

**Experiment title:**

Determination of partial structure factors in Ge-Sb-Te Phase Change Materials

Experiment number:

HD-603

Beamline:

BM-02

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18

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Report:

We have recently started a research project aiming to explore characteristic structural trends of different liquid and amorphous Ge-Te-Sb alloys. In the ternary phase diagram these compounds are situated on the pseudo-binary conjunction between GeTe and Sb_2Te_3 (see Fig. 1). They are known as excellent Phase

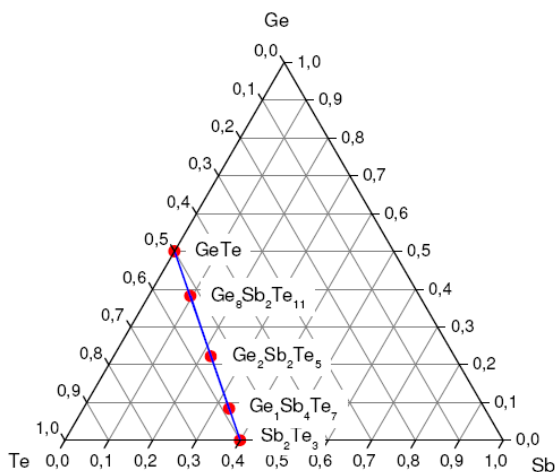


Figure 1: Ternary phase diagram of the Ge-Sb-Te system.

Change Materials (PCMs), i.e. they can reversibly switch back and forth between a meta-stable polycrystalline and an amorphous phase within some ten nanoseconds. Some of these materials are already commercially used to manufacture optical storage devices as e.g. the DVD-RW or the Blu-Ray Disc. However, the microscopic mechanisms enabling these remarkable features are still not fully understood. One reason is that detailed structural information on both of the phases is still lacking and the relation between the crystal-structures and the spatial alignment of the atoms in the respective amorphous phases is still controversially discussed.

To examine the structural changes in the amorphous phase along the *tie*-line, we have proposed to measure the materials with the nominal compositions $\text{Ge}_8\text{Sb}_2\text{Te}_{11}$ and $\text{Ge}_1\text{Sb}_4\text{Te}_7$ in order to investigate a GeTe-rich example (GST-8,2,11) and an example with a low GeTe content (GST-1,4,7), using Anomalous X-ray Scattering which allows to obtain partial structural information of the multicomponent amorphous system.

It was intended to measure the materials at the K-absorption-edges of the respective elements; however, since we encountered problems with the high energy monochromator at the beamline, only the low-energy Ge-K-edge of the samples was accessible for the experiment, and we were not able to measure the Sb- and Te-edges. We therefore decided to measure Ge-rich samples only (i.e. the GST-8,2,11 and, instead of the GST-1,4,7 sample, we measured GeTe (1:1), which represents another member along the *tie*-line) since we already had preliminary results from previous measurements available for the Te-K-edges (see experimental report HD-510) for these materials, so that we now are able to start first computer simulations without the lack for the high-energy data. Subsequent more accurate measurements of the high-energy edges will thus enable us to refine these preliminary simulations.

This way, we will be able to accurately examine the structural changes that occur with only a minimal deviation from the pure GeTe case, which are known too be huge in the case of the crystalline phases, where they are accompanied by a transition from a conducting phase (GeTe) to a semiconducting phase (GST-8,2,11), and we will examine whether such changes are also visible in the corresponding amorphous phases. Figures 2 and 3 depict the obtained preliminary structure factors at the Ge-K-edge; compared with previous measurements at this comparably low energy, the quality of the data has been greatly enhanced due to the new experimental setup at D2AM.

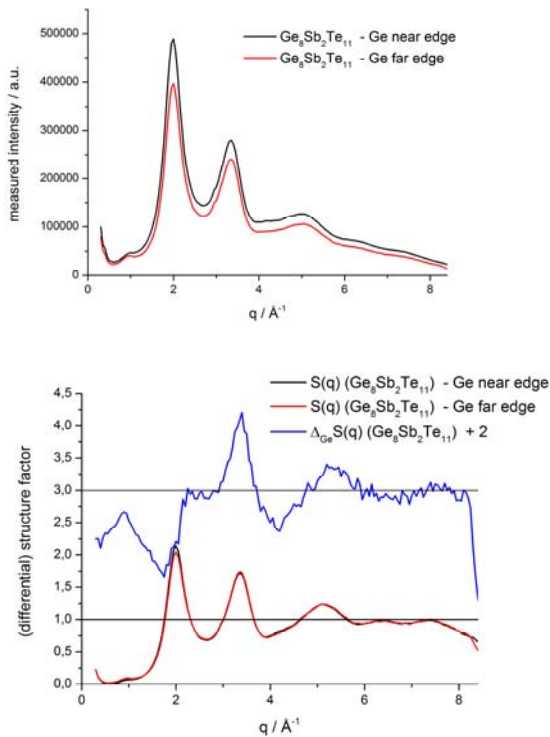


Fig 2: Raw data for the measurements of a-Ge₈Sb₂Te₁₁ at the near- and far-edge measurements at the Ge-K-edge (top). The bottom graph shows the obtained structure factors and the corresponding differential structure factor.

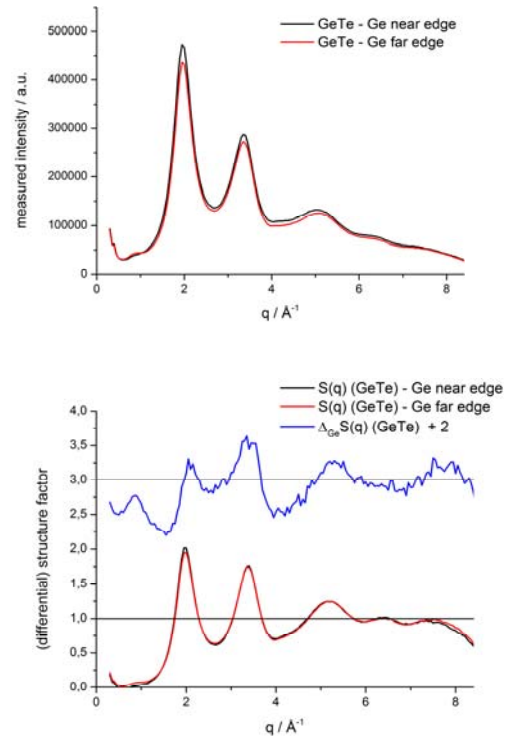


Fig 3: Raw data for the measurements of a-GeTe at the near- and far-edge measurements at the Ge-K-edge (top). The bottom graph shows the obtained structure factors and the corresponding differential structure factor.