Programming and Read-back Processes on Phase-Change Materials during Surface Scanning

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Abstract

Scanning probe methods, based on micro-electromechanical (MEMS) devices, have been employed to store data at ultrahigh densities (>Tbit/sq.in) with low power consumption. The use of microscopic conductive tip in contact with phase-change materials (PCM) is one such approach, with the aim to record data as amorphous or crystalline marks on a sample medium down to the nanometer scale. These applications rely on the reversible phase transition property of PCM between amorphous and (poly)crystalline state. Writing data is a complex process which involves electrical, thermal and phase-transition phenomena that determine the final size and shape of the written mark. Reading is based on the detection of the large difference between electrical conductivities of the two states of the phase-change medium. Towards a better understanding of these processes, numerical models, based on finite element methods (FEM), have been developed to simulate and analyze such a system. The objective of this paper is to present a theoretical study based on computational calculations, in order to predict the spatial distribution of amorphization during writing and derive the basic waveform of the read-back signal.

Keywords: scanning probe data storage, phase change materials, MEMS.

1. Introduction

In recent years, techniques like scanning probe microscopy (SPM) and atomic force microscopy (AFM) have been widely investigated and experimented in various scientific areas. Applications based on Micro-Electro-Mechanichal Systems (MEMS) combined with scanning probe techniques that make use of nanometer scale tips, is an emerging technology for developing data storage systems and micro-sensor based applications. MEMS have been identified as one of the most promising tools, based on the fabrication of micro/nano-integrated devices, that combine mechanical and electronic components, in order to sense, control and manipulate matter at nanoscale. Scanning probe methods are mainly used for measuring a physical property or for manipulating and modifying a sample material. With such techniques, we have the capability not only to 'write' data on the sample, but also to 'read' the previously stored information [1].

Nowadays, phase-change materials (PCM) that employ chalcogenide alloys, such as *GeSbTe/AgInSbTe*, are used to store data in optical storage systems and non-volatile solid-state memory applications [2], relying on the reversible transition property of PCM between amorphous and crystalline state via joule heating. The use of PCM technology has made rapid progress in a very short period of time, surpassing other competing technologies in terms of scaling, retention, endurance and performance. Recently, scanning-probe techniques using a conductive tip in contact with a phase-change film have also been developed to record data, as amorphous or crystalline `marks'. Information is stored across a track as a sequence of `mark' and `no mark' corresponding to the basic information unit ‘0’ or ‘1’, respectively.

Storing information on a PCM surface is a complex process. Storing (usually referred as *write*) operation couples complex electrical, thermal and phase transition phenomena that determine the bounds of the transformed region. There are two alternative writing options: writing amorphous marks at an initially crystalline field or crystalline marks at an amorphous background ([3],[4]). In this study, we analyze and investigate the case of writing amorphous marks in a PCM surface, that has experimentally verified and reported in [5]. The temperature distribution produced by Joule heating, in addition to thermodynamic properties of the coupled materials, determines the final size and shape of the recorded mark.

Read operation is based on sensing the large difference in electrical conductivity between the two states by applying a `low' amplitude voltage relative to *write* process, to avoid recrystallization. The basic characteristics of the read-back waveform, during *read*, are mainly determined by the marks' size and the tip-medium electrical contact area. *Read* is usually performed by scanning the surface with a constant velocity relative to the medium. The scanning velocity may also exhibit random fluctuation due to external disturbances. Signal processing of the read-back signal can be used in applications to estimate the motion dynamics by scanning a known data pattern, previously stored in the PCM medium.

The objective of this work is to theoretically investigate and to explore by accurate simulations the mechanisms of *write/read* operations in a scanning probe recording system, based on phase-change materials. For this purpose, two-dimensional analytical models have been developed based on finite element methods (FEM) and numerical algorithms to simulate the electrical, thermal and phase transition dynamics of such a system. Results from the writing model are used to predict the spatial distribution of the amorphous phase inside the PCM layer that eventually determines the density of the stored data in the medium. On the other hand, the reading model provides information about the basic form of the read-back pulse obtained by sensing an amorphous mark. In this content, it is examined how geometric and structural parameters, such as the size of the tip-medium contact area and/or the size of the mark, affect the basic characteristics of the read-back signal. Scanning velocity and sampling rate are the two basic factors that affect the read-back signal resolution, and they are also analyzed in details.

