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# MODELING OF PHASE CHANGE MEDIA SURFACE SCANNING

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**Abstract.** *In recent years, techniques like scanning probe microscopy (SPM) and atomic force microscopy (AFM), have been widely investigated for being applied to various scientific fields. Scanning probe techniques based on micro-electromechanical (MEMS) devices have demonstrated their ability to store data at ultrahigh densities (>Tbit/sq.in). Phase change materials (PCM) have been recently used to write and read 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 crystalline state. Write operation combines electrical, thermal, phase-transition phenomena that determine the final size and shape of the written mark. Reading depends on sensing the huge difference of the electrical conductivity of these two PCM states. Both operations use conductive tips in contact with the medium that move relative to it, during surface scanning. In this paper, we present a theoretical study using computational tools in order to describe and analyze the processes that take place in such a system and unveil the mechanisms that determine the properties of the stored information and readout signal.*

## 1 INTRODUCTION

Over the last few decades, there is an increased demand for developing ultra-high density data storage systems and micromachined sensors based on micro/nano-technology. Many of the devices and systems used in modern industry and in our everyday lives are becoming progressively smaller. Micro-electromechanical systems (MEMS) are a promising future technology that seems to cope with such demanding applications. With MEMS devices we are able to develop techniques that allow us to manipulate a sample material down to the nanometer scale. Techniques such as scanning probe microscopy (SPM) and atomic force microscopy (AFM) have been extensively investigated and have been proved to be incorporated well with MEMS devices. Nowadays, tools based on scanning probe methods (SPM) are applied in a wide range of applications in order to modify or sense nano-structures with the aim to store and retrieve information, respectively. These techniques make use of nanoscale sharp tips in contact or close proximity with a sample material and using a physical mechanism they can modify the surface or alter some physical properties of the material or at a later stage detect these changes. The most well-known scanning-probe based approach for data storage is that of IBM "*Millipede*" system [1], where a 2-dimensional array of almost one thousand thermomechanical probes is applied to write, read and erase indentations in a thin polymer film.

Recently, phase-change materials that employ chalcogenide alloys, such as *GeSbTe* (referred elsewhere as GST) or *AgInSbTe,* are widely used in rewritable storage systems (e.g CD/DVD-RW). They are also proved to be potential candidates and as alternatives to silicon non-volatile solid-state flash memories, the so-called phase-change RAM (PCRAM) devices. In both applications, data storage relies on the reversible transition property of phase-change materials between amorphous and crystalline state via heating. Information retrieval can be achieved by sensing the changes in refractive index or electrical conductivity associated with the two states, respectively. PCM technology has made rapid progress and passed in a short time older ones in terms of scaling, retention, endurance, system performance and cost.

Current research progress of scanning-probe techniques based on phase-change materials aims to develop systems with the ability to record data at the nanometer scale. Generally, these systems consist of a conductive probe/tip in contact with the medium, so that electric current passes from probe through the PCM. Information is stored across a track as a sequence of "*mark*" or "*no mark*" by applying a short and intense electric pulse. The presence or absence of an amorphous/crystalline mark corresponds to a logical unit of information '1' or '0', respectively. Replay is achieved by applying a relatively low voltage and detecting the differences in electrical resistance between the two states of the medium.

The *read*/*write* operations of such a system depend on mechanical scanning with a velocity that affects the resolution of the system. The objective of this paper is to analyze and theoretically investigate using computational tools the characteristics and the behavior of such a system during write/read operations. Especially, we focus on the amorphization process during writing an amorphous ‘bit’ into a crystalline medium and on the readback pulse obtained by reading a previously written mark. Finally, it is also examined the case of reading a ‘bit’ sequence with a velocity-dependent scanning method.

## 2 GENERAL SYSTEM ARCHITECTURE

The basic system architecture, as illustrated in Fig.1, is comprised of a two layer structure: the uppermost layer, which is the PCM storage medium and a highly conductive underlayer that forms the bottom electrode. The physical mechanisms that determine the *write/read* performance of the system involve electrical, thermal and phase transition processes. During *write* the probe moves relative to the medium and an electric voltage pulse is applied between the tip and the bottom electrode at specific time instants. As a consequence, a current flows from the tip through the medium and heats locally the PCM, just beneath the tip-medium contact area. If the pulse amplitude and duration are sufficient, the PCM will reach the required melting temperature and the phase transition process will be initiated.

