	Experiment title: Partial structure factors of liquid amalgams: existence of chemical orders in liquid metal alloys	**Experiment number**: HS 1115
Beamline: BM02	**Date of experiment**: from: 15 Nov. 2000 to: 20 Nov. 2000	**Date of report**: 14 February 2001
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Report:

Since the pioneering work of Fuoss *et al.* [1], anomalous x-ray scattering using synchrotron radiation has widely been utilized for investigations on local structures of non-crystalline multicomponent systems. However, partial structure factors $S_{ij}(Q)$s of sufficient statistical quality could not yet been obtained with this method, except in those studies where reversed Monte Carlo technique was additionally employed [2] or where combined synchrotron- and neutron experiments were carried out. The determination of $S_{ij}(Q)$s is still the domain of neutron scattering. There, appropriate isotopes are needed which, however, restrict such investigations only to a limited number of elements. Although intense x-rays are nowadays available from third generation synchrotron facilities, this situation has not much changed yet.

In order to obtain $S_{ij}(Q)$s of good statistical quality, there are two requirements which need to be fulfilled: 1) A sufficient energy resolution of the detector to discriminate the elastic scattering signal from the fluorescence or Compton scattering contribution, and 2) a sufficient number of scattered photons in a reasonable acquisition time. For example, provided that 30,000 counts at the Q position of first $S(Q)$ maximum give enough statistical quality, and the element under consideration contributes about 20% to the intensity in $S(Q)$, then 600,000 counts are necessary to obtain the differential structure factors $\Delta_i S(Q)$s of identical statistical quality, because the contrast in the vicinity of the absorption edge is only about 5%. Three times more counts would even be needed to obtain the $S_{ij}(Q)$s. During the reported beamtime, we selected and optimized the detector system at BM02 to satisfy the above conditions using glassy (*g*-) Ge-Se samples. They have similar edge energies to those of liquid Rb-Hg system, which we plan to investigate within this project [3] in the future.

The experiments were carried out at two energies below the K edge of each element using a normal θ–2θ diffractometer. We chose a graphite analyzer crystal with a 40 cm detector arm. Fig. 1 shows rocking curves measured close to the Se K edge at Q = 6 Å^{-1}, where the contributions from the Se K_β fluorescence and from Compton scattering to the elastic signal are very large. The energy resolution of this detector was about 90 eV. As seen in the figure, the Se K_β fluorescence- or Compton contributions can be estimated to be less than 0.3% at those energies where the elastic spectra were measured (arrows in Fig. 1). Ge or InSb crystal analyzer has a much better resolution of less than 10 eV, which enables us to completely remove these contributions. In turn, however, their count rates are very low, which result in acquisition times of much more than two weeks for reasonable statistics.

We measured g-$Ge_{19.5}Se_{80.5}$ and $Ge_{23}Se_{77}$ in steps ΔQ of 0.05 Å^{-1}. For the measurements close to the Ge K edge, about 600,000 counts were acquired for about 4 hours, and near the Se K edge, about 200,000 counts in about 6 hours (due to the strong x-ray absorption). Fig. 2 shows $\Delta_i S(Q)$s for g-$Ge_{19.5}Se_{80.5}$ together with $S(Q)$ measured at 200 eV below the Se K edge. Apparently, the statistical quality of the $\Delta_i S(Q)$s is so high that an interpretation of the underlying structural information can easily be given. For example, since $\Delta_{Ge}S(Q)$ originates from about 75% $S_{GeSe}(Q)$, 15% $S_{GeGe}(Q)$, and 10% $S_{SeSe}(Q)$, while $\Delta_{Se}S(Q)$ about 80% $S_{SeSe}(Q)$, 20% $S_{GeSe}(Q)$, and no $S_{GeGe}(Q)$, it is obvious that the prepeak at 1.1 Å^{-1} is a result of the pure Ge-Ge correlation. A detailed discussion will be given elsewhere [4].

In order to obtain $S_{ij}(Q)$s, however, the quality of $\Delta_{Ge}S(Q)$ seems not to be sufficient due to the small concentration of Ge. An acquisition time at least three time longer would be needed to obtain 2 million counts at the $S(Q)$ maximum as already estimated above. Nonetheless, total duration for one complete experiment (4 energies) would still remain less than two days. We plan to make use of this opportunity in our future experiments on liquid amalgams and also in a new project where g-Ge-Se alloys will be investigated over a wide concentration range.

[1] P. H. Fuoss *et al.*, Phys. Rev. Lett. **46**, 1537 (1981).
[2] Y. Waseda *et al.*, J. Phys.: Condens. Matter **12**, A195 (2000).
[3] S. Hosokawa *et al.*, ESRF Report SC-500.
[4] S. Hosokawa *et al.*, Phys. Rev. B, in preparation.

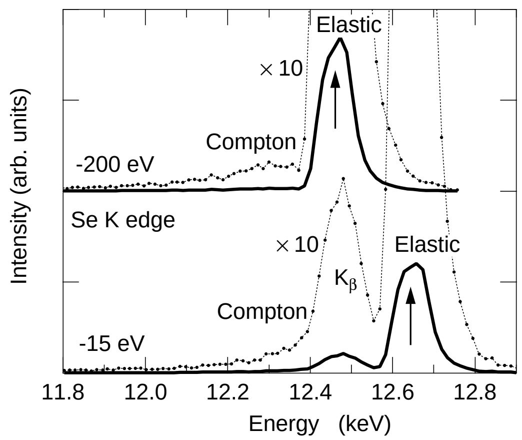

Fig. 1

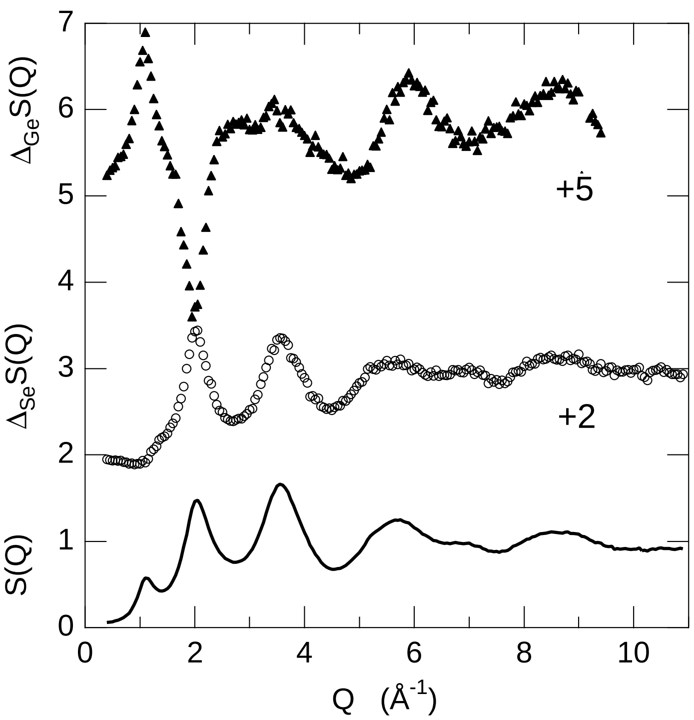

Fig. 2