



	Experiment title: The structure of liquid III-VI semiconductors (EXAFS study)	Experiment number: HS-1198
Beamline: BM29	Date of experiment: from: 27/04/00 to: 02/05/00	Date of report: 26/07/00
Shifts: 12	Local contact(s): M. Borowski	<i>Received at ESRF:</i>
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Report:

The lack of long range order has a strong influence in the electronic transport properties of liquids and amorphous systems that needs to be coupled to the local and medium range order of these materials. Even if some modelshave shown to produce rather good results in the case of charge-transfer-type liquid semiconductors (Tl-Te system for instance) unexplained transport anomalies remain in the same III-VI family of compounds. Our objective is to couple structure determination experiments with modeling efforts to determine the origin of the transport anomalies in systems like ℓ - InSe or ℓ - GaSe.

In order to accelerate the sample homogeneity, solid alloys at different composition were prepared in lab. After melting, the liquid In-Se samples were inserted into the gap between the X-ray windows made of quartz glass cell which are polished to 0.35 mm thickness. The gap -sample thickness- is optimized for an absorption step of one in the transmission experiment and varies between 35 and 90 micrometers depending on the alloy composition and of the absorption edge. The samples were heated at temperatures just above the melting point (< 1000 C) in an adapted furnace inserted into the beamline. Because of the active evaporation of the Se-rich side, measurements were carried out under a pressure of 3 bar argon gas. Extended x-ray absorption spectra with an optimized energy mesh with a constant spacing in the photoelectron wavevector scale, k-space were used as acquisition mode. Both In and Se k-edge were measured.

Fig shows the obtained EXAFS signal as a function of the concentration of indium for the nominal sample composition. The measure of both edges allows to correct this values for any disproportionation.

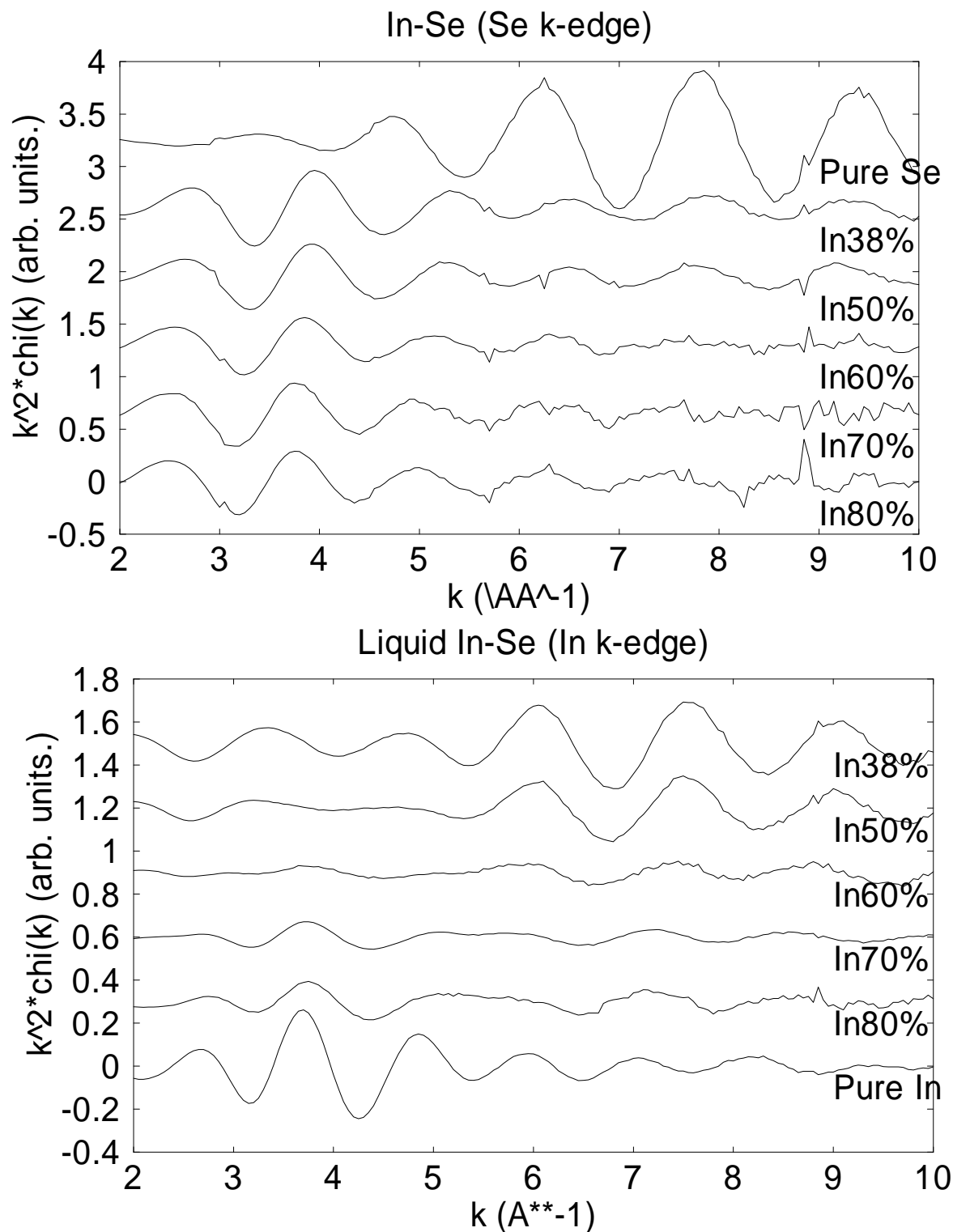


Fig 1. EXAFS signal of liquid In-Se alloys as a function of composition at the Se and In K-edge.

Molecular Dynamics simulations are currently under way for the study of the structure and dynamics of the alloy in conjunction of the present EXAFS data. In any case, it is apparent from the data that the Selenium environment in the liquid alloy is well stabilized for all composition and it does not contain dimers. On the contrary the Indium environment shows a progressive evolution.