ESRF	Electronic structure of amorphous silicon	**number:** HE-1370
Beamline: ID16	**Date of experiment:** from: 31/01/2003 to: 03/02/2003	**Date of report:** 26/02/2004
Shifts: 9	**Local contact(s):** G. Vanko	*Received at ESRF:*

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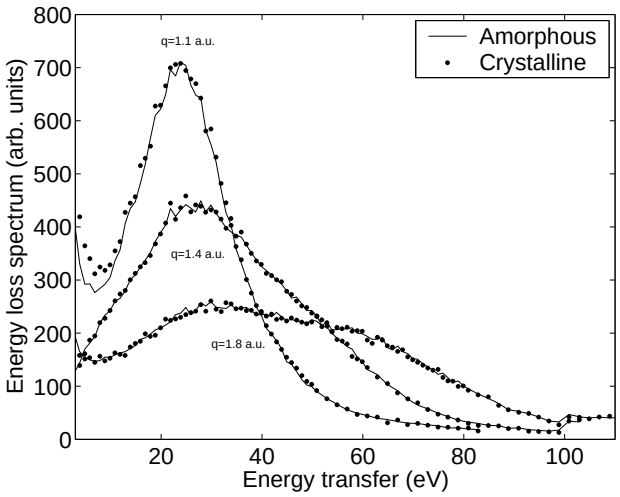
Report:

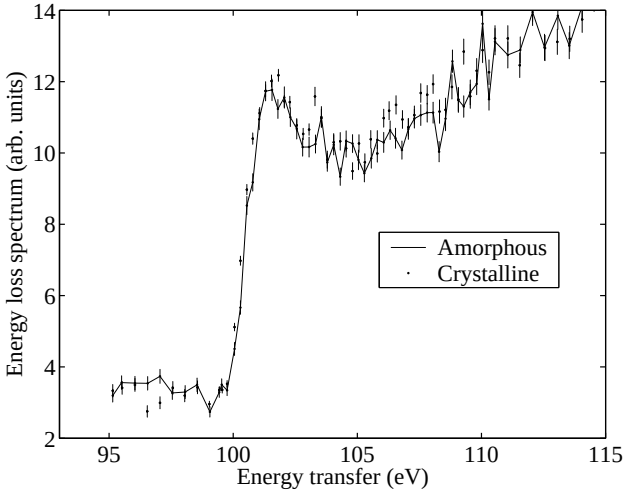
We studied the difference between the electronic structures of polycrystalline and amorphous silicon by utilizing non-resonant inelastic x-ray scattering (NRIXS). The experiment was performed at ID16. The amorphous silicon samples were manufactured in Laboratoire de Physique des Interfaces et des Couches Minces, École Polytechnique, France, and crystalline Si powder was obtained from Alfa Aesar. Our priority plan was to study structures near the Fermi level, i.e. the density of states within the first 1-2 eV of the elastic line, where the largest differences between the samples were to be expected. For this we needed a high energy resolution of about 0.2 eV which we achieved by using the Si(111) premonochromator and Si(220) channel-cut postmonochromator working with photon energies of 8 keV. However, the tangent arm where the channel-cut was mounted, failed to work properly. Thus from the 9 allocated shifts we used 6 to fix the tangent arm but didn't succeed. The arm could not reproduce its movements, and so tuning the incident photon energy, crucial for the experiment, was not successful.

For the last day of the beamtime, we had to change plans and to resort to plain Si(111) premonochromator, producing an energy resolution of about 1 eV. During the last two shifts, we studied electron energy-loss spectrum (dynamic structure factor $S(q,\omega)$) with different momentum transfer values. Schülke et al. [1] have studied the **q**-vector orientation dependence of $S(q,\omega)$ in single-crystalline Si and found that it indeed has orientation dependence arising from band-structure effects.

However, we didn't find any difference between the $S(q,\omega)$ of amorphous and polycrystalline samples in the range of q,ω that we had time to study (Figure 1). This is probably a manifestation of the fact that even small-range order is adequate to create band-structure effects relevant to $S(q,\omega)$ with our experimental accuracy. This result contradicts those obtained by Compton scattering from similar samples [2], where a 10% difference was observed between amorphous and crystalline silicon.

The fact that we were only granted 9 shifts instead of the requested 15 combined with problems with the channel-cut made it rather difficult to us to observe any differences between the amorphous and crystalline samples, given the statistical accuracy of the data gained with 1 eV energy resolution. The only difference we observed was a 0.5 eV shift in the Si $L_{2,3}$ edge energy (Figure 2). To study this effect more closely, better resolution and statistical accuracy are required, and new experiments are being currently planned.





Left: Figure 1. The $S(q,\omega)$ for three momentum transfer values.

Right: Figure 2. The Si $L_{2,3}$ edge of the two sample materials. The edge was observed to be 0.5 eV lower in the crystalline than in the amorphous sample. Data gathering time was about 4 hours.

[1] W. Schülke et al. Phys. Rev. B 52, 11721-11732 (1995)
[2] Ch. Bellin et al. Solid State Comm. 104, 193-197 (1997)