2. Scanning Probe Storage System Architecture

The general system architecture being considered in this study is illustrated in Fig.1. The system consists of two basic elements: the probe with the tip attached to it and a two-layers structure. The upper layer constitutes the phase-change storage medium, while the under layer forms the bottom electrode.

During *write,* the probe is moving relative to the storage medium with a constant velocity, while a voltage is applied between the tip and the bottom electrode at predetermined locations. Consequently, this results in a current flow from tip through the medium that heats locally the PCM, just beneath the tip-medium contact area. If the pulse's amplitude and duration are sufficient, the phase transition mechanism is activated, resulting to a mark formation.

Read is based on a similar concept. The tip scans the surface of the storage medium, while a voltage is applied to the tip. The resulting current flows through the medium and provides the read-back signal. The current is inversely proportional to the resistance of each specific location. The equivalent resistance of the system, as stated from the Ohm's law, depends on the special conductivity of the PCM, just below the tip-medium contact area, which in turn is associated with the phase of the material. The presence or absence of a mark during scanning leads to the detection of the logical unit '1' or '0', respectively.

It is important to note that in electrical probe recording on PCM, the size and shape of the written 'bit', as well as the read-back signal characteristics are primarily determined by the size of the tip-medium contact area and the specific electrical and thermal properties of the system's materials. The size of the written bits determines also the data storage density. Another important parameter that should also be taken into account is the scanning speed that affects the read-back signal resolution. As a consequence, the *read/write* data rates dependent on the density of the written bits and the scanning speed which affect the overall system performance.

3. System Model

In order to analyse and explore the *write/read* mechanisms of such a system, appropriate simulation models have been developed. These models are based on finite element numerical methods and have been implemented using the computational tool *COMSOL Multiphysics* under the control of *Matlab* functions.

A two-dimensional design of the model architecture is illustrated in Fig.2, which consists of three basic elements. The tip positioned at the top of the structure and a two-layered stack below. The upper layer of the stack corresponds to the PCM, which is considered here to be $Ge_2Sb_2Te_5$ (referred later as GST), with 60-nm in thickness. The under layer constitutes the highly conductive ($\sigma=10^6$ S/m) bottom electrode. It should be noted here that the width of the stack is considered to be large enough (500nm) compared to the tip-width and the tip-scanning area assumed for the simulations. In both *write/read* operations a voltage pulse is applied to the tip with respect to the bottom electrode, which is held to ground potential.

The basic physical mechanisms that govern the *write/read* operations of the scanning probe system, involve electrical, thermal, and phase transition phenomena.

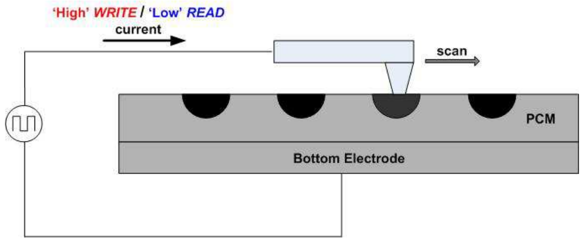

Fig. 1 Scanning-probe system architecture.

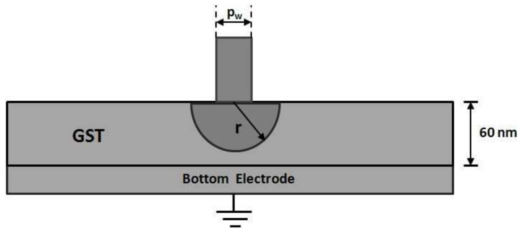

Fig. 2 The 2D geometry of simulation model. The semi-spherical shape just beneath the tip, represents a written amorphous mark with radius ***r.***

The electro-thermal process determines the current density throughout the whole structure, producing a temperature distribution, during write, that leads to amorphization. The readout process is basically electrical and depends on material properties.