Reading is done using a similar concept. As demonstrated in Fig.1, during *read* the tip scans the surface over the written ‘bits’ with a constant velocity, while a constant voltage is applied to the tip. This results in an electric current flow, the intensity of which provides the readback signal. The applied voltage is lower than that of the writing process, so that any produced heating is insufficient to stimulate phase transition phenomena. The *read* process relies on the vast difference between electrical conductivities of the amorphous and crystalline phase of the PCM layer. The readback signal basically represents the equivalent resistance of the whole structure as stated from Ohm’s law (R=V/I). It is important to note that in scanning-probe recording the written ‘bit’ size and the readback signal resolution are primarily determined by the tip-medium electrical contact area, as well as the electrical properties of the coupled elements.

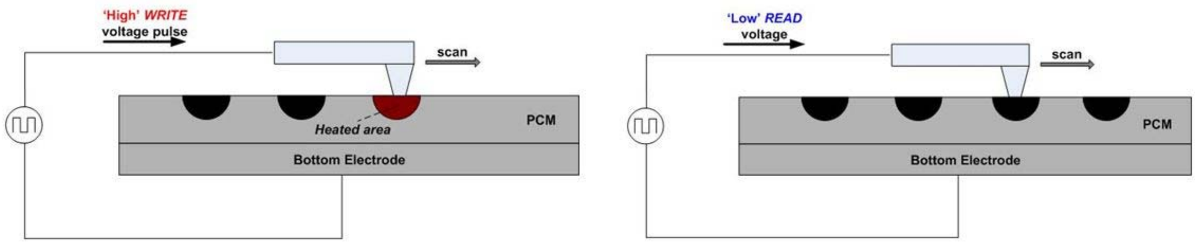


Figure 1. Schematic diagram of a scanning-probe system, illustating the write (left) and read (wright) operation

*Write/read* operations are performed using a scanning mechanism, whereby the probe moves relative to the medium with a constant velocity. It should be mentioned that the scanning velocity of *read* operation may differ from that of the *write* operation. Fast and accurate motion of the nanopositioning scanner is crucial to achieve high data rates and maintain high spatial resolution. The scan trajectory and pattern may also vary on a case-by-case basis and depend on the specific requirements that must be satisfied for each application. The most frequently used scheme is the raster-based scan trajectory by applying triangular or sawtooth signals to actuate the x/y axis with respect to the plane of the PCM medium. Another approach that has been proposed as a nanopositioning scheme is that of a spiral-based pattern (see [2]). In this case the probe follows an archimedean spiral trajectory, where the distance between symbols and the spatial resolution are maintained constant. Additionally, another method ([3],[4]) based on lissajous pattern can be applied by actuating the x/y scanner with two single-tone harmonic waveforms of constant or variable frequency and amplitude. This results to an extremely narrow frequency spectrum that allows imaging with high speed and low noise levels.

According to the above analysis, it is clear that data recording on a PCM can be done in different ways concerning the size of the written symbols and the trajectory where the bit sequence is stored. These parameters determine the density of the recorded data, which in turn have an impact on the readout signal resolution. Readout resolution also depends on the geometric (e.g tip-medium contact area) and physical (e.g amorphous/crystalline electrical conductivities) characteristics of the system. Consequently, the maximum data rate that can be achieved and determines the overall system performance depends on the scanning speed which is constrained by the minimum specified resolution requirements.

## 3 THE SIMULATION MODEL

As mentioned before, *write/read* operations combine complex electrical, thermal and phase transition physical processes, as well as moving parts. To investigate these phenomena in detail and explore the performance of such a system, we have developed appropriate simulation models. These models enable a systematic numerical analysis and description of the system's processes. In order to produce an integrated model for *write* and *read* operations, we used a computational graphical tool (Comsol multiphysics [5]) based on finite element numerical methods (FEM) in collaboration with the Matlab software [6].

