ESRF	**Experiment title:** Short range order in liquid Ag_2Se using EXAFS.	**Experiment number:** HS-526
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Report:

The structure of the superionic conductor Ag_2Se in its alpha, beta and liquid phases has been probed. Structural information at the partial level has already been determined using NDIS for the liquid phase [l] and suggestions for the structure of the other two phases are summarized elsewhere [2].

The compound was fabricated by melting the elements together in an evacuated silica ampoule and quenching in water. Optimal effective thicknesses of 18 microns (for the Se K-edge) and 35 microns (for the Ag K-edge) dictated that the powder should be very fine. The powder was prepared by grinding the solid billet using fine (1200 C) SiC paper and the larger particles were rejected using the method of sedimentation followed by filtration. This was then mixed with an inert BN Matrix in the approximate ratio 1:20 and pressed into a small disc shaped pellet.

Temperature scans confirm the presence of the solid alpha-beta phase transition at 406 K as well as exhibiting the expected hysteresis. The solid -liquid phase transition was also clearly visible. A phase transition within the alpha phase at 370 K was also detected at both edges. Evidence of this has been discovered before in measurements of C_p [3].

Transmission EXAFS measurements were taken at both Ag and Se K-edges in the energy

ranges 12.5 keV to 14.3 keV and 25.2 keV to 28.2 keV. The temperature range was 300 K to 1220 K facilitated by an evacuated chamber with an electrically heated graphite crucible. The samples proved to be good with a signal to noise ratio of 10^{-4} or lower.

Figure 1 shows the EXAFS oscillations for the sample for the alpha, beta and liquid phases at the Se K edge. The Se-Se correlation being at significantly higher r than the Ag-Se correlation meant that the structural information gleaned from this edge could be taken to be almost exclusively the Ag-Se correlation. There is a clear distinction between all 3 phases in both amplitude and phase.

This work is still very much in progress as the 'GNXAS' ab initio multiple-scattering software is currently being applied to try to fit the experimental oscillations. Initial results are encouraging with the characteristic asymmetry in the first coordination peak of the Ag-Se correlation function appearing in the Fourier transforms of both the theoretical and experimental EXAFS functions.

References:

[l] A. C. Barnes et. al., J. Phys.: Condens. Matter 9 6159-6173 (1997).

[2] M Kobayashi, Solid State Ion. 39 121 (1990).

[3] Y. Baer et. al., Z. Naturforsch. 17 886-889 (1962).

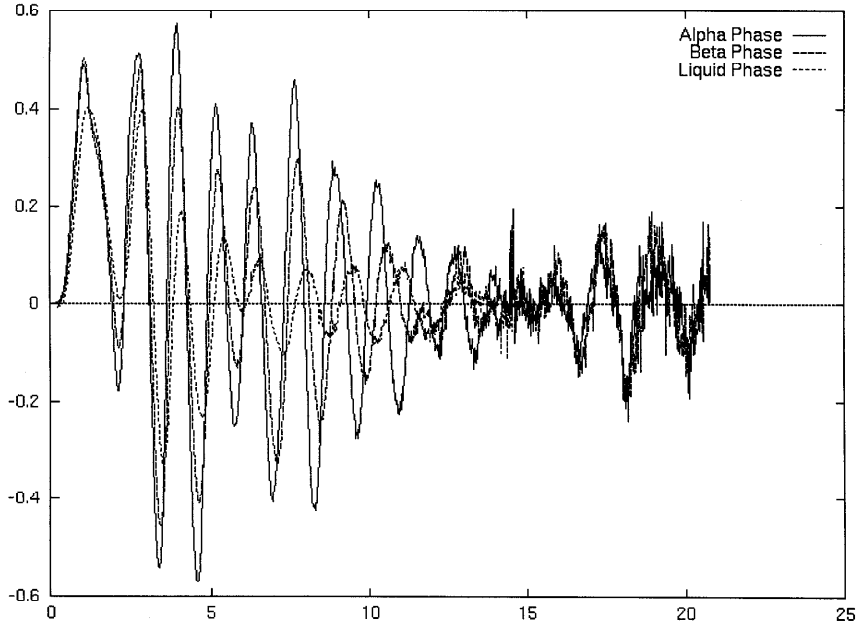

Figure 1