The models perform calculations, solving the time-dependent Laplace equation of the electric field theory:

$$\nabla \cdot \left[\sigma(x,y) \nabla V\left(x,y,t\right) \right] = 0 \quad (1)$$

where $\boldsymbol{\sigma}$ is the electrical conductivity and $\boldsymbol{V}$ the electric potential. The solution of Laplace equation provides us with information about the electric potential $\boldsymbol{V}$, electric field $\boldsymbol{E}$, and the current density $\boldsymbol{J}$ of the whole system.

The temperature distribution inside the structure of a material can be estimated by solving the heat conduction equation:

$$C\left(x,y\right)\frac{\partial T\left(x,y,t\right)}{\partial t} = \nabla \cdot \left[K(x,y) \nabla T\left(x,y,t\right) \right] + Q\left(x,y,t\right) \quad (2)$$

where $\boldsymbol{C}$ is the material heat capacity and $\boldsymbol{K}$ the thermal conductivity. The quantity $\boldsymbol{Q}$ corresponds to the heat source which is associated with electric current density and equals to $|J|^2/\sigma$.

4. Write mechanism

Recording of an amorphous mark in an initially crystalline material, requires heating of the GST layer above the melting temperature (T_m=616 ^{o}C) followed by rapid cooling, with a rate in the order of a few tens of K/ns. Heating is achieved by applying a voltage pulse with sufficient amplitude and duration. The pulse has a rectangular shape with 0.5-V in amplitude and 50-ns duration. In order to achieve fast cooling rates, a falling edge of about 5-ns has been considered.

The conditions that have to be satisfied for forming an amorphous region inside the crystalline material, are the following two: reaching the melting temperature and sufficient cooling rates. As a consequence, these two conditions will eventually define the bounds of the transformed region.

The time when the material reaches its maximum temperature, is just before the voltage pulse begins to drop, and particularly, in this case at 45ns. In Fig.3 is given the contour of isothermal curves, just before the beginning of the falling edge of the writing pulse. The region that finally exceeds the melting temperature ($T(x,y) \geq T_m$) is localized at the top of the GST layer and below the tip-medium contact area, since the current density is higher, as we get closer to the tip.

The second condition, that is related to the cooling rate, gives us the final bounds of the amorphization area. The trailing edge of the writing pulse begins to fall and that results to a rapid cooling of the molten material. During cooling, the points of the material that will finally solidify to amorphous state, are those at which the cooling rate exceeds 5×10^{10} K/sec [6]. In Fig.4 are demonstrated some snapshots from the simulation model that present the evolution of the spatial distribution of amorphization. At the pulse end (t=50ns), the formed amorphous mark has an almost semi-spherical shape, localized just beneath the tip-medium contact area.

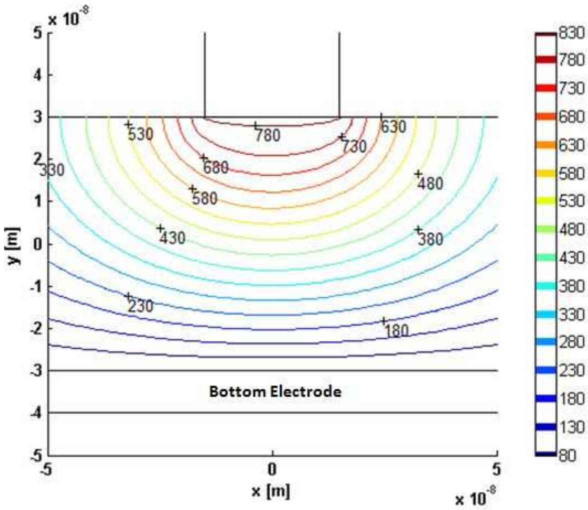

Fig. 3 Isothermal contours showing the temperature distribution throughout the GST layer, after the application of a voltage pulse with amplitude 0.5-V for 45 nsec.

