ESRF	**Experiment title:** Differential structure factors of amorphous and liquid DVD material $Ge_2Sb_2Te_5$ by anomalous x-ray scattering	**Experiment number:** HD-380
Beamline: BM02	**Date of experiment:** from: 28 Oct 2009 to: 03 Nov 2009	**Date of report:** 01 Mar 2010
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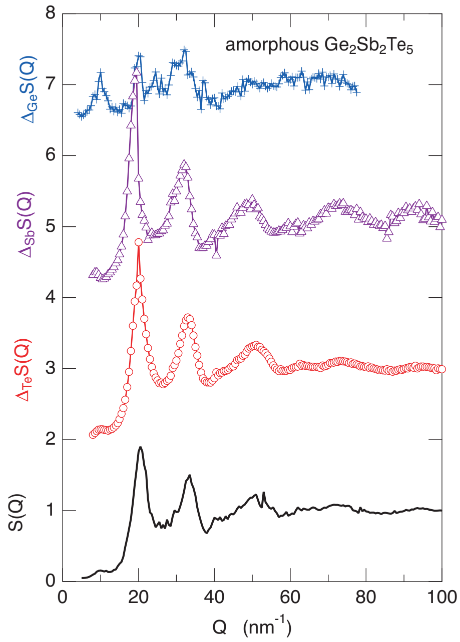
Report:

Rewritable optical storage devices like Digital Versatile Disk - Random Access Memory (DVD-RAM) are nowadays common media for data storage and are widely used in all areas of daily life. The writing/erasing process is thereby attained by a reversible laser induced crystalline-amorphous transition in these materials, such as $Ge_2Sb_2Te_5$ (GST). It occurs on a timescale of a few nanoseconds and is accompanied by significant changes in the optical and electrical properties. This property is the basis for the reversible data storage ability. However, the underlying microscopic processes enabling the fast change from crystalline to amorphous and vice versa are not yet understood.

Some structural models exist in the literature, which are currently controversially discussed. Kolobov et al. [1] investigated the local structure around each element in the crystalline and amorphous phases of GST by XAFS. From their data, they proposed the so-called umbrella flip mechanism for the fast transition where the Ge atoms switch from an octahedral arrangement in the crystal to a tetrahedral environment in the amorphous phase. On the other hand, Kohara et al. [2] measured the total structure factor, $S(Q)$, of the amorphous phase by using high energy x-rays, and analyzed the data using a reverse Monte-Carlo (RMC) calculation. They proposed that the amorphous phase can be regarded as an even-menbered ring structure, and suggested that the resemblance of the ring structure is related to the fast phase change process. However, the key information on the intermediate structure in the amorphous phase is still lacking at present.

In order to investigate the local- and intermediate range order in the amorphous



phase of GST, an anomalous x-ray scattering (AXS) experiment was carried out at energies close to the Ge, Sb, and Te K edges. The amorphous sample was contained between two extremely thin walled ($\sim 50\mu$m) sapphire plates with a thickness of $\sim 50\mu$m for the Ge K edge experiment, or in a quartz glass capillary with an inner diameter of 0.2 mm and a wall thickness of $\sim 10\mu$m for the Sb and Te K edges experiments. The AXS experiments were carried out by using a standard $\omega - 2\theta$ diffractometer installed at the BM02 at two incident x-ray energies below each K edge (-20 eV for Ge, -30 eV for Sb and Te, and -200 eV for all). For discriminating the elastic signal from the K_β fluorescence and Compton scattering contributions, a graphite crystal analyzer was mounted on a 50 cm long detector arm. The feasibility of this setup is described elsewhere [3,4].

The figure shows differential structure factors, $\Delta_i S(Q)$, obtained close to the Ge (crosses), Sb (triangles), and Te (circles) K edges, together with $S(Q)$ given by the solid curve. A prepeak is observed in $S(Q)$ at about $Q = 10$ nm^{-1}, indicating the existence of an intermediate-range atomic correlation. At the prepeak position, $\Delta_{\rm Ge}S(Q)$ has a prominent peak, while $\Delta_{\rm Sb}S(Q)$ and $\Delta_{\rm Te}S(Q)$ show only small peaks. Thus, the intermediate-range correlations originate from the atomic correlations related to the Ge cations. This clear assignment could undoubtedly be drawn from the present AXS measurement for the first time. In addition, there is almost no contribution from $\Delta_{\rm Ge}S(Q)$ to the first peak in $S(Q)$, while the other two $\Delta_i S(Q)$s have large peaks there. It should also be noted that the shapes of $\Delta_{\rm Ge}S(Q)$ and $\Delta_{\rm Te}S(Q)$ in this amorphous material resemble those of $\Delta_{\rm Ge}S(Q)$ and $\Delta_{\rm Se}S(Q)$, respectively, in Ge-Se glasses [4]. From the obtained results, a RMC modeling will be applied to obtain the three-dimensional atomic configurations in the amorphous phase of GST.

[1] A. V. Kolobov et al., Nature Materials **3**, 703 (2004).

[2] S. Kohara et al., Appl. Phys. Lett. **89**, 201910 (2006).

[3] S. Hosokawa and J.-F. Bérar, AIP Conf. Proc. **879**, 1743 (2007).

[4] S. Hosokawa et al., Z. Phys. Chem. **216**, 1219 (2002); Phys. Rev. B, submitted.