The model architecture, as illustrated in Fig.2, consists of three basic elements: the tip (up) and a two-layers substrate (down). The tip-width is not associated with the physical sharpness of the tip, but with the electrical tip-medium contact area. In a real system, it is possible to have tips with small electrical contact interface but relative large physical radius [7],[8]. As already mentioned, the electrical contact area plays a crucial role in the determination of shape and size of the written bit. The two-layers rectangular structure beneath the tip comprises the GST (upper layer) material, which is 60 nm thick and the highly conductive ($\sigma=10^6$ S/m) bottom electrode (under layer). It should be noted here that the width of the substrate is considered to be large enough (500 nm) compared to the tip-width and the tip-scanning area assumed for the simulations (~ +/-100 nm). The model incorporates all the physical processes referred previously by solving the proper time-dependent equations. Since the model parameters change during each time step, the model simulation time-interval has been chosen to be sufficiently small ($\Delta T$=20 psecs) in order to achieve high calculation accuracy.

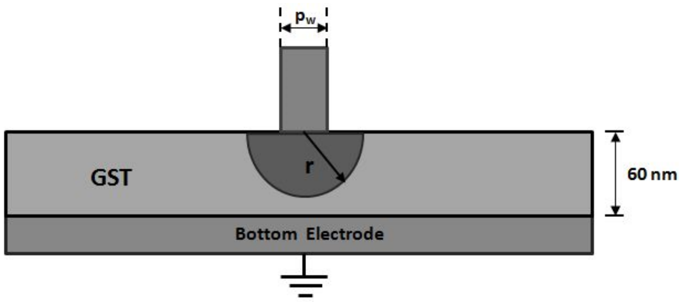


Figure 2. Geometry of simulation model. The semispherical shape, just beneath the tip in the GST layer represents a written amorphous mark of radius **r**

The basic physical mechanism that dominates the operations of a scanning-probe PCM system is the electrothermal process. The electrical process determines the current flow which is responsible for the temperature distribution due to joule heating. During write, the spatial temperature distribution determines the region inside the PCM medium where the 'bit' is going to be formed. The readout process is purely electrical and depends on the total current that passes through the structure, depending on the material phase beneath the tip-medium contact area. To understand these processes from a mathematical point of view, we will briefly discuss their basic equations.

The electrical behavior of this model is derived by solving the Laplace equation of a conductor:

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

where $\boldsymbol{\sigma}$ is the electrical conductivity and $\boldsymbol{V}$ the electric potential. Solving the above time-dependent equation we are able to calculate the potential $\boldsymbol{V}$, electric field $\vec{\boldsymbol{E}}$ and current density $\vec{\boldsymbol{J}}$ throughout the whole system's structure.

The temperature distribution within a material structure can be evaluated from the heat conduction equation:

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

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 induced by electric current and equals to $|J|^2/\sigma$.

The electrical behavior of this model is determined by the electric potential and electric field, as well as the current density distribution over the whole system's structure. Subsequently, the electrical characteristics are used as input at each time step to the thermal computational model, resulting to the calculation of the temperature distribution. Finally, the temperature distribution determines the region inside the GST where the phase transition phenomena are taking place. During simulation of *write* process, it was assumed that the tip was stationary above the storage medium. This approximation is not far from reality where in a scanning probe system the tip-medium displacement is relatively small compared to the displacement during a typical *write* pulse duration which is on the order of a few tens of nanoseconds.

## 4 THE WRITING PROCESS

There are two alternative recording strategies used in scanning-probe PCM systems: either writing amorphous marks in a crystalline material or crystalline marks in an amorphous surrounding environment. In this study, we will focus on the first case that has been verified experimentally in [9].

In order to activate the amorphization process of an initially crystalline material, the PCM must be heated locally above its melting temperature ($T_m$=616 $^oC$ for the GST) by applying an electric pulse with sufficient amplitude and duration. Specifically, there is a restricted region, just below the tip-medium contact area that manages to reach the melting temperature and has the potential to be transformed to amorphous state. A subsequent rapid cooling of the molten material, below its glass transitions temperature ($T_g$=380 $^oC$), forces it to solidify to amorphous state. The degree of amorphization is predominantly determined by the cooling rate of the molten material which must become larger than $5\times10^{10}$ K/s, until the temperature falls below the glass transition temperature, in order to prevent recrystallization of the medium. The region of the GST, where the previously described conditions are satisfied, determines finally the boundaries of the amorphous mark.