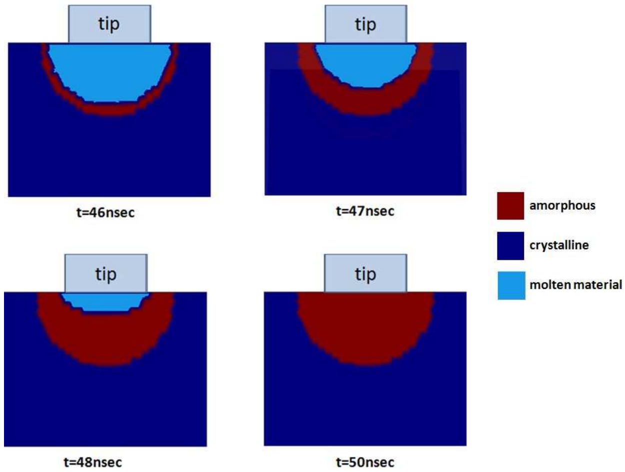

Fig. 4 Spatial distribution of amorphization during cooling process.

5. Read mechanism

As discussed previously, the *read* process relies on the vast difference of electrical conductivity between the amorphous and crystalline phases of the GST layer. During *read*, the tip scans over the surface of the PCM, while a voltage is applied to the tip with respect to the bottom electrode. The voltage's amplitude in this case, is relatively lower compared to that of the writing process, in order to avoid recrystallization via heating.

To investigate the readout process and obtain the read-back signal of a written bit, a 2-D model similar to that of writing has been developed, where some assumptions have been made. An isolated amorphous mark was considered with an idealized semi-spherical shape of radius ***r***, localized at the upper portion of the GST layer, as shown in Fig.2. During *read*, it was assumed that the tip was stationary above the PCM medium, while a voltage pulse was applied to the tip at each position. This approximation is not far from reality, as the tip-medium velocity is results to a negligible displacement, during *read*.

For representing the read process a rectangular voltage pulse with 0.2-V amplitude and 20-nsec duration was considered for the simulations. The Laplace equation was solved for each tip position, calculating the current density throughout the whole structure. Consequently, this results to the evaluation of the equivalent resistance after integration. The above described process was repeated at all space-steps (=1nm), until the surface area around the written amorphous mark was scanned. This process provides information about the equivalent resistance with respect to the displacement, representing the read-back waveform of a single written mark. Fig. 5 illustrates the read-back pulse obtained from simulation by scanning an isolated amorphous mark of radius ***r****=30nm*.

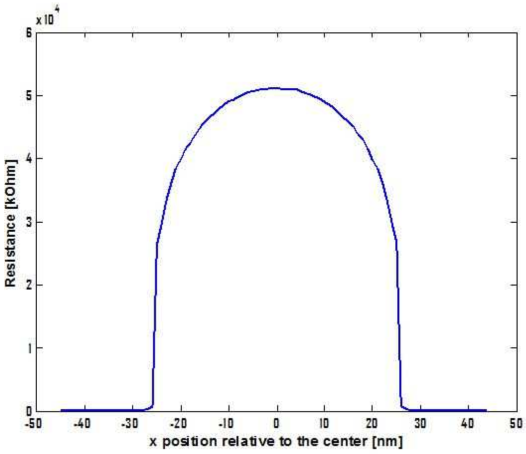

Fig. 5 A typical read-back signal pulse obtained by reading a single amorphous mark with radius ***r****=30nm.*

In general, the shape of the read-back pulse has the basic form shown in Fig. 5, independent of the size of the written amorphous mark. However, the magnitude of some features of the pulse seems to change according to some structural parameters of the system. To be more specific, the maximum amplitude of the read-back pulse is related with the radius of the written mark and the size of the tip-medium electrical contact area. In Fig. 6, it is shown the dependence of the maximum amplitude R_{max}, which is located at the centre of the bit, from the quantity a_r that equals to the ratio of tip-width p_w to the mark-radius r and considering the mark-radius as a parameter. As it can be seen, the larger the value of a_r, which means larger tip-medium contact area, the lower the maximum amplitude obtained. This is due to the fact that

