Inverse heat conduction problem in a phase change memory device

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Abstract. An inverse heat conduction problem is solved considering the thermal investigation of a phase change memory device using the scanning thermal microscopy. The heat transfer model rests on system identification for the probe thermal impedance and on a finite element method for the device thermal impedance. Unknown parameters in the model are then identified using a nonlinear least square algorithm that minimizes the quadratic gap between the measured probe temperature and the simulated one.

1 Introduction

In a previous study [1], we demonstrated that the scanning thermal microscopy (SThM) is a very efficient tool to perform the thermal investigation of a phase change memory device at the microscale. In previous studies, the thermal properties of each material involved in a phase change memory as well as the thermal boundary resistances (TBR) at the interfaces between those materials have been measured in specific configurations, generally as thin films [2-4]. It is then questionable about the reliability of those properties, mainly at the level of the TBR, considering the device itself. The goal of this paper is to implement an inverse approach in order to identify the parameters that are involved in the model for the heat transfer within the SThM experiment.

The phase change material (PCM) is the Ge2Sb2Te5 (GST) very well known alloy [6] that shows a rapid and reversible phase-change switching from amorphous (α) to face centered cubic (fcc) metastable and hexagonal close packed (hcp) stable crystalline phases. The amorphous-to-crystalline transition is achieved by heating the GST above the glass transition temperature that is 130°C for α to fcc transition while it is around 300°C for the fcc to hcp transition. A remarkable, and one of the most interesting features concerning the practical implementation of the PCM in microelectronics, is that the GST electrical resistance varies along decades according to the crystalline state [7]. The practical functioning of the device is described in [1]. During the past ten years, PCM attracted large attention thanks to their maturity and their amazing performances. Nevertheless, numerous challenges remain regarding the bit retention time at elevated temperature that implies a highest thermal stability of the amorphous state at high temperature, the fastest transformation speed with a low pulse current, the cyclability and finally the scalability implying that the switching properties have to be maintained at dimensions well below tenth of nanometers. With those objectives, it has been shown that confinement of phase change materials, in a µ-trench for instance as presented in the paper of Lai et al. [8], enhances Joule’s effect efficiency and highly reduce the reset current. However, we have to mention that other solutions are envisaged as that of implementing the phase change material as a nanowire with very low cross-section area [9]. The device developed by CEA-LETI (see Fig. 1) is constituted around a cylindrical trench of crystalline GST surrounded by silicon nitride. The layer under the GST is the classical titanium nitride layer that will play the role of the bottom electrode, namely the heater. The PCM is surrounded by silicon nitride (SiN) that acts as the electrical and thermal insulator, with the additional feature to limit the thermal cross-talk between neighbourhood memory cells. The thickness of the GST cylindrical wall is 30 nm and its thickness at the bottom is 60 nm. Thermal properties of the materials at room temperature have been the subject of previous studies and they have been reported in Tab. 1.
Figure 1. At the left: small area of the memory device pattern; At the right: cross-section of one phase change memory cell (cylindrical revolution). Device developed at CEA-LETI.

Table 1. Thermal properties of materials involved in the phase change memory cell ($k$: thermal conductivity, $\rho$: density and $C_p$: specific heat, $\Theta_D$: Debye temperature, $v_T$: phonon transverse velocity, $v_L$: phonon longitudinal velocity) at room temperature. *Cu content being very low in the AlCu alloy, data for Al have been considered.

