

# Phase change memory: *the future of computer memory?*

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Every user of a personal computer or laptop knows the frustration caused by the delay between switching on the computer and starting to use it. Customary random access memory (RAM) is “volatile”, and its content is lost when the power is switched off. Disk storage limitations and the mechanical failure of disk drives that rotate at high speeds are also known to many. Phase change materials (PCM), which switch between *amorphous* and *ordered* structures when an electric current or a laser pulse is applied, are widely viewed as the most promising candidates for the memory of the future, although details of the structures involved are available in few cases. We have used the new IBM BlueGene/L computer to perform extensive simulations on the amorphous and ordered states of an alloy of germanium, antimony, and tellurium (GST) that is already used in DVD-RW optical disks. These simulations provide insight that can be obtained by no other means.

Memory devices that are independent of a power supply have obvious advantages, and some are familiar to us all. The ubiquitous USB-sticks can already be bought with 16 GB capacity, and SD memory cards can be used in digital cameras to store thousands of high resolution pictures. These devices are examples of flash memory, which is based on arrays of Si-SiO<sub>2</sub> junctions. The limitations of flash memory - in particular, the lower reliability that has accompanied scaling to smaller dimensions - have stimulated the search for other “non-volatile” memory devices.

The rapid and reversible transition between ordered and amorphous forms is the basis of phase change (PC) memory materials such as rewritable optical disks. In thin films of many such materials, amorphization can be driven by localized and short (~ 1 ns) laser heating to a temperature above the melting point  $T_m$ , and longer laser heating (~ 50 ns) to below  $T_m$  but above the glass temperature  $T_g$  leads to a metastable “crystalline” form. The phase change can be monitored by the accompanying large changes in resistivity or optical reflectivity. A memory cell where the phase change is driven by a current pulse is shown in Fig. 1. PC materials are widely viewed as prime candidates for the memory mate-

rials of the future, which ideally will be fast (~ 10 ns switching time), dense (bit diameter  $\ll$  50 nm), stable (several years per lost bit), long-lived ( $>$  10<sup>12</sup> cycles per lost bit), and - naturally - with low manufacturing cost and power consumption. Such bit diameters would result in storage densities far in excess of those found in current commercial devices, such as those based on giant magnetic resonance (GMR).

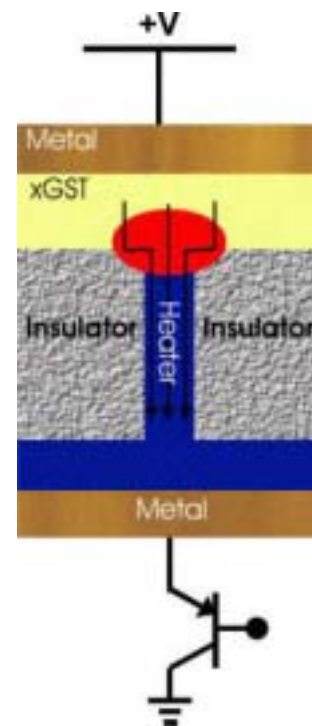


FIG. 1: Cross section of one type of PC memory cell [1]. The localized phase change in the GST film [red area] is driven here by a current pulse.

To satisfy these criteria, PC optical memory materials require: (a) an absorption edge in the visible or near infrared that changes with the transition, (b) a melting point  $T_m$  that is high enough to prevent spontaneous crystallization, but accessible to laser heating, (c) a rapid and stable transition. Work has then focused on semiconductors and semimetals with  $T_m$  between 500 and 1000°C, large atomic mobilities, and structures that are similar in the amorphous and crystalline phases. For more than a decade [2],

the pseudobinary compounds GeTe-Sb<sub>2</sub>Te<sub>3</sub> have attracted much attention, and one of them (Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>, GST) is already the basis of digital versatile disc-random access memories (DVD-RAM).

Central to the understanding of the properties of GST is a knowledge of the structures of the different phases, but these are difficult to obtain in a ternary alloy with a significant number (~ 20%) of vacancies. Yamada [2] proposed that the metastable phase has a rock-salt structure with Te atoms on all sites of one type, with the other site occupied randomly by Ge and Sb atoms and vacancies. However, as noted recently, “the local structural order of glasses in the ternary system Ge<sub>x</sub>Sb<sub>y</sub>Te<sub>1-x-y</sub> is not well established” [3]. It is striking that systems whose structures are “not well established” should already be the basis for mass commercial products. We can expect that an improved understanding of the structures and the transitions between them will lead in turn to a much deeper understanding of material properties and ways that they can be improved.

The study of phase change mechanisms in ternary alloy systems is very difficult for both theory and experiment, and the analysis of the latter often requires wide-ranging assumptions about the atomic arrangements. The metastable nature of amorphous GST (bulk samples crystallize) has also restricted experimental studies of this material. A number of calculations have been performed on GST materials in recent years, and they have provided important clues to the phase change mechanism. Nevertheless, they have focused on a restricted range of structures using unit cells (typically ~ 60 atoms) that may be too small to describe the details of the mechanism. The simulation times (typically a few picoseconds) are probably too short to describe vibrational and other thermodynamic properties reliably.

The installation and availability of the new supercomputer in Jülich has enabled us to extend the range of density functional calculations on GST and related systems substantially. We have performed calculations on Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> in a unit cell containing 460 atoms, and we have carried out simulated annealing from a high temperature in order to avoid bias towards particular structural types. We have also simu-

lated rock-salt (ordered) structures of Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>, the corresponding liquid and amorphous structures (at 900 K and 300 K, respectively), as well as two well-studied forms of the Ge-Te alloy system: Ge<sub>0.50</sub>Te<sub>0.50</sub> and Ge<sub>0.15</sub>Te<sub>0.85</sub>, the second of which has the lowest melting point (650 K) of Ge-Te alloys.

The calculations have resulted in a huge amount of data that we are still analyzing. Since we know the positions of each atom throughout the simulations, we can determine the pair correlation functions for all atom types. The structure factors derived from these agree remarkably well with the results of scattering experiments (x-rays, neutrons) where available. The vibration frequencies can be determined from well-equilibrated structures and from analysis of correlation functions obtained from long simulation trajectories. We would welcome more experimental information of the vibrational properties. The structures of the amorphous and ordered phases show similarities, as we expect from such a rapid phase change. A recent paper [4] pointed out that the ring statistics in amorphous GST were dominated by four- and sixfold rings, as found in the crystal phase, and similar patterns are evident in our work. A crucial component of these materials (and essential for an understanding of their properties) are the vacancies. The calculations provide us with insight into their distributions as well.

More details are not yet available, but this situation will change soon. We shall have plenty to say in the Annual Report next year, so you should return to this space then.

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