A rectangular voltage pulse of 0.5 V in amplitude and 50 ns duration with linear rise/fall times 5 ns was considered to be applied to the top boundary of the tip for the simulations. Supposing that even the tip-medium velocity is relatively large e.g. *1 mm/sec,* the displacement in this case during write cycle will be *0.05 nm*. This is a very small distance, so that the tip can be considered stationary above the GST during *write*. The aforementioned requirements that must be satisfied in order to define the region that has the potential to amorphize are basically two: the melting temperature and the cooling rate. The spatial coordinates of the GST layer that exceed the melting temperature can be defined at the time, when the temperature distribution reaches its maximum value. This state occurs just after the beginning of the falling edge of the write pulse. Fig.3 depicts a cross-sectional view of the temperature distribution when the pulse begins to drop (at t=45nsec). As it can be seen, the region of the molten material ($T(x,y) \geq T_m$) is mainly located just below the tip-medium contact area, as a result of the current density distribution that attains its maximum value inside the GST in the vicinity of the tip.

When the voltage of the pulse starts to decrease with high rate (after t=45nsec), the heated material begins to cool down rapidly. The melted region that cools with a rate exceeding the required threshold rate for amorphization, finally solidifies to the amorphous state. Fig.4 shows the evolution of amorphization for four distinct time instants, during cooling process. At the end of the pulse (t=50nsec), it can clearly be seen that it has been formed a region of amorphous material with a semi-ellipsoidal shape and a surface diameter of about 50nm.

## 4 THE READING PROCESS

The *read* process is mostly electrical based on a similar concept as writing. The surface of the PCM is scanned with a constant velocity while a constant voltage is applied between the tip and the bottom electrode. The form of the readback signal depends mainly on the material's physical properties and the system's configuration. Specifically, the readout process is determined by the electrical conductivity of the amorphous/crystalline material, the tip-medium contact area and the shape/size of the written mark. To obtain the readback signal of a single written bit, a model has been developed in order to simulate the read process. For the sake of simplicity, it was assumed that an isolated mark with a semispherical shape of radius $\boldsymbol{r}$ has been formed into the GST medium (see Fig.1).

In order to simulate the scanning mechanism, it was considered that the tip was stationary above the medium for each simulation time-step and moving forward with a space-increment of *1 nm* for the next step. During each time-step, a constant voltage with 0.2 V in amplitude was applied at the top boundary of the tip. This choice was made in order to avoid re-crystallization of amorphous material via heating. As a consequence, the applied voltage results in a current density distribution throughout the system's structure. The ratio of the applied voltage amplitude $V_p$ to the total current $I_T$ that flows from tip to medium, equals to the equivalent resistance of the whole structure. Therefore, the calculation of the total current at each discrete position of the tip provides us with an estimate of the equivalent resistance with respect to displacement *x* and can be expressed as $R_{eq}(x)$. In this study, we will investigate and analyze the basic form of the readback pulse that is obtained by reading a single written 'bit' and for different system design configurations. One of the design parameters that will be examined here is the size of the tip-medium electrical contact area that is related to the tip-width $\boldsymbol{p_w}$, shown in Fig.1.

The basic waveform of the readback pulse that is acquired from a single written 'bit' of 30 nm radius is depicted in Fig.5. As it can be seen, the readback pulse should be divided into three main zones with respect to the resistance level and the transition points. We can consider that there are two main resistance levels: the low-resistance level (close to zero) and the high-resistance level $\left(H_o \leq R_{eq}(x) \leq R_{max}\right)$. In addition, there are the transition states from low-to-high and vice versa that take place between the two levels in a very narrow region on the order of *1nm*.

