Phase-Field Simulations for RF Switches: Highlighting the Benefits of GeTe over GST

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***Abstract*— To better understand the crystallization mechanism of phase change material, the phase field method is used for the first time in simulations of the switching dynamics of RF switches. This method allows reproducing the nucleation and growth of the crystalline phase during amorphization and crystallization of the PCM. In this work, the quenching behavior of GeTe is compared with that of GST. The presented observations are consistent with the expected crystallization behavior and kinetics of each material. This work demonstrates the interest of the phase field model in PCM RF Switches simulation and highlights the interest of using GeTe rather than GST to obtain better amorphization quality in phase change materials.**

Keywords—Phase field, COMSOL, RF switch, PCM, GeTe, GST

I. INTRODUCTION

For RF signal transmission between antennas, several types of RF switches can be used for signal routing. The work presented here focuses on RF switches using phase change materials (PCMs). The switch relies on reversible transitions between the amorphous and crystalline phases of the PCM material, which exhibit highly contrasted electrical conductivities at room temperature. The crystalline phase, characterized by high conductivity, is obtained by heating the PCMs up to their crystallization temperature and for sufficient time for the atoms to rearrange into the crystalline structure. In contrast, the highly resistive amorphous phase is obtained by heating the PCMs to their melting point, followed by rapid quenching during which the PCM, having no time to recrystallize, solidifies into the amorphous phase. The Phase Field Method (PFM) can be used to simulate the phase changes in PCMs. The first part of this paper presents an implementation of the phase field method coupled with an electrothermal solver and applied for the first time, to our knowledge, to RF switches simulation. It provides a better understanding of the differences in phase change mechanisms between materials. Finally, a comparison between GeTe and GST is presented in the second part.

II. ELECTROTHERMAL SIMULATIONS

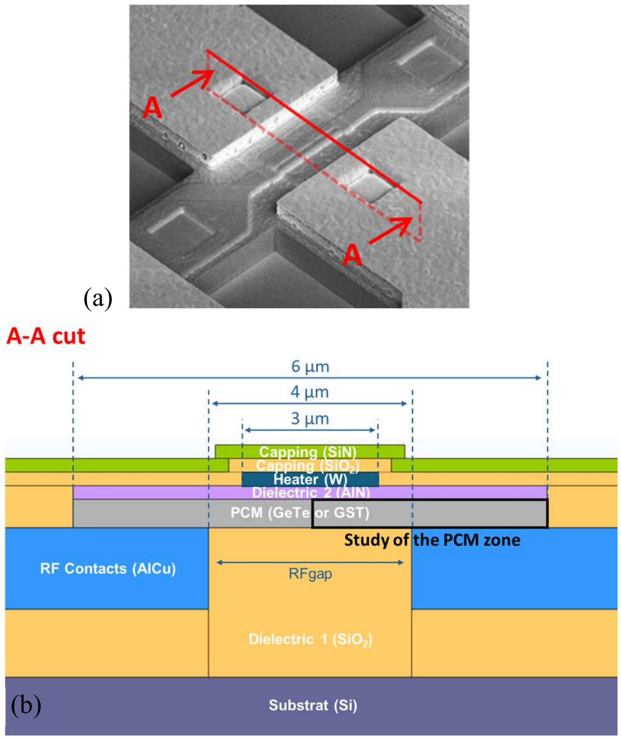

Fig. 1(a) Photograph of a PCM RF switch with a red rectangle representing the plane in which the layout in (b) was designed.

Our model was designed using the Finite Element Method (FEM) with COMSOL Multiphysics®. It represents a 2D cross-section of a PCM RF switch, taken at its mid-length, as shown by the red rectangle in Fig. 1(a). The structure of the model is presented in Fig. 1(b). A PCM (GeTe or GST) connects two RF contacts and allows to either block or transmit signals between the electrodes. The heat required to change the state of the PCM is provided by a heat source applied to a thermo-resistive element called "heater." This heat is mainly dissipated from the PCM by the RF contacts and the substrate, which are excellent thermal conductors. The other layers are dielectrics used to confine or diffuse heat and electrically isolate the heater from the rest of the switch. More details on the role of each layer and ways to modify the switch performance are provided in [1].