| Material   | $k$  (W.m$^{-1}$.K$^{-1}$) | $\rho$ (kg.m$^{-3}$) | $C_p$  (J.kg$^{-1}$.K$^{-1}$) | $\Theta_D$ (K) | $v_T$ (m.s$^{-1}$) | $v_L$ (m.s$^{-1}$) |
|------------|--------------------------|----------------------|-----------------------------|----------------|-------------------|-------------------|
| Si         | 131                      | 2329                 | 700                         | -              | -                 | -                 |
| SiO$_2$ [10] | 1.4                     | 2200                 | 787                         | -              | -                 | -                 |
| AlCu*      | 238                      | 2700                 | 900                         | -              | -                 | -                 |
| Ti [5]     | 13                       | 4500                 | 540                         | -              | -                 | -                 |
| TiN [5]    | 33.6                     | 5400                 | 220                         | 580            | 5110              | 10200             |
| GST (α) [3] | 0.18                    | 5870                 | 218                         | 136            | 1350              | 2250              |
| GST (fcc) [3] | 0.45               | 6270                 | 205                         | 197            | 1914              | 3190              |
| a-Si$_3$N$_4$ [10] | 2.1                 | 2900                 | 400                         | 985            | 6200              | 10300             |

The thermal boundary resistance (TBR) at the different interfaces between the GST and the surrounding material are more or less well known. They cannot be ignored since a fast calculus shows that they are comparable to the ratio between the thickness and the thermal conductivity of the GST. The TBR at the interface between the GST and the TiN has been the subject of several studies and it was found that it varies significantly according to the GST state. In addition, it was found to be higher than the prediction based on the diffuse mismatch model (DMM) whose asymptotic expression for the high temperature in the Debye approximation is [11]:

$$\tau^\text{DMM}_{\text{GST-SiN}} = \frac{4}{\tau^\text{SN-ST}_\text{Sn,TiN} \quad \rho^\text{ST}_\text{Sn,TiN} \quad C^\text{ST}_p,\text{Sn} \quad v^\text{ST}_T}$$

where

$$\tau^\text{SN-ST}_\text{Sn,TiN} = \sum_{j=1}^{3} v_{j,\text{Sn}}^{-2} \left( \sum_{j=1}^{3} v_{j,\text{Sn}}^{-2} + \sum_{j=1}^{3} v_{j,\text{TiN}}^{-2} \right)$$

denotes the phonon transmission coefficient that is calculated from the longitudinal and transverse phonon velocities for the two materials separated by the interface. The TBR at the interface between GST and SiN has not been measured so far to our knowledge. Using the DMM leads to a relatively low TBR as $5 \times 10^{-4}$ K.m$^{-1}$.W$^{-1}$. However, the Debye temperature for SiN is larger than that of TiN that is already high compare to that of GST. Therefore, a higher TBR at the GST-SiN interface is reasonably expected.

2 Scanning Thermal Microscopy (SThM) technique

The SThM has been implemented within the $3\omega$ mode with the frequency ranging from the DC up to 5 KHz [12]. Anasys Comp. provided the commercial probe that is a Si$_3$N$_4$ cantilever on which is deposited a palladium (Pd) strip at the tip. The curvature radius of the apex is about 100 nm. We used
a commercial AFM provided by Nanosurf Company. The experimental setup is rather classical although lot of caution have to be put on the electronics that allows extracting and measuring the third harmonic of the voltage drop that is related to the probe temperature thanks to the thermal coefficient of the Pd.

3 Heat transfer model and sensitivity analysis

A model of the heat transfer in the SThM experimental configuration is built and represented on Fig. 2 using the thermal impedances formalism [13]. At each frequency \( f \), the thermal impedance \( Z_p(\omega_2) = A_p(\omega_2) \exp(i \delta_p(\omega_2)) \), with \( \omega_2 = 4 \pi f \), of the probe is deducted from the measurement of the amplitude \( A_p(\omega_2) \) and the phase \( \delta_p(\omega_2) \) when the probe is out-of-contact from the surface of the sample. Indeed, we consider that the model bias from this “system identification” approach is much smaller than that obtained from an analytical solution based on a simplified geometry of the probe. The electrical resistance of the probe at room temperature is denoted \( R_0 \) and the current passing through the Pd wire is \( i_0 \). Approaching the probe tip to the surface and ensuring the contact by monitoring the force applied on the cantilever, a very small part of the heat flux generated within the probe can flow the sample. A thermal contact resistance \( R_c \) occurs at the interface that has been studied by several colleagues in order to understand all the physical phenomena that are involved regarding the heat transfer at the interface. Among them, the solid-solid contact, the water meniscus formation and the diffusion through air surrounding the contact are well identified. In addition, regarding the method we used to derive the probe thermal impedance, this thermal resistance will also account with the thermal gradient that occurs at the probe tip in the contact mode. In a previous study [5] we observed that the identified thermal contact resistance \( R_c \) on calibrated samples did not vary significantly when the thermal conductivity of the material varied from 0.2 to 40 W/m/K. We identified \( R_c = 1.2 \times 10^{-8} \text{ m}^2 \text{K} \text{W}^{-1} \) from frequency dependent probe temperature measurement (not represented here) when the probe is in contact with the SiN material and we assume that this value remain constant all over the device whatever the material in contact.