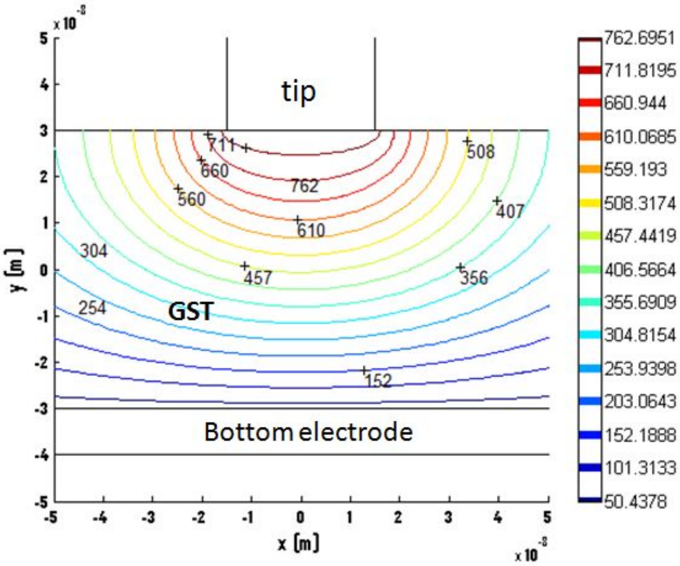


Figure 3. Cross-sectional view of temperature distribution (contours) just before the falling edge of the writing pulse at t=45nsec.

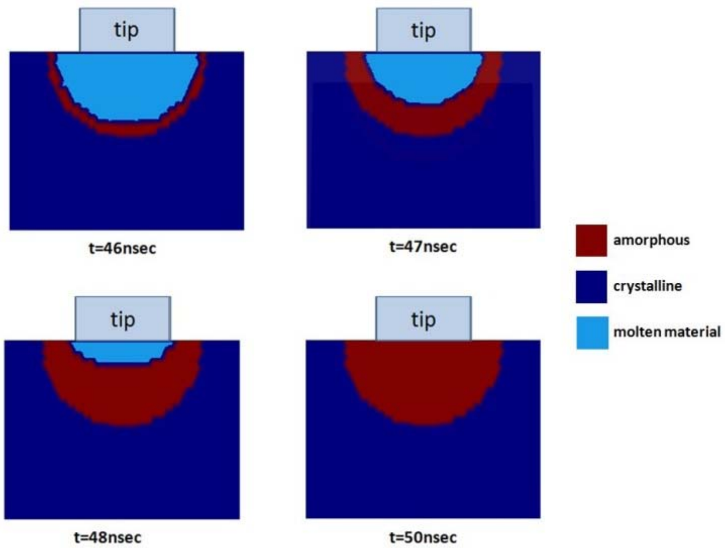


Figure 4. Amorphization distribution for four different time instants during cooling period (falling edge of the pulse).

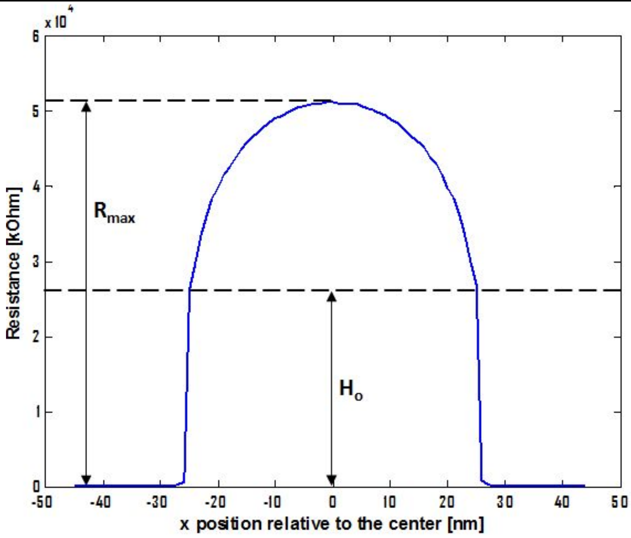


Figure 5. Typical waveform of the equivalent resistance pulse

The reason that the transition between the two levels occurs abruptly can be explained if we take a closer look at the states just before and after this transition. Fig.6 illustrates two snapshots taken from the simulation model corresponding to the low-to-high transition points. As it can be seen, in Fig.6(a) the tip is mainly above the amorphous area, but it is still in contact with a small region (left) of crystalline material. Hence, there is a highly conductive path, whence a relatively large amount of current can pass from tip to the medium, resulting in a low resistance level. At the next scanning step, as shown in Fig.6(b) the tip is completely above the amorphous area with high resistivity that forces the current density to be decreased radically.