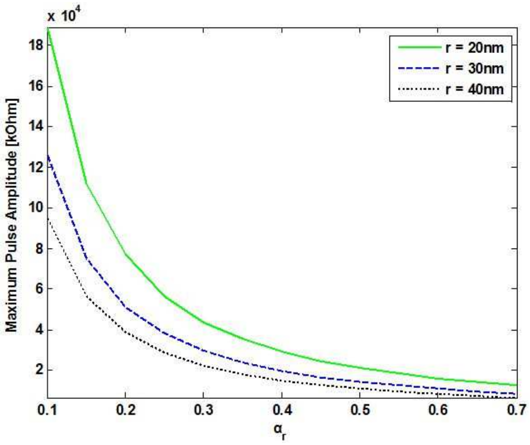

Fig. 6 Maximum pulse amplitude versus $\boldsymbol{\alpha_r}$ for 3 written mark-radiuses.

the total current passing from the tip through the medium, that finally determines the equivalent resistance of the system, is determined by the size of tip-medium contact area.

The read-back signal of a real scanning probe system is not actually a continuous waveform but a discrete set of values, taken at regular time intervals. Therefore, the resolution of the read-back signal is a function of the sampling interval T_s and the scanning velocity u_s that is assumed to be fixed for a specific system configuration. The spatial resolution of the signal is associated with the density of the samples taken within a space interval.

Assuming that the distance that has to be scanned is *D*, with a scanning velocity u_s and a sampling period T_s, then the number of samples N_s acquired during *read* process are given by

$$N_s = \frac{D}{u_s \cdot T_s} \quad (3)$$

Eq.(3) implies that the resolution of the read-back signal is inversely proportional to the scanning velocity for a fixed sampling rate. Towards a better understanding of the effect of the scanning velocity to the read-back signal, in Fig.7 are shown two graphs, representing the signals obtained by scanning a sequence of bits with two different velocities. In Fig.7(b) scanning has been performed with a velocity u_2 larger than u_1 corresponding to that of Fig.7(a). As it can be seen the read-back signal in Fig.7(b) seems to be compressed in time, compared to that of Fig.7(a).

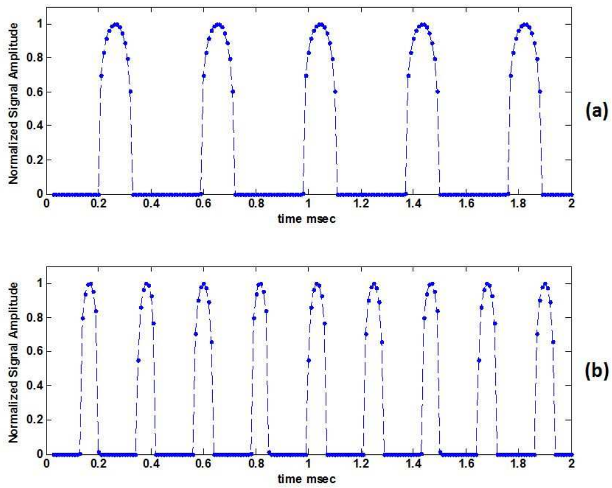

Fig. 7 Read-back signal acquired during scanning **(a)** with velocity u_1 and **(b)** with velocity u_2, where $u_2>u_1$.

This can conceptually be seen as a time–scaling transformation with a scale factor that equals to u_2/u_1. This latter conclusion can be used to develop a method, based on signal processing techniques, in order to estimate the velocity of a scanning process by comparing the obtained signal with an apriori known, but with unknown phase shift and/or timing difference.

6. Conclusions

In this work, comprehensive numerical models of an electrical scanning probe recording system on phase- change media have been developed, in order to explain the electrical, thermal, and phase transition processes during *write/read* mechanisms. The models allow us to predict the degree of amorphization of an initially crystalline PCM medium, during *write* and derive the basic form of the read-back pulse by reading a previously written amorphous mark. Although, the basic form of the read-back pulse remains the same, simulations showed that the amplitude of the pulse depends on the size of the amorphous mark, as well as the tip-medium electrical contact area. Finally, it was examined the impact of the scanning velocity to the resolution of the read-back signal and how it affects its time representation producing replicas scaled in time.

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