\[
\frac{1}{Z_r(\omega_2)} = \frac{1}{R_c + Z_m(\omega_2)} + \frac{1}{Z_p(\omega_2)}.
\]

Finally, due to the complexity of the domain geometry, the thermal impedance \( Z_m(\omega_2) \) for the device has been calculated here using the finite element method. As represented on Fig. 3 the geometry has been first simplified since we verified that, in the working frequency range [100-5000] Hz, the TiN,
AlCu and Ti layers as well as the TBR between those layers can be merged to form the thermal resistance $R_i$ between the SiN and the thermal SiO2 layer at the top of the Si substrate. This former must be considered as a semi-infinite medium within the finite elements technique (node Infinite Domain with COMSOL Multiphysics code). The mesh of the domain appeals to 458096 degrees of freedom (DoF), the system is solved using an iterative multigrid algorithm based on the generalized minimal residual method. The temperature is integrated over the heated area using a 4-order numerical integration technique. As presented also on Fig. 3, a crucial choice has to be made on the value of the characteristic dimension $a_{cell}$ of the cell that is expressed according to the GST tank diameter.

![Figure 3](image)

**Figure 3.** Simplification of the device geometry: the Ti, AlCu and TiN layers are merged to form the thermal resistance $R_i$, including the TBRs at the interfaces between the layers.

We assumed a contact area between the probe and the surface as a disk; the radius $r_0$ of the disk was determined using the step technique presented in the paper of Puyoo et al. \[14\]. It is about 100 ± 10 nm and we assumed this value for our configuration. The probe is assumed passing from the SiN onto the GST trench along the $x$-direction. The $x$-dependent reduced sensitivity functions of the probe temperature according to the parameter $\theta$ are represented in Fig. 4, $\theta$ being either the probe thermal impedance $Z_p$, the geometrical factor $\beta$, the TBR at the GST-SiN interface and the thermal conductivity $k_{GST}$ of the PCM have been calculated from the classical finite difference:

$$S^\ast(x,\theta) = \theta \frac{dT_p(x,\theta)}{d\theta} - \theta \frac{T_p(x,\theta + \delta\theta) - T_p(x,\theta)}{\delta\theta}$$

![Figure 4](image)

**Figure 4.** Reduced sensitivity functions of the probe temperature according to the probe thermal impedance $Z_p$, the geometrical factor $\beta$, the TBR at the GST-SiN interface and the thermal conductivity $k_{GST}$ of the PCM.
Obviously we found that the sensitivity on $Z_p$ is huge, meaning that making a small error on this parameter will lead to a very high deviation on the calculated temperature of the probe. Fortunately, we observe that the four sensitivity functions are linearly independent since:

$$\mathcal{J}(a_0, a_1, a_2, a_3) \neq 0 \text{ as: } a_0 S'(Z_p) + a_1 S'(\beta) + a_2 S'(k_{GST}) + a_3 S'(TBR_{SiN-GST}) = 0$$

Therefore, we proposed to identify the four parameters by minimizing the quadratic gap $J = \sum (T_p(x) - \tilde{T}_{p,i})^2$ between the measured temperature, denoted $\tilde{T}_{p,i}$, and the calculated one using the Levenberg Marquardt algorithm [15].

