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| | Experiment title: In situ XRD study of temperature-dependent structural changes in liquid Ge-Sb-Te alloys | Experiment number: MA-3124 |
| Beamline: ID11 | Date of experiment: from: 02/11/2016 to: 06/11/2016 | Date of report: 06/02/2017 |
| Shifts: 12 | Local contact(s): Dr. Jonathan Wright | <i>Received at ESRF:</i> |
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Report:

Ge-Sb-Te chalcogenide alloys are important for applications in advanced (non-volatile) random-access memory based on a reversible switching between the crystalline and amorphous phases. As the amorphisation occurs via the liquid state, a detailed knowledge of the liquid structure is essential for understanding the glass formation.

The X-ray diffraction measurements of liquid Ge-Sb-Te alloys were carried out successfully for the six alloys on the pseudo-binary line between GeTe and Sb_2Te_3 (GeTe, $\text{Ge}_8\text{Sb}_2\text{Te}_{11}$, $\text{Ge}_2\text{Sb}_2\text{Te}_5$, $\text{Ge}_1\text{Sb}_2\text{Te}_4$, $\text{Ge}_1\text{Sb}_8\text{Te}_{13}$, Sb_2Te_3), as well as the eutectic composition $\text{Ge}_{15}\text{Te}_{85}$. The samples were sealed with 250 mbar Argon gas in 2 mm quartz-glass capillaries and mounted vertically above the hot-air blower (Cyberstar) available at ESRF. The incident radiation with 120 keV provided a sufficient signal in transmission mode despite the high absorption of the sample material. The scattered intensities were measured continuously in the temperature range between 1100 K and the solidification, depending on the composition (995 K - 650 K).

The temperature dependence of the total structure factors have been mainly analyzed so far, while the analysis of the concentration dependence is in progress. Fig. 1 shows the change of the total structure factor $S(Q)$ of liquid GeTe over temperature. The first peak shows a linear behaviour, which fits well with the density and viscosity measurements.

The XRD structural data will be modeled together with ND data by the reverse Monte-Carlo and ab-initio molecular dynamics simulations in order to determine the partial pair correlation functions.

These XRD results are supplemented by neutron diffraction data carried out at the LLB CEA CNRS Saclay (France) and ISIS (UK) as well as by the measurements of the mass density (Niigata University) and dynamic viscosity (IFW Dresden).

A paper on the liquid GeTe is in progress and will be submitted for publication soon. The other data are under treatment and will be published in future as well. Furthermore the results of the study will make a part of a PhD thesis of one of the proposers (H.W.) at the TU Dresden.

The experiment at the ID11 was excellently prepared. We want to thank our local contact Jonathan Wright for the support during the experiment as well as with the data treatment.

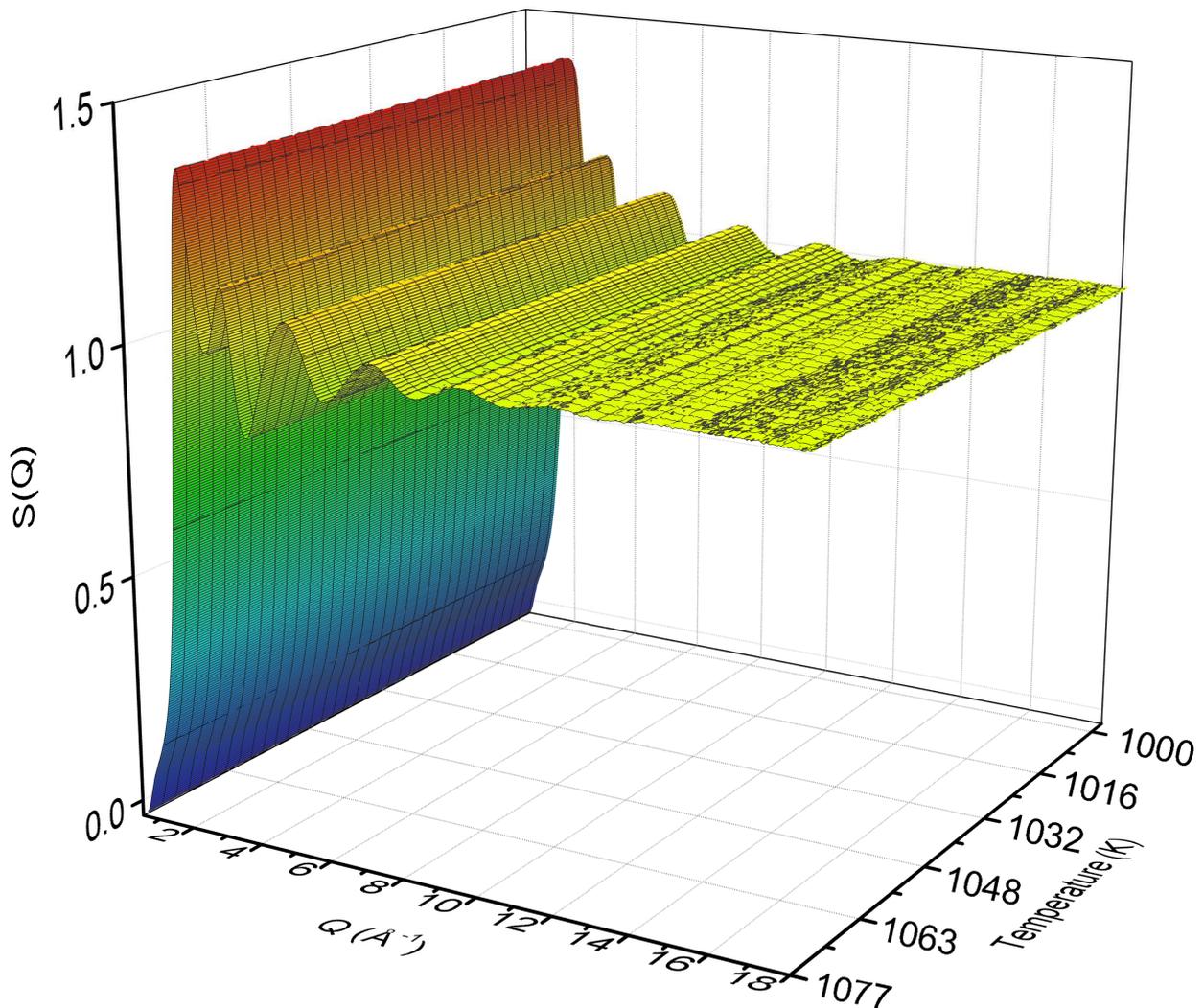


Fig. 1: Total structure factor $S(Q)$ of liquid GeTe over wavevector Q (0-18 \AA^{-1}) and over a temperature range between 1000 and 1077 K. The first peak shows a linear decrease and a linear shift with temperature.