Phase change memory materials: an update

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Phase change (PC) materials remain leading candidates for future computer random access memory (RAM) and rewritable storage devices. The battle to replace the current standard in the world of optical recording material, the digital versatile disk (DVD), was decided in 2008, when the Blu-ray Disk (BD) became the de facto world standard. The recording medium of all BD products comprise PC materials, where a write/erase cycle involves the reversible switching between amorphous and ordered states in nanosized “bits” in a polycrystalline layer. The state can be identified by monitoring the optical or electrical properties. The transition between different structures is crucial, and we have used density functional methods to simulate several materials in widespread use. As in other areas of materials science, improving our understanding of the processes that occur on an atomistic length scale should result in materials that are better or can be prepared more cheaply. Crucial to our studies of amorphous and ordered alloys has been the availability of the BlueGene/P (Jugene) and Jüropa supercomputers.

Phase change (PC) materials are familiar to us all as rewritable media (CD-RW, DVD-RW, DVD-RAM, and now BD). Many know that laser light is involved, but fewer seem to know how the information is recorded and read. The “active” parts of all these devices comprise thin layers of an alloy (often containing Ge, Sb, and/or Te) that undergo a rapid and reversible transition between the crystalline and amorphous forms of nanoscale bits (⩽ 100 nm) that arise from quenching after a localized and short (∼ 1 ns) laser annealing to a temperature above the melting point. Longer laser heating (⩽ 50 ns) to above the glass transition temperature but below the melting point leads to a metastable crystalline form.

Many alloys used in PC storage and memory materials can be seen in Fig. 1. Alloys along the (GeTe)₁₋ₓ(Sb₂Te₃)ₓ line (often containing Ge, Sb, and/or Te) that undergo a rapid and reversible transition between the crystalline and amorphous forms of nanoscale bits (⩽ 100 nm) that arise from quenching after a localized and short (∼ 1 ns) laser annealing to a temperature above the melting point. Longer laser heating (⩽ 50 ns) to above the glass transition temperature but below the melting point leads to a metastable crystalline form.

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The Blue Gene supercomputers in Jülich have enabled us to perform simulations for a unit cell with hundreds of atoms over several hundred picoseconds. Starting from a high temperature liquid in order to avoid any structural bias, we showed that amorphous GST has many structural units (“ABAB squares”, A: Ge or Sb, B: Te) that are also present in the ordered state. Substantial numbers of cavities (vacancies, voids) provide the space needed for the structural phase change to occur in a few nanoseconds. The original calculation showed good agreement with x-ray diffraction measurements of researchers at SPring-8, the world’s most powerful x-ray source [1]. Together with our Japanese colleagues [2], we have developed a procedure for refining our structure to reproduce even better the measured structure factors and radial distribution functions (Fig. 2).

There is good contrast between the optical properties of the amorphous and ordered phases near the GeTe end of the pseudobinary line GeTe-Sb₂Te₃, but the crystallization process is slow. The reverse is true at the Sb₂Te₃ end: short crystallization times, but poor optical contrast. Ge₁₋ₓSbₓTe₃ has been adopted by many as a compromise, but alloys nearer to GeTe appear to be even better. Ge₈Sb₂Te₁₁ is used in Blu-ray Disc applications, and we have simulated it with 630 atoms in the unit cell over 400 picoseconds [3]. The properties of Ge₈Sb₂Te₁₁ are generally similar
to those of Ge$_2$Sb$_2$Te$_5$, but it crystallizes even more rapidly. The addition to GeTe of a small amount of Sb has a remarkable effect, and such “GeTe-rich” alloys are much favoured by manufacturers such as Panasonic.

Alloys of Sb and Te with compositions near the eutectic (Sb$_{0.70}$Te$_{0.30}$) are used for CD-RW and DVD-RW applications, usually including small amounts of Ag and In. Here the amorphous marks crystallize by growth from the edge (rather than nucleation from inside, as in GST alloys). We have simulated the liquid phase of a common composition of this alloy (Ag$_{3.5}$In$_{3.8}$Sb$_{75.0}$Te$_{17.7}$), and the comparison with new experimental data from SPring-8 was very encouraging [4]. A snapshot of part of the structure is shown in Fig. 3, and the work (experimental and theoretical) is being extended to the amorphous phase.

Almost all of the alloys used commercially as optical storage materials contain tellurium, which itself has properties that are no less remarkable: it crystallizes rapidly, and it has a very unusual density maximum just above its melting point. Te shares this behaviour with water, the most important liquid on Earth, and the structure of Te in the supercooled phase could shed light on the (still controversial) structure of water. A detailed study of Te is almost complete, and you should come back to these pages next year for a report.

The Jülich supercomputers allow us to perform calculations on length and time scales that are much closer to physical reality than were previously possible. Nevertheless, materials science and condensed matter physics play much smaller roles on Jugene than elementary particle physics. One of the most eminent elementary particle physicists, Steven Weinberg, noted that this field “has no direct applications that anyone can foresee” [5]. By contrast, materials scientists are challenged on a daily basis by problems with direct applications. Our experiences with PC materials and the work of many others show just how exciting such applications can be.

**FIG. 2:** (a) Structure factor $S(Q)$ in amorphous GST. Red: x-ray diffraction, blue: calculated. (b) Total radial distribution function $g(r)$.

**FIG. 3:** Snapshot of t-AIST (Ag: silver, In: magenta, Sb: blue, Te: yellow). Ag and In are depicted with small spheres, the cavities are shown in red.

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