4 Results and analysis

Using the experimental data presented already in [1], we performed the identification of the four parameters and we found: $Z_p(523\text{ Hz}) = (11.10 \pm 0.025) / P_0 \text{ K.W}^{-1}$; $TBR_{GST-SiN} = (2.0 \pm 0.2) \times 10^{-8} \text{ m}^2.\text{K.W}^{-1}$; $k_{GST} = 0.46 \pm 0.1 \text{ W.m}^{-1}.\text{K}^{-1}$; $\beta = 3.3 \pm 0.1$ All the known parameters have been reported in the Tab. 2.

We represented on Fig. 5, the measured and simulated temperature of the probe using the identified parameters. The standard deviations for the parameters have been calculated from the Hessian matrix at the end of the minimization process and the residuals [15]. The value we found for the identified $Z_p$ is exactly the same than that we measured in the out-of-contact mode. As expected we found a value of the TBR at the GST-SiN interface that confirms that the value estimated from the DMM was too low. The GST thermal conductivity is that of the fcc state measured when the GST is deposited as a thin film. We observed on Fig. 5 that the change in the temperature probe is only $0.2^\circ\text{C}$. This comes from the fact that the thermal conductivity of both the amorphous SiN and the GST in fcc state are not very different although the amorphous SiN is a little bit more conductive. The increase observed after the GST barrier is obviously due to the heat confinement within the GST micro trench. Considering the thermal properties of the amorphous GST instead of the crystalline ones is clearly visible on the simulated probe temperature on Fig. 5.

![Figure 5](image)

**Figure 5.** Fit between the experimental data (dots), when the probe follows the direction represented in the inset, and the simulated probe temperature (red line) using the identified values of the four parameters at the end of the minimization process. The simulated probe temperature is calculated from the thermal conductivity of the GST (green line) in order to demonstrate the sensitivity to this parameter for instance.

| Table 2. Known parameters. |
|---------------------------|
| $f$ (Hz) | $523$ | $TBR_{AICCu-TiN}$ (DMM) | $3 \times 10^{-7} \text{ m}^2.\text{K.W}^{-1}$ |
| $r_0$ (nm) | $100$ | $TBR_{SiO2-AICCu}$ (DMM) | $3 \times 10^{-9} \text{ m}^2.\text{K.W}^{-1}$ |
| $R_0$ (Ohm) | $125$ | $TBR_{SiO2}$ [16] | $5 \times 10^{-9} \text{ m}^2.\text{K.W}^{-1}$ |
| $R_c$ (m$^2$.K.W$^{-1}$) | $1.2 \times 10^{-8}$ | $TBR_{GST-TiN}$ [17-18] | $2 \times 10^{-8} \text{ m}^2.\text{K.W}^{-1}$ |
| $i_0$ (µA) | $800$ | | |
5 Conclusion
As it was demonstrated already in previous studies, SThM appears to be reliable to investigate the thermal properties of devices even if the characteristic dimensions of the constitutive elements are lower than the probe spatial resolution. This study shows that the implementation of an inverse approach leads to exploit better the experimental measurements. First, it leads identifying the sensitive thermal parameters in the model that are the thermal conductivity of the PCM (GST), the TBR at the PCM-Dielectric (SiN) interface and also additional parameters as the probe thermal impedance and the geometrical domain of investigation. Retrieving the thermal impedance of the probe measured using the out-of-contact mode leads also to be confident with the TBR at the interface between the probe and the surface as well as the contact radius area, that have been both measured in a different configuration. On the other hand, such a characterization allows verifying the reliability of the thermal properties that have been measured in different configurations (as thin films) that than met in the device. However, the main drawback in this approach is related to the CPU time required to complete the identification process. Indeed the minimization algorithm appeals to the simulation of the finite element model a lot of time that makes the process very time consuming. In the present study, only very small amounts of data have been exploited whereas the SThM image is composed from (256x256) pixels. Therefore, further work is designed to reduce strongly the computation times.

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