

# Industrial Applications

## XAFS STUDY OF LOCAL STRUCTURAL CHANGES IN Ge-Sb-Te DURING OPTICAL RECORDING BELOW THE DIFFRACTION LIMIT

Continuing progress in multimedia has led to the need for ever increasing storage density requirements with fast data recording/access. One of the most promising solutions to these stiff requirements is phase-change optical data storage. The latest industrial implementation of optical data storage is the re-writable digital versatile disc (DVD), a medium that allow storage up to 4.7 Gb of information on a single-layer disk. The recording (phase change) medium of a DVD is either  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (DVD-RAM) or a quaternary Ag-In-Sb-Te (DVD-RW) alloy.

The phenomenology of optical recording is very simple. CW-laser light crystallizes the recording layer while an intense laser pulse melts the material that is subsequently quenched into the amorphous state. The recorded bits are thus amorphous marks against a crystalline background.

Although the idea of phase-change recording has been around for almost 40 years and DVDs have been commercially available for over a decade, it has only been recently that the nanoscale structure of the recording material and its modification upon the amorphous-crystalline phase transition started to emerge.

Earlier X-ray diffraction studies suggested that – although the stable structure of  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  (GST) is hexagonal – thin GST layers crystallize into the rocksalt structure with a rather large isotropic temperature factor [1]. Whilst this was a very important finding it left several very important questions unanswered.

We have carried out X-ray absorption fine structure (XAFS) measurements of crystallized and laser-

amorphized GST layers at beamline **BL01B1** and – which is important – our measurements were performed on real-device structures. For the crystalline state we found that Ge and Sb atoms were not located on the ideal rocksalt sites (in the center of the Te face-centered cubic (fcc) sublattice) but were somewhat displaced from the center, i.e., similar to the GeTe structure, a distorted rocksalt, or rhombohedral structure. An immediate consequence of this is that GST in its metastable crystalline state possesses a net dipole moment, i.e., is a ferroelectric [2,3].

It was found that the “amorphization” of GST produced a structure with bonds *shorter and stronger* than in the crystalline phase as evidenced by comparison of Fourier-transformed extended X-ray absorption fine structure (FT EXAFS) spectra (Fig. 1) for the two phases. The results of a detailed data analysis are summarized in Table 1. Such a change is highly unusual for covalently bonded solids and suggests that the “amorphization” of GST is not a simple disordering of the structure but involve much more drastic changes [2].

To get more insight into the structural transformation we have also performed X-ray absorption near-edge structure (XANES) measurements and simulations. The best agreement between the experiment and simulations was obtained when Ge atom was placed into a tetrahedral symmetry position within the Te face-centered cubic (fcc) sublattice [2].

The structure of the crystalline and amorphous phases of GST are schematically illustrated in Fig. 2, which shows fragments of the structure with a Ge

