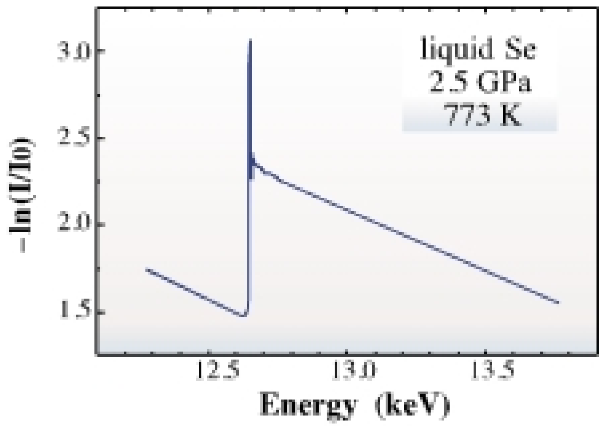

Fig. 1: XAFS spectra for liquid Se measured at pressure of 2.5 GPa and temperature of 773 K.

decrease in the amplitude of the EXAFS oscillation for liquid Se was observed above 1050 K. The decrease was larger than that expected from the normal thermal effect, and it indicates that the two-fold covalent bonds in liquid Se weaken and/or break under high-temperature. The change occurred near the boundary of the reported semiconductor-to-metal transition. This confirms that the transition is accompanied by a structural change.

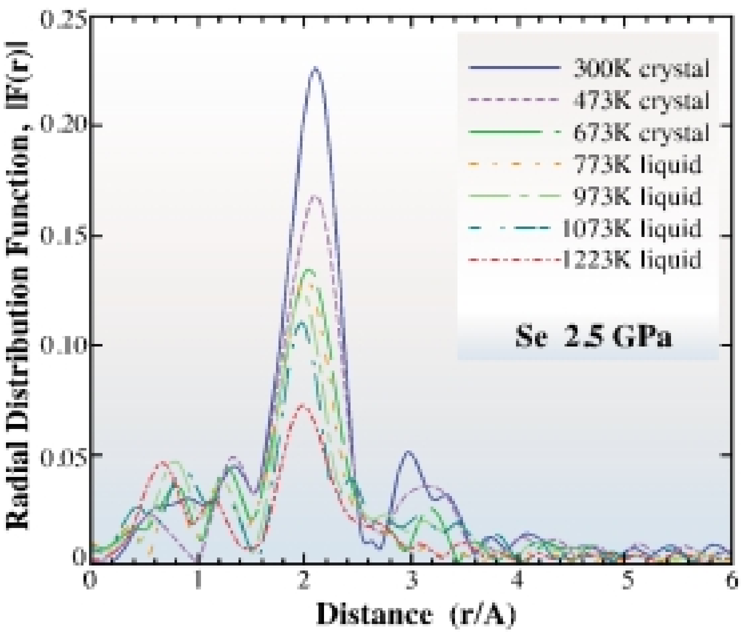

Fig. 2: Temperature dependence of radial distribution function, |F(r)|, obtained from EXAFS spectra, for crystalline and liquid Se at 2.5 GPa.

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References

[1] Y. Katayama et al., to be published in *J. Non-Crystalline Solids.*
[2] V.V. Brazhkin *et al., Phys. Lett. A* **166** (1992) 383.

XAFS SPECTRA IN THE HIGH ENERGY REGION

There is sufficient photon density even at 100 keV from a bending magnet at the SPring-8 storage ring. This enables qualitative XAFS spectra to be observed near K absorption edges for almost all heavy elements. Since an EXAFS signal above an L_{III} absorption edge is followed by an L_{II} absorption edge, the energy range is limited for the analysis. Therefore, EXAFS spectra with K absorption edges are anticipated in order to improve the accuracy of local structure parameters for elements, *e.g.*, lanthanoids. However, it has theoretically been pointed out that the finite lifetime of a core hole smears out EXAFS oscillations, and that this effect becomes more serious for K absorption edges of heavier elements [1,2].

