ESRF	**Experiment title:** The structure of liquid Tl-Se compounds	**Experiment number:** HS32
Beamline: **BM16**	**Date of experiment:** **from:** 28-10-1996 to: 30-10-1996	**Date of report:** **16-4-1997**
Shifts: **9**	**Local contact(s):** E. Doryhee and A.Fitch	*Received at ESRF:* 21 AVR. 1997

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Report:

The Structure of Liquid Tl-Se Alloys.

Liquid Tl-Se alloys are a particularly interesting class of liquid as their electronic properties lie on the border between semiconducting and metallic behaviour. Their conductivity remains very low over the composition range Tl_2Se-Tl_2Se_3; behaviour which is believed to due to the formation of charged Se pairs and chains in the liquid. Neutron diffraction experiments with isotopic substitution are at the limit of current techniques and give particularly poor resolution of the Se-Se partial structure factor. In this experiment we were concerned with measuring accurate X-ray diffraction patterns for these alloys which could be combined with the neutron diffraction results. It is notoriously difficult to do this using conventional diffractometers due to the problems involved in correcting for Compton and. multiple scattering from the materials. In this experiment we took advantage of the highly monochromatic incident beam, coupled with high energy resolution of the scattered beam, in order to eliminate and minimise these corrections. Due to the high mass of the Tl atom it was also advantageous to use a high incident energy (38 keV) in order to reduce the sample self attenuation. The high θ resolution of BM16 allowed us to do this with minimal loss of Q-space resolution due to the small scattering angles involved.

Figure 1 shows the normalised X-ray diffraction patterns for the background, empty silica container and the liquid TlSe sample in the silica container (after the 9 detectors had been combined). The background observed at small Q was disappointingly high and difficult to control as the beam stop was a rather ad hoc affair. With a careful design of the beam stop we are sure these problems could be considerably reduced. Nevertheless, we have been able to carry out the fist stages in the data analysis and the results look very encouraging. The scattering has been corrected for background, container scattering and self attenuation. Figure 2 shows the partial structure factors obtained from a neutron diffraction and isotopic substitution experiment using the most favourable isotope combinations available - $^{n}Tl^{n}Se$, $^{203}Tl^{76}Se$ and $^{205}TlSe$ - on the D4 diffractometer at the ILL. As can be seen the statistical accuracy is poor and the partial structure factors need to be heavily smoothed before real space transforms can be obtained. Figure 3 shows the equivalent partials obtained, at the first attempt, for the same material using the $^{203}Tl^{76}Se$, $^{205}TlSe$ neutron diffraction data and the X-ray data collected in this experiment. As can be seen the statistical accuracy of the data is considerably improved, and the partials show typical binary liquid characteristics. Transformation into real space reveals a very good Tl-Se partial g(r) and a well resolved Se-Se peak at 2.34 clearly indicating Se-Se pairs or chains. We are currently refining the data analysis before publication.

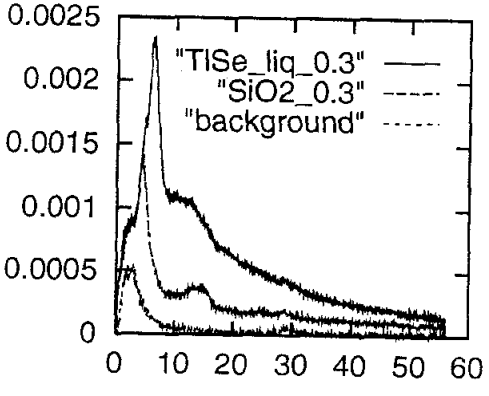

Figure 1.

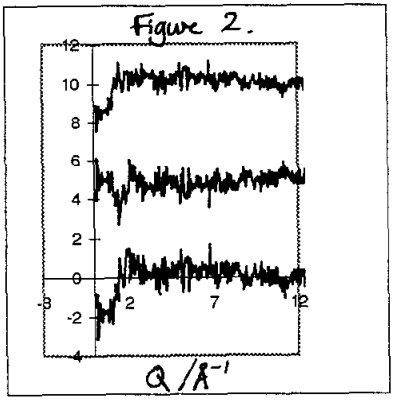

Figure 2.

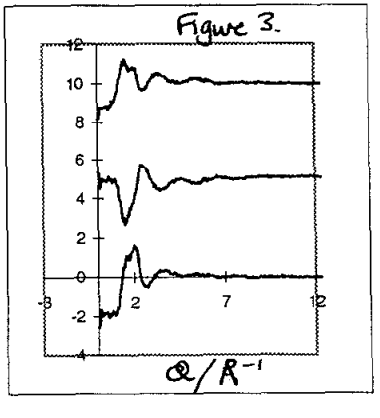

Figure 3.