The stability of the OFF-state is directly improved with the size of the amorphous domain which, itself, results from the shortest possible quenching time. Power handling, OFF-state capacitance (C_{OFF}) and resistance ratio between OFF and ON states (R_{OFF}/R_{ON}) can also be improved by accelerating quenching. A thermodynamic phase-change model is needed to assess the impact of quenching changes on RF switches performance. We could not find a suitable thermodynamic phase field solver in commercial tools and

TABLE 1 : MICROSCOPIC PARAMETERS OF GST AND GETE

Description	**Symbol(unit)**	**GST**	**GeTe**
Density	$\rho\ (kg/m^3)$	6150	5770
Interatomic distance	d (A)	3	3
Melting temperature	$T_m\ (K)$	880	997
Latent heat of melting	$L\ (J/m^3)$	$1.1\ 10^9$	$1.36\ 10^9$
Glass temperature	$T_g\ (K)$	353	373
Viscosity parameter a	a	4.2	4.9
Viscosity parameter b	b	2.4	2.7
Interface energy cristal/amorphous	$\sigma_{ac}\ (J/m^2)$	0.1	0.13

TABLE 2 : THERMODYNAMIC PARAMETERS OF CRYSTALLIZATION MODEL

Description	Symbol	Expression
Free energy difference	$\Delta G\ (J/m^3)$	$\frac{L(T_m - T)}{T_m}$
Nucleation barrier	$\Delta G^*(J)$	$4\frac{\sigma_{ac}^3}{27\Delta G^2}$
Nucleation rate	$I(x,y,t)\ (s^{-1}m^{-3})$	$C_N \exp\left(-\frac{\Delta G^*}{kT}\right)$
Growth velocity	$V_g(m/s)$	$d\mu\left(1-\exp\left(\frac{\Delta G d^3}{kT}\right)\right)$

decided to adapt the phase-field model presented in [2] to RF switches.

III. COUPLING WITH THE PHASE FIELD METHOD

We have coupled the electrothermal solver of the FEM software with a phase change model based on the phase field method completed by a stochastic nucleation model.

The phase field method relies on an order parameter η that represents the local crystallinity of the PCM:. $\eta = 0$ in the amorphous phase and $\eta = 1$ in the crystalline phase. The phase microstructures evolution is determined by the Allen-Cahn equation:

$$\frac{\partial \eta}{\partial t} = -L_\eta\left(\frac{\partial f(\eta)}{\partial \eta} - \kappa\nabla^2\eta\right)$$

where L_η is the rate of this evolution, $\frac{\partial f(\eta)}{\partial \eta}$ is the evolution of the free energy potential, and $\kappa\nabla^2\eta$ represents the energy costs necessary to maintain a diffuse interface between the two phases. The kinetic coefficient L_η can be calculated from the crystalline growth velocity V_g by:

$$L_\eta = \frac{V_g R_c}{\kappa}$$

where R_c is the curvature radius of the interface that we will consider as equal to the radius of critical nuclei.

The PFM is completed by a stochastic nucleation model, which ensures the apparition of crystal nuclei inside the amorphous phase, which relies on the classical nucleation theory. The expected number of critical nuclei generated during dt in each unit volume h^3 is calculated by:

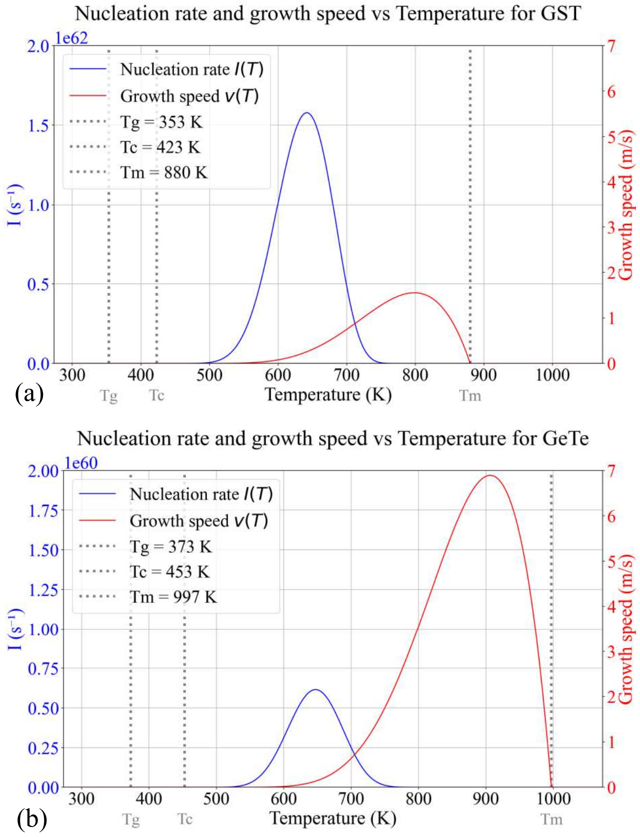

Fig. 3 Evolution of the nucleation rate and growth velocity along the temperature for (a) GST and (b) GeTe

