

# X-RAY ANALYSIS FOR BETTER OPTICAL STORAGE MATERIALS

**M**aterials called “chalcogenide glasses” have been at the forefront of a revolution in optical data storage. Of special interest is the compound  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (GST), which exhibits the very useful ability to switch reversibly between amorphous and crystalline phases on exposure to light or electrical pulses. Because the properties of these phases are different and can represent data bits, GST is being studied for data-storage-device applications. To engineer optimum switching performance, however, materials scientists seek a detailed understanding of the mechanism responsible for the amorphous-crystalline transition. Recently, a team of researchers from North Carolina State University and the Colorado School of Mines used the MR-CAT 10-ID beamline at the APS in conjunction with powerful theoretical tools to study the bonding mechanisms in the amorphous phase of GST. Their results underscore the ability of high-brilliance x-ray beams, such as those from the APS, to provide atomic-scale measurements for clarifying phase transition mechanisms of technological interest.

Samples of GST were fabricated by radio frequency sputtering 2.7- $\mu\text{m}$  films onto aluminum foils. The foils were sectioned into 10 mm x 4 mm pieces and stacked to create layered specimens with a total thickness of 22  $\mu\text{m}$ . Extended x-ray absorption fine structure (EXAFS) spectra were obtained at MR-CAT beamline 10-ID. Spectra near the K edges of Ge, Sb, and Te were collected in transmission mode. Fitting of the Fourier transformed spectra was carried out with standard analysis codes to yield atomic bond distances and coordination numbers consistent with tabulated values.

These measurements were analyzed in the context of bond constraint theory, which provides a framework for characterizing amorphous materials in much the same way that periodicity serves to characterize crystalline materials. In this theoretical picture, a material is good for forming glass if the average number of constraints (that is, stretching or bending motions) per atom is equal to the dimensionality of the amorphous network. Atoms are constrained to remain where they are unless energy is provided to stretch or bend the bonds that hold them in place, and bond constraint analysis quantifies this concept. Materials that are either too constrained (stressed and rigid) or not constrained enough (floppy) will not be good candidates for easily switched structural transitions. Structural probes such as EXAFS can be used to construct a detailed picture of the bonding arrangements for each of the atoms in GST. When the average constraint numbers for each of the constituent atoms are added together, the result is a total of 3.07, which is in good agreement with the dimensionality of the network  $D = 3$ .

Bond constraint analysis based on the EXAFS results shows that GST is an intermediate region of the ternary phase diagram where entropy effects in the amorphous phase and enthalpy effects in the crystalline phase balance out to allow reversible transitions. With this information, it should be possible to fine tune the GST composition for optimum switching.

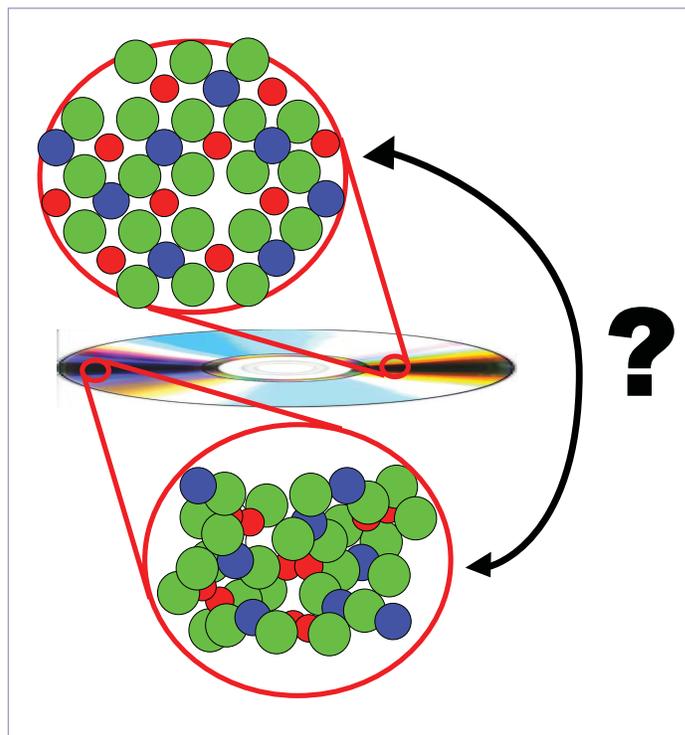


Fig. 1. The two phases of GST that are used for data storage. The lower, amorphous phase consists of  $\text{Ge}_2\text{Te}_3$  units and  $\text{Sb}_2\text{Te}_3$  units interconnected by an amorphous tissue of two- and three-fold coordinated Te. The upper diagram shows the well-characterized crystalline phase.

The findings show the value of detailed atomic-scale measurements in elucidating phase transition mechanisms of technological interest, especially when the measurements can be performed at high-brightness third-generation synchrotrons such as the APS. — David Voss

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