and Fig. 10.

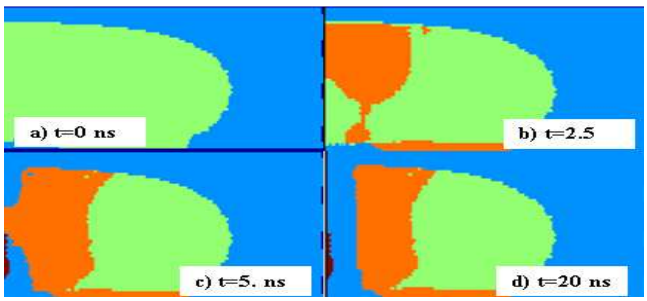

Figure 9. Visualisation of the phase (blue: crystal, green: amorphous off-state, orange: amorphous on-state, brown: melted)

The formation of this filament creates a path of conduction from the heater to the crystalline GST. The size of the filament increases, and the high density of current in the on-state amorphous GST progressively induces thermal conditions where nucleation and growth are highly probable. At t = 20 ns, part of the amorphous GST has crystallized (Fig.9d). Our tool is efficient in giving an insight on dynamics of crystallization.

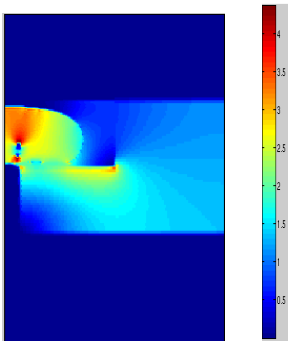

Figure 10. Electric Field (V/m) at t=2.5 ns

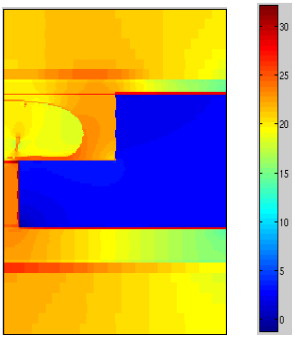

Figure 11. Log of current density (A/m^2) at t=2.5 ns

VI. CONCLUSION

A macroscopic model for Ovonic Threshold Switching and improved analytical models for GST electrical conductivity are introduced in a Finite Volume electro-thermal solver. The models for GST electrical conductivities are calibrated. We demonstrated the ability of our model to reproduce qualitatively the electronic switch (typical of phase change material), the conduction in the on-state and the possible recovery of the off-state. Simulations on µtrench device are presented to illustrate the local occurrences of electronic switching and how it opens the way to crystallized domains. This electro-thermal model, coupled to a local and transient crystallization model, can be extended to other chalcogenide materials starting directly from parameters extracted from electrical results. Our simulation tool is developed to help the engineering process of our PCM devices, by foreseeing the electrical behaviour of new device structures and its dependency on new phase change materials.

REFERENCES

[1] A. Glière, O.Cueto, J.Hazart, "Coupling the Level Set Method with an electro-thermal solver to simulate GST based PCM cells," SISPAD 2011, Sept 2011 Osaka, Japan "

[2] G.Navarro et al., "unpublished,"

[3] D.Ielmini, Y.Zhang, "Analytical model for subthreshold conduction and threshold switching in chalcogenide-based memory devices," Journal of Applied Physics vol. 102, 054517 (2007)

[4] M. Nardone, V.G Karpov, D.C. S. Jackson, I.V. Karpov , "A unified model of nucleation switching,"Applied Physcis Letters 94, 103509 (2009) .

[5] M. Nardone, V.G Karpov, I.V. Karpov, "Relaxation oscillations in chalcogenide phase change memory," Journal of Applied Physics vol. 107, 054519 (2010)

[6] E. Voronkov, "Calculation of threshold voltage for phase-change memory device", Journal of Non-Crystalline Solids, vol. 353, 2591-2594 (2007)