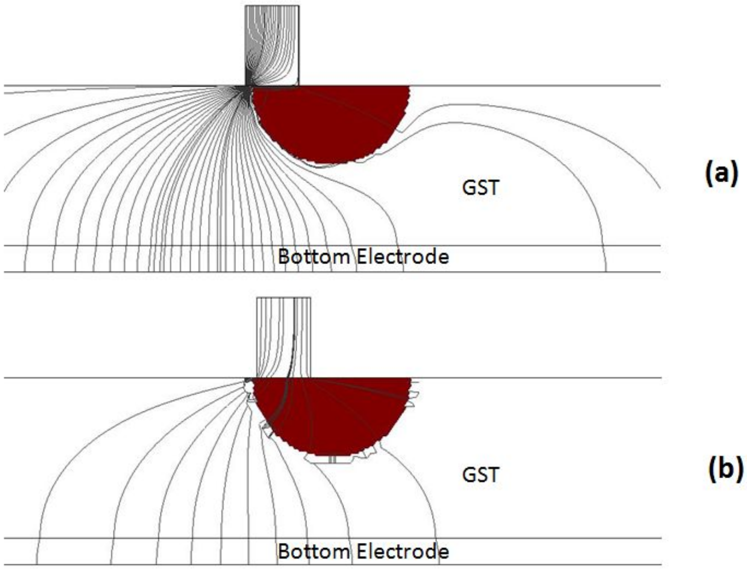


Figure 6. Snapshots of the current density (streamline) (a) just before the tip is positioned entirely above the amorphous area and (b) just after it.

Although the basic form of the readback pulse is generally maintained, there are some factors that affect specific features of the pulse. Particularly, the final form of the pulse depends on the size/shape of the written 'bit', the electrical conductivities of amorphous/crystalline material, the tip-medium contact area and the scanning velocity. As it is expected the size of the mark has an impact on amplitude and duration of the readback pulse and more specifically, the larger the mark-size the larger will be its amplitude and its duration for a fixed scanning velocity (Fig.7). Furthermore, the pulse's amplitude depends on the electrical conductivity of the amorphous region. Later, we will discuss and analyze in more detail, the dependence of the readback pulse from the electrical contact area and the scanning velocity.

The tip-medium electrical contact area is a function of the tip-width. In order to examine the effect of the size of the contact area independent of the written mark-size, we defined the parameter $\boldsymbol{\alpha}$ that equals to the ratio of the tip-width $\boldsymbol{p_w}$ to the radius $\boldsymbol{r}$ of the amorphous mark. Fig.7 illustrates the equivalent resistance obtained during reading a mark with 30nm radius and for two different values of $\boldsymbol{\alpha}$**.** As it is shown, the pulse's amplitude increases for smaller values of $\boldsymbol{\alpha}$ (smaller tip-width) and this is due to the limitation of the total current through the tip. It has been considered in this figure that the displacement of $x$ axis is measured using as a reference point the left corner of the tip for the left side of the pulse (with respect to the center) and the right corner for the right side, respectively. This is done in order to have a common reference frame to compare the pulses for different tip-size.

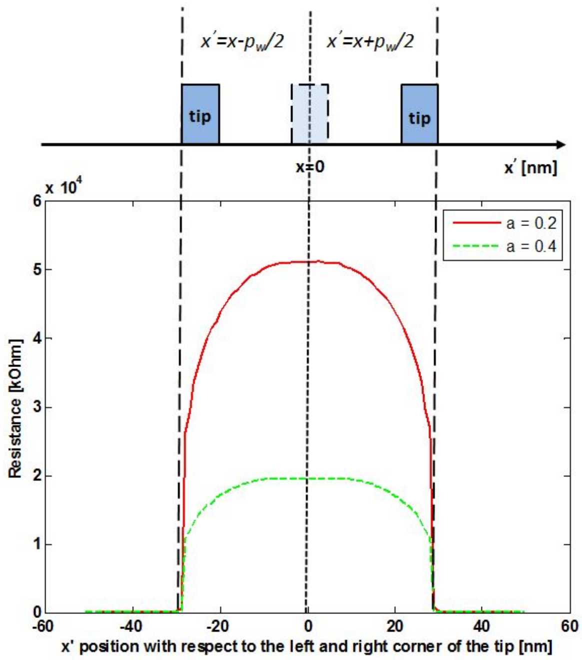


Figure 7. Equivalent resistance pulse for an amorphous mark of 30nm radious and for two values of $\boldsymbol{\alpha}$.

