XAFS study on liquid Te and I under high temperature and high pressure

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Crystalline Te and Se have the same crystal structure. They consist of helical chains arranged parallel in a hexagonal array. Each atom is covalently bonded to two atoms within a chain. Crystalline Te and Se are thus semiconductors. On the other hand, their atomic configuration in liquid states is different: the two-fold coordinated chain structure of Se is largely preserved in the liquid state while that of Te is modified upon melting. The metallization of liquid Te proceeds with pressure. We measured XAFS of liquid Te under high-pressure in a previous beamatime (1997B0064-NX-np) and found that the EXAFS oscillation for liquid Te under pressure was very small, which was typical of liquid metal. Recently metallization of l-Se under high-pressure has been reported [1]. It is interesting to study if there is structural change associated with the change in electronic property of liquid Se. In this study, we measured XAFS of Se at pressure 2.5 GPa and at temperatures up to 1073 K.

A large-volume Paris-Edinburgh press was used to generate high-pressure high-temperature conditions. Mixture of Se powder and BN powder was put in a BN capsule, which was surrounded by a gasket made of Boron and Epoxy. The sample was heated using two graphite disk-type heaters inside the gasket. Experiments were carried out at XAFS station on BL01B1. X-ray absorption spectra near Se K-edge (12.7keV) were measured. X-ray beam was monochromatized using Si(111) reflection. The beam was focused vertically by a mirror. The size of the x-ray was reduced to 0.3(H) x 0.2(V) mm^2 by slits in the experimental station. The intensities of the incident and transmitted x-rays were measured by ionization chambers.

Figure 1 shows temperature dependence of radial distribution function, $|F(r)|$, which was obtained by the Fourier transform of the EXAFS function $\chi(k)$ multiplied by k, for crystalline and liquid Se at 2.5 GPa. The main peak corresponds to the covalent bonds. The peak height decreases continuously with increasing temperature due to Debye-Waller factor. The radial distribution function changes little upon melting, indicating that the two-fold chain structure is largely preserved in the liquid. The peak height decreases abruptly above 973K. The decrease is attributable to weakening and/or breaking of covalent bonds. The change occurs at the reported boundary where the electrical resistance decreases.

[1] V. V. Brazhkin, *et al.*, Phys. Lett. A 166 (1992) 383.

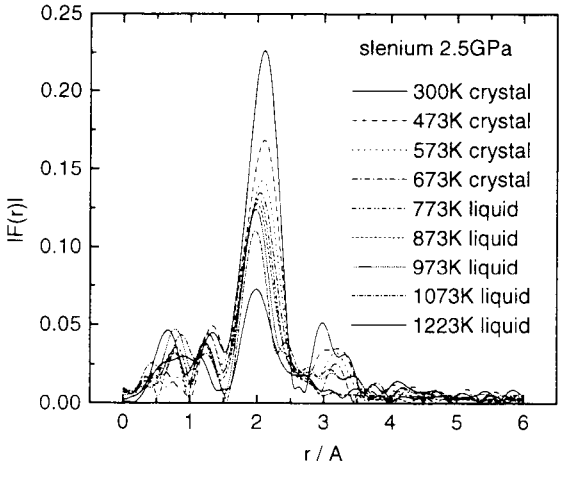

Fig.1 Temperature dependence of radial distribution function |F(r)| for crystalline and liquid Se at 2.5 GPa.