ESRF	**Experiment title:** **Density anomaly and local order in $Ge_{.15}Te_{.85}$ alloy**	**Experiment number**: HS-1953
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Report:

Let first recall some of the important features of Ge_xTe_{1-x} liquid alloys around the eutectic composition. Similarly to the well-known case of liquid water, those liquids (x=0.15) contract upon heating as evidenced by the density measurements [1] presented on figure 1. This density anomaly is accompanied by a sharp maximum on the specific heat [2], which suggests that structural changes occur in the liquid state (fig. 1). However the recent thermodynamic assessment on the GeTe [3] system could not give any clue to understand these unusual results in the thermodynamics response functions.

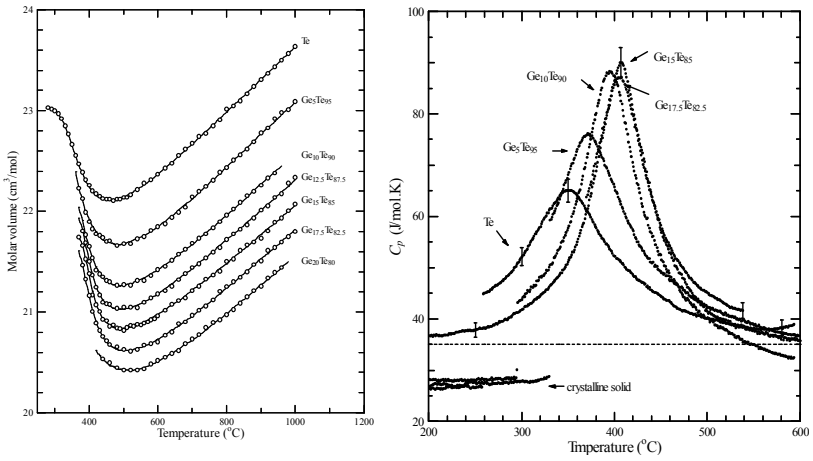


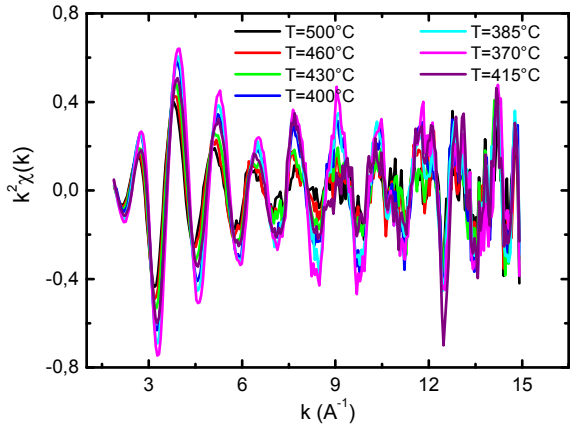
Figure 1 : Density (right) and specific heat (left) measurements on Ge_xTe_{1-x} liquid alloys around the eutectic composition

Although numerous neutron and X-ray scattering experiments have been performed on this system [4-7], no clear picture emerges of the structural mechanisms involved, essentially because none of them gave access to the partial structure factors, thus making the interpretation of the measured total structure factors difficult. Very recently, *ab-initio* calculations of the structure of liquid $Ge_{0.14}Te_{0.86}$ alloys have been performed [7] and seem to indicate that the major changes concern the Ge-Te partials, the Te-Te partials remaining essentially unaffected by the structural change.

The aim of the experiment reported here was to gain a better understanding of the structure of the liquid Ge_xTe_{1-x} and of the structural mechanisms responsible of the anomalous behaviour of density. We performed EXAFS measurements at the Ge K-edge on $Ge_{.15}Te_{.85}$ alloy in to study the evolution of the local atomic environment.

The experiments were performed using the new high pressure and high temperature vessel recently developed by the Laboratoire de Cristallographie. This cell is specially devoted to EXAFS measurements in fluorescence mode and was necessary here because of the high absorption of the elements.

The evolution of the liquid structure has been studied for temperatures ranging from 350°C up to 500°C. As those alloys investigated present a non-negligible vapour pressure in this temperature range, an external pressure of 30 bar was applied against the saturated vapour pressure of the elements. We present in figure 2 our preliminary results by plotting the evolution of $k^2\chi(k)$ function. First we note the high quality of the data in spite of the high absorption coefficient of the liquid and the very good reproductibilty of the spectra when varying the temperature.



Evolution of $k^2\chi(k)$ when varying the temperature.

Secondly we observe that the amplitude of the oscillations increases with decreasing temperature and that the phase shift toward smaller values of k. This phase shift corresponds to a change in the local atomic ordering around Ge atom and ca be seen, in the reciprocal space, as the onset of neigbhours at larger distances (ie a second spehere of coodination). Such results would be consistent with ab-initio calculations [7] but of course a detailed analysis has to be perform.

References :

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This report was submitted a first time in April 2003 but as I could not load it, it has been submitted again in February 2005