$$N(x,y,t) = I(x,y,t).dt.h\text{^}3.$$

As given in TABLE 2, the nucleation rate and the crystalline growth velocity both rely on the main microscopic thermodynamical parameters of the PCM. The parameters C_N (respectively μ), is a pre-factor of the nucleation rate (respectively of the growth velocity). μ depends on the temperature and represents the frequency of accretion of atoms to the nuclei. In Fig. 3, nucleation rate and crystalline growth velocity are plotted for GST and GeTe from the microscopic parameters given in TABLE 1 and the formula given in TABLE 2. GST nucleation rate is higher than that of GeTe meanwhile the crystalline growth velocity is lower. The differences in the crystallization mechanisms observed for GST and GeTe come from the differences in these microscopic parameters.

Further details on the crystallization model and its implementation are provided in [2].

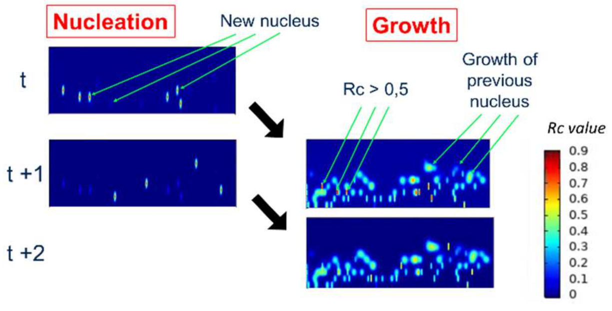

Fig. 2 Illustration of the nucleation and growth mechanisms

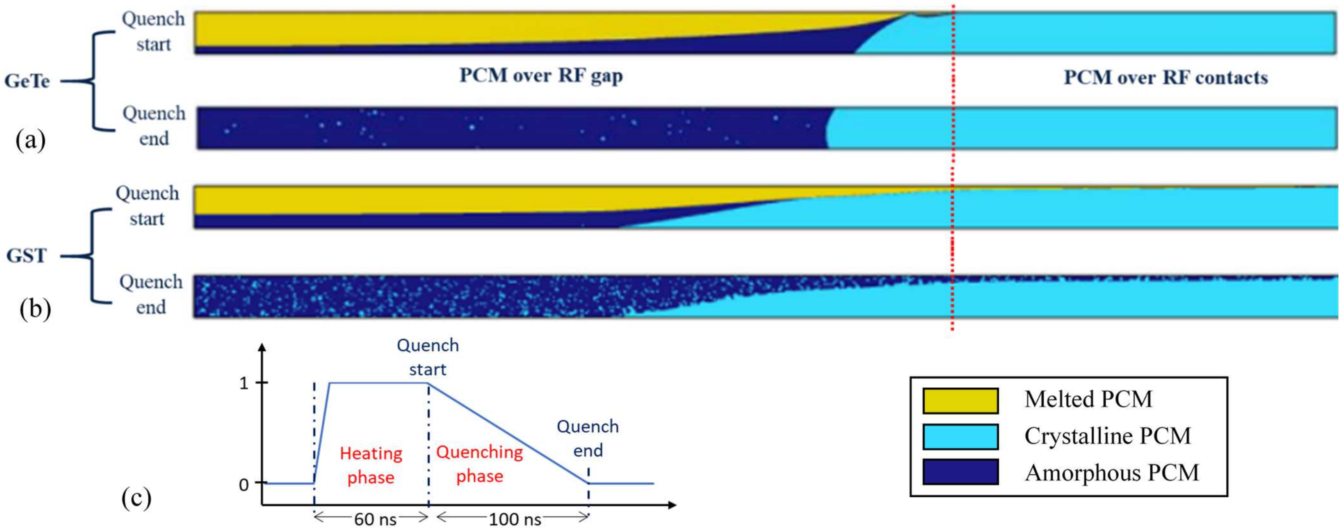

Fig. 4 (a) States of GeTe at the start of the quench and after the quench. (b) States of GST at the start of the quench and after the quench. (c) (left) Amorphization pulse used to actuate the PCMs. (right) Association of the states to the colors used in Fig. 2.a. and Fig. 2.b