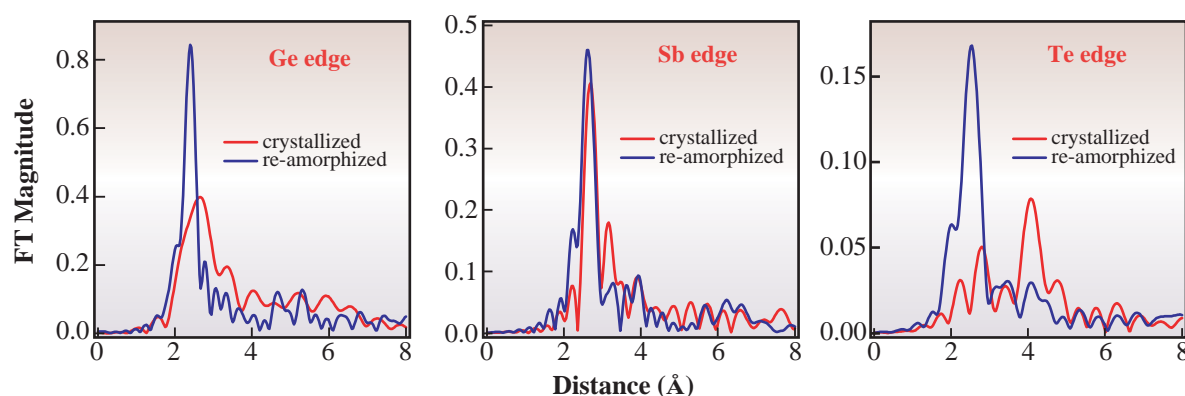


Fig. 1. FT-EXAFS spectra of crystalline and amorphous areas measured at Ge, Sb, and Te K-edges (after [2]).

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atom located either in a octahedral (crystalline) or tetrahedral (amorphous) symmetry positions. As a double check of the amorphous structure, one can estimate the Ge-Te bond length assuming the Ge atoms are in tetrahedral symmetry positions. Based on the lattice parameter obtained by X-ray diffraction, this bond lengths is expected to be 2.61 Å, a value identical to the experimentally measured result (Table 1).

The phase-transition thus primarily consists in an umbrella flip of Ge atoms between the octahedral and tetrahedral symmetry positions without major structural rearrangement. It is the fact that the Te sublattice is preserved while only the Ge atoms switch position that accounts for the ultra-fast recording/erasing rates and the overall media stability [2,3].

It is interesting that the same materials, namely GST and Ag-In-Sb-Te alloy (AIST), are also the best-performing materials in the optical discs of new generation, the so-called super resolution near-field structure (Super-RENS) optical discs currently developed by our Center [4]. At present, bits with a characteristic size of less than 100 nm with a carrier-

to-noise ratio (CNR) over 40 dB can be recorded with an inexpensive standard “red” diode laser. A significant difference between the DVD and Super-RENS structures is that in the latter the GST layer is crystalline in both recorded and non-recorded areas. Intensive investigations of the underlying mechanisms behind super-RENS recording and read-out are currently underway [5].

**Table 1.** Bond lengths and mean-square relative displacements (MSRD) obtained for crystalline and amorphous Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>.

Bond	Bond length (Å)/MSRD (Å <sup>-2</sup> )	
	Crystal	Amorphous
Te-Ge	2.83 ± 0.01 / 0.02	2.61 ± 0.01 / 0.008
Te-Sb	2.91 ± 0.01 / 0.02	2.85 ± 0.01 / 0.008
Te-Te (2 <sup>nd</sup> )	4.26 ± 0.01 / 0.01	

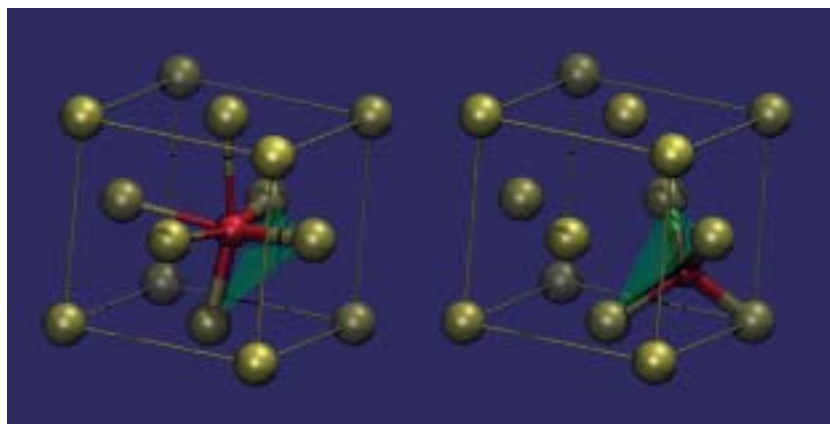


Fig. 2. Fragments of crystalline and amorphous structures. During the transition Ge atom switches between octahedral and tetrahedral symmetry positions (after [2]).

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