The readback signal in a real system is not actually a continuous waveform but a discrete set of samples taken at regular time instants. Therefore, the readout resolution depends on the sampling interval and the scanning velocity. To be more specific the number of samples/symbol, denoted here as $\boldsymbol{N_s}$, acquired during reading of an amorphous mark with a surface-diameter $2r$, sampling rate $\boldsymbol{f_s}$ and scanning velocity $\boldsymbol{\upsilon_s}$ is:

$$N_s = \frac{2r}{\upsilon_s} f_s \tag{3}$$

Consequently, samples that are taken with a sampling rate $f_s$ correspond to a space-step that equals to $L_s = \upsilon_s / f_s$. So far, it has been considered that the velocity during scanning in probe-based system is maintained constant. In fact, velocity is not always constant but it may exhibit rapid fluctuations due to the induced noise from the scanner's control system or external vibrations. Velocity changes affect the resolution of the readout signal as it can easily be deduced from equation (3), where $\boldsymbol{N_s}$ is inversely proportional to the scanning velocity. That means that the number of samples increases as velocity decreases and vice versa. Consequently, the waveform of the readback signal (for fixed sampling rate) appears to become compressed or stretched in time relative to that obtained for constant velocity. The implications of a non-constant velocity to the readback signal in a scanning-probe system can be seen in Fig.8, where it was assumed that scanning has been performed introducing an accelerated motion. Particularly, scanning begins initially with a constant velocity for some time and then increases linearly until it becomes about 2.32 times higher than the initial value and remains constant to the end. One can observe that readback signal during accelerated motion period seems to be compressed progressively until scanning velocity reaches its final value.

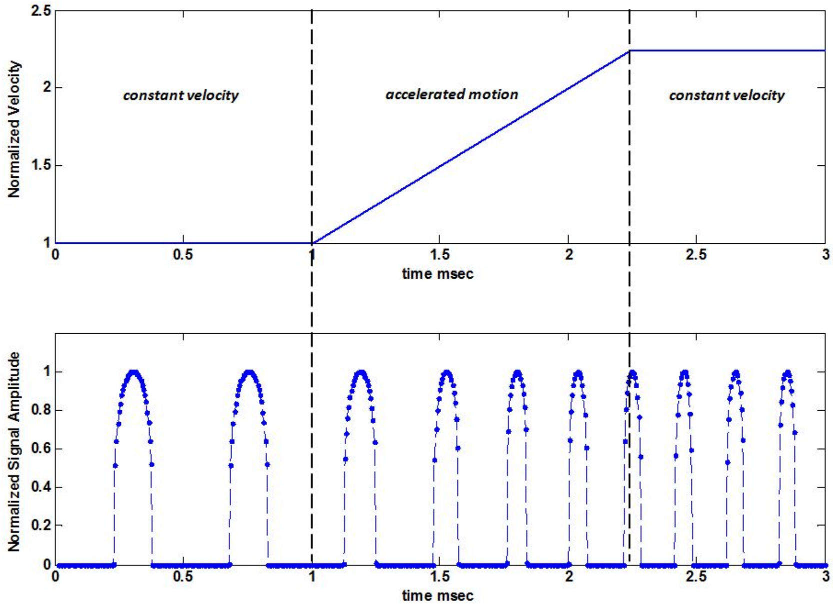


Figure 8. Scanning velocity motion profile (up) and the corresponding readback signal (down).

## 5 SUMMARY

In this study, simulation models have been developed to analyze the write/read processes of an electrical probe-based recording system using finite elements computational tools. The models allow us to deeply investigate the mechanisms of writing an amorphous mark in a previously crystalline material involving electrical, thermal and phase transition phenomena and predict its final size and shape for a specific system design configuration. We are also able to approximate the readback signal during scanning of a written 'bit', as well as to examine the changes of the basic form of the readback pulse for different sizes of tip-medium electrical contact area. Finally, it has been theoretically shown that signal resolution is a function of the sampling rate and scanning-velocity of the system and that the signal exhibits compression/expansion when scanning is performed with variable velocity. This final conclusion can be used for sensor-based applications in order to evaluate the acceleration induced by external forces in such a system with prestored data patterns.

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