The PFM is a diffuse interface method that requires meshing the interface between the amorphous and crystalline domains with a cell size of approximately 1 nm^2. This numerical constraint on the cell size induces a prohibitive simulation time for a transient simulation over the whole amorphization pulse. To overcome this issue, a two-step simulation approach is used: the heating phase of the switch is performed using a stationary approach, while only the quenching phase is performed through a transient approach. The downward ramp of the heat source pulse, representing the quenching phase, is limited to 100 ns. This limits the duration for which the PCM can remain between the melting and the crystallization temperature, but remains sufficient for crystallization to occur.

The component used in the first step, modeling the entire switch in two dimensions, is used to drive the amorphization pulse through the heat source applied to the heater. All parts that reached the melting temperature adopted the properties of a highly resistive PCM, i.e., the amorphous state. This first component also played the role of nucleation, allowing the random introduction of critical nuclei in the amorphous domain at each time step. The second component, modeling only the PCM part, was used to simulate the growth mechanism both from nuclei and from the neighboring elements. The mesh was finer in this component due to the resolution of the Allen-Cahn equation. This resolution, as previously introduced, requires a meshing of the interfaces. During the simulation, the two components were alternately run, as shown in Fig. 2.

During crystallization, nucleation and growth interplay and our algorithm reproduces that. First, nuclei were randomly introduced in the PCM amorphous parts. The apparition of critical nuclei take place if the temperature in the amorphous phase is between the crystallization and melting temperatures. Then, at the next time step, the nuclei introduced at the critical size (corresponding to nuclei with a value greater than 0.5) can grow, while the smaller ones disappear. The simulation then returned to the first component to perform a new nucleation, before moving to the next timestep and repeating the process until the end of the amorphization pulse. During this process, all the PCM parts transformed into nuclei adopted the properties of a crystalline PCM.

IV. APPLICATION TO PCM RF SWITCHES MODELS

GeTe is currently regarded as the best phase change material for implementing PCM RF switches. Compared to other chalcogenides such as GST, used in Non-Volatile Memories, GeTe allows to realize RF switches with higher R_{OFF}/R_{ON} ratio (about 10^4) and higher ON-state conductivity for better signal transmission. In addition, GeTe crystallization temperature is higher than that of GST, thus improving phase stability. Finally, upon quenching, its recrystallization is growth-dominated, unlike that of GST, rather nucleation-dominated [3]

A comparison of the behavior of GeTe and GST, used as the PCM in an RF switch, during an amorphization pulse was carried out (Fig. 4). The PCM area observed in these simulations is illustrated by the red rectangle in Fig. 1(b). The stationary studies during the heating phase were first carried out so that, for both PCMs, the central part is melted and the part above the contacts remains crystalline. The transient studies were then performed for the quenching phase. The states of both PCMs, observed at the start and end of their quenching processes, are shown in Fig. 4.a and Fig. 4.b. As can be seen, the crystallization in GeTe mainly occurs through the growth of pre-existing crystalline regions with few crystalline nuclei appearing in the amorphous region. Conversely, nucleation is the main crystallization mechanism observed for GST with almost no growth. These behaviors align with the expected characteristics of both PCMs, represented in Fig. 3.

V. CONCLUSION

We have coupled a FEM electrothermal simulation of a switch RF with a phase change model based on the phase field method. It is the first time, to our knowledge, that the phase field method is applied to RF switches simulation. Although this method remains qualitative, due to the uncertainty around the microscopic parameters it relies on, it provides a better understanding of the crystallization dynamics of GeTe and GST. We explained, in this work, that the different crystallization dynamics in GeTe and GST come from differences in microscopic parameters of the two PCMs. GeTe has a much lower nucleation rate than GST; consequently, the lower amount of crystalline nuclei in the GeTe amorphous region after the quench will induce a higher breakdown voltage of the amorphous phase. This confirms that this material is more suitable than GST to deliver good power handlings in RF switches. More detailed observations could be obtained if the downward ramp of the heat source pulse was extended, allowing for more recrystallization in both PCMs. An improvement in the accuracy of the thermal simulations could be achieved by a 3D coupling of the PFM with the electrothermal solver. However, this would result in considerably longer simulation times.

VI. ACKNOWLEDGMENT

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