



	<b>Experiment title:</b> Influence of the pressure on the liquid-liquid phase transition in GexTe1-x alloys : an XAFS study	<b>Experiment number:</b> HS-2460
<b>Beamline:</b>	<b>Date of experiment:</b> from: 02/02/05 to: 08/02/05	<b>Date of report:</b> 03 march 05
<b>Shifts:</b>	<b>Local contact(s):</b> O. Mathon	<i>Received at ESRF:</i>
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## Report:

Let recall that chalcogenide semiconductors are good candidates as materials for optical memories and optical data storage. Te-based semiconductors have the ability to easily crystallise and amorphise under the action of a laser pulse, basic process of commercial phase change optical disks. During this process, the crystal is locally melted to obtain an amorphous spot; this spot can be recrystallised by using a less intense laser beam. Recently, many theoretical studies were performed examining the precursor liquid phase on both the eutectic composition  $\text{Ge}_{15}\text{Te}_{85}$  [1] and GeTe compound [2,3]. It has been shown that the liquid phase at both compositions exhibits a liquid-liquid (L-L') phase transition within 200K above the melting point. In both compositions, the L phase is shown to be locally similar to the low temperature threefold coordinated crystalline phase ( $\alpha$ ) while the L' phase is locally similar to the high temperature sixfold coordinated crystalline phase ( $\beta$ ).

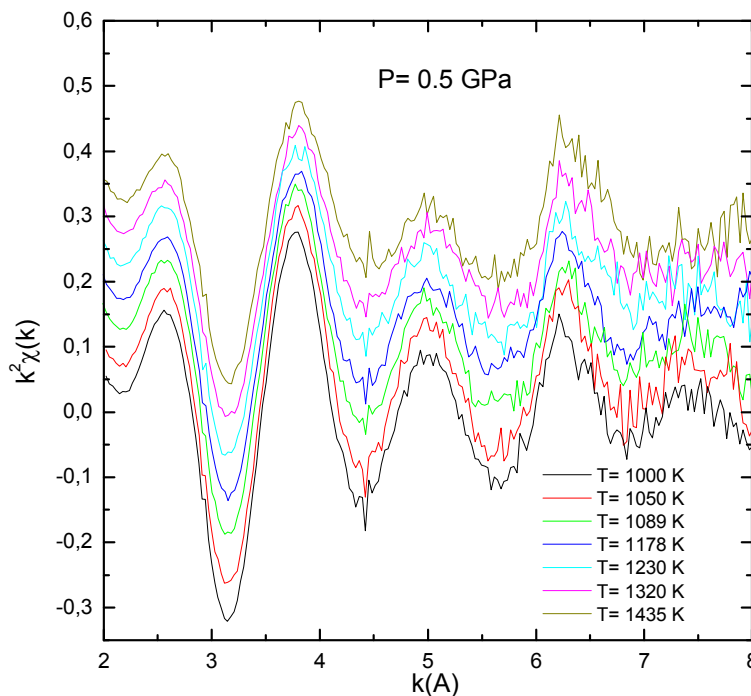
The aim of the performed experiment was to study the liquid-liquid transitions in both GeTe and  $\text{Ge}_{15}\text{Te}_{85}$  liquids and to study the influence of the pressure on the L-L' transition line. Our thermodynamic assessment of the phase diagram under pressure suggest that for pressure up to 5 GPa the relative stability of the compound and the eutectic is not modified, which justify such experiments.

In the given time (18 shift), we were able to study the structure of GeTe liquid for a pressure varying between 0.5 and 5 GPa and at different temperatures. For each thermodynamic state, EXAFS spectra were

measured at the Ge-K edge and a near edge absorption spectra at the Te-K edge was collected in order to check the composition of the sample. Precise EXAFS acquisitions at the Te-K edge were not possible as the thickness of the sample was optimized for Ge-Kedge. Moreover for each thermodynamic state a X-ray diffraction pattern was recorded in order to determine the pressure (diffraction of BN matrix), to verify the state of the sample (solid/liquid) and to follow the recrystallisation of the sample when increasing pressure/decreasing temperature. In addition, by using SEXAD (single energy x-ray absorption detection) we were able to map the liquidus curve with increasing pressure.

Figure 1 represents one of the series of the  $k^2\chi(k)$ . Let us note that we do not present all the data obtained during the experiment. The presented data were obtained for a pressure of 0.5 GPa, the temperature varying from 1000 K up to 1435 K. As a first result we can conclude that the local order is the liquid undergo important changes as the temperature is increased.

The amplitude of the oscillations decrease with increasing temperature and strong and rapid changes are observed in the shape of the oscillations (peak around  $5 \text{ \AA}^{-1}$ ). This could correspond to a change in the local atomic ordering around Ge atom and could be consistent with a liquid-liquid transition. Such results would be consistent with ab-initio calculations [2,3] but of course a detailed analysis has to be performed.



*Figure 1 : Evolution of  $k^2\chi(k)$  as a function of the temperature for a fixed pressure equal to 0.5 GPa*

## References

- [1] C. Bichara et al., J. Phys. Cond. Matt., 15 (1), S167-173 (2003)
- [2] J.Y. Raty et al., Phys. Rev. B, 65, 115205 (2002)
- [3] J.Y. Raty et al., Phys. Rev. Lett. 85(9), 1950 (2000)