



Experiment title: Structure determination of liquid Ga-Te using combined x-ray and neutron scattering.	Experiment number: SC-359	
Beamline: BM 16	Date of experiment: from: 6 th Dec. 1997 to: 9 th Dec. 1997.	Date of report: July, 1998.
Shifts: 9	Local contact(s): Dr. Andrew Fitch	<i>Received at ESRF:</i> 19 AOUT 1998

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Report:

This experiment was initially carried in July 1997, but failed due to the failure of the BM16 furnace that was running near its temperature limit. The experiment was repeated in December 1997 with a new furnace arranged in a new geometry to avoid overheating. The furnace worked well in this configuration. The samples were mounted in thin walled 0.5mm diameter silica capillaries. Small experimental problems occurred due to the migration of the sample in the silica tube as it melted. This led to approximately only half of the intended sample volume being illuminated. Nevertheless, satisfactory diffraction patterns were obtained from the liquid Ga-Te sample.

Data was collected for the composition Ga_2Te_3 at 3 incident beam energies: 31604 eV, 31795 eV and 31805 eV. These energies corresponded to 210, 20 and 10 eV below the Tellurium K absorption edge.

The raw data (shown in figure 1) have been corrected for self attenuation and the empty silica and background scattering[1]. No Compton scattering correction was made as this will be eliminated by the high resolving power of the analysing monochromators on BM16.

Figure 1

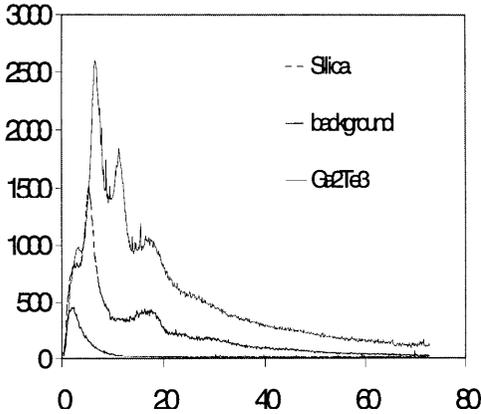
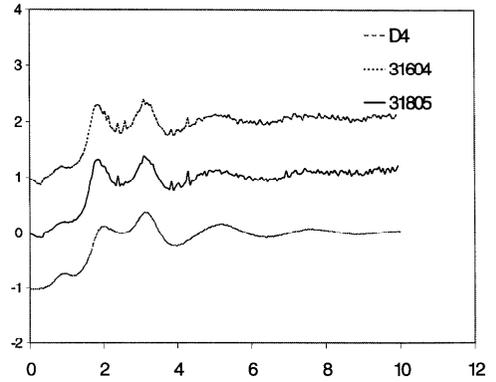


Figure 2



Neutron data has already been collected for these alloys by this group at D4 at the ILL (experiment reference: 6-03-206). This in itself was a development on previous work [2] in that data was collected at lower Q and higher resolution. This was also the case with the x-ray data collected here. The normalised $S(Q)$'s for the x-ray data compare well with the D4 neutron data in terms of the position of the peaks. There is also a clear contrast in intensity of the peaks (due to the anomalous scattering) between the 2 sets of X-ray data shown in figure 2. We are currently carefully analysing the data to the partial structure factor level by combining the neutron/x-ray data. Certainly, the preliminary partial structure factors are encouraging and are reminiscent of the ab-initio dynamical simulation results for Ga_2Se_3 [3].

Partial structure factors have been obtained by this group for liquid TlSe using 1 x-ray measurement and 2 neutron measurements on different isotopes [4]. More recently, partials have been obtained for GeO_2 at room temperature using 2 x-ray measurements at 2 energies below the Germanium K-edge and one neutron measurement [5]. This experiment has represented the next stage in the development of using x-rays in the traditionally neutron-dominated field of structural determination of disordered materials.

References:

- [1] Paalman and Pings: (1962) *J. Appl. Phys.* 33 (8) 2635.
- [2] Hoyer et. al.: (1984) *Phys. Stat. Solidi* 84, 11.
- [3] Hollender and Gillan (1996) *Phys. Rev. B*.
- [4] Barnes et. al.: accepted for publication in *J. Phys. Condens. Matt.*
- [5] Price et. al.: submitted to *Phys. Rev. Letts.*