Measurements were carried out at the beamline **BL01B1** in the transmission mode with the Si (511) planes of an adjustable inclined double-crystal monochromator, which is the standard monochromator at SPring-8 and can provide a wide energy range from 4.5 to 110 keV by inclining a pair of crystals. The incident and transmitted X-ray intensities were monitored with flowing Kr gas ionization chambers. It took 5 sec to monitor the X-ray intensities for each data point. The counting of higher-order harmonics was estimated to be less than 1% in comparison with that of the K edge energy, by considering both the photon flux of the source and the efficiency of the detector.

The highly brilliant X-rays of the third generation synchrotron radiation source enable us to measure XAFS spectra with better energy resolution than before. Accordingly, the energy resolution near the Pt K edge was estimated to be 7 eV from the vertical size of the X-ray source (0.1 mm) and the width of the vertical slit at 47 m from the source (0.2 mm). Such an energy resolution allows us to discuss the EXAFS function even at low-k values. Since the width of the rocking curve of the monochromator crystal is sharp, the first crystal holder is equipped with a piezo-actuator to keep the crystals in parallel during a scan.

Figure 1**(a)** shows the X-ray absorption spectrum of Pt at room temperature. The width of the edge jump is as wide as 100 eV and dependent on the width of the initial state of the K level, Γ_K. The blunt edge jump makes it difficult to extract the EXAFS signal at low-k values, while the EXAFS signal is defined well up to 20 Å^{-1}, as shown in the inset.

The near-edge-structure is unusual in the ordinary sense. The energy at which the absorption saturates on average is converted to the wave number k = 6 Å^{-1}; the photoelectron has enough kinetic energy to transit between the central and neighboring atoms. The EXAFS oscillation of the outer shells seems to smear out. In particular, the amplitude of the EXAFS oscillation is reduced significantly at low-k values. It has been shown that local structure parameters such as the interatomic distance and the Debye-Waller factor obtained for the K edge are in good agreement with those obtained for the L_{III} edge.

Figure 1**(b)** shows the XAFS spectrum of the same sample at 12 K. The amplitude of the EXAFS oscillation increases considerably against the smearing effect due to the finite lifetime of the core hole, indicating that it is very sensitive to the Debye-Waller factor at high-k values. It has been shown that the K edge XAFS measurement in the high energy region is useful, which so far has been difficult. Very recently, we have succeeded in observing EXAFS oscillations above the Pb K edge (88.0 keV) at low temperatures.

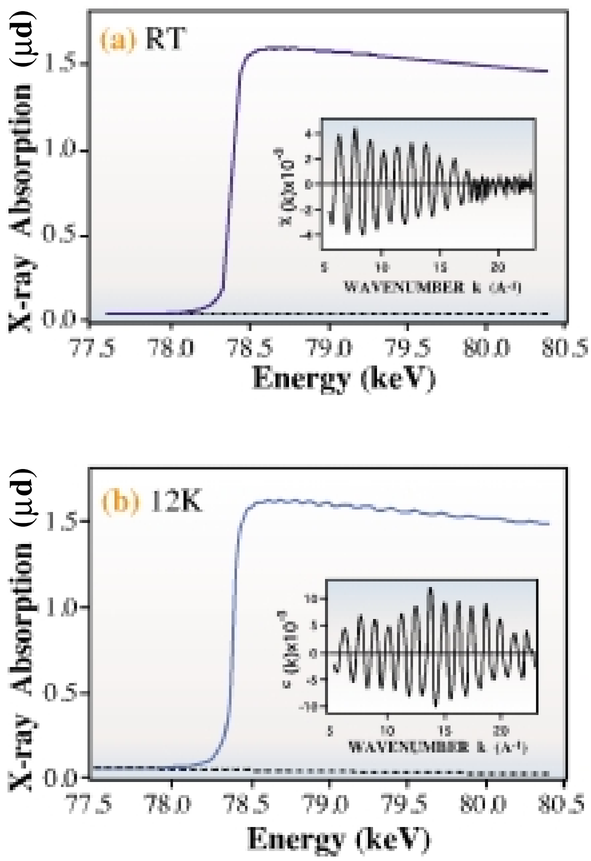

Fig. 1: XAFS spectra at the Pt K-edge for Pt foil ***(a)*** *at room temperature and* ***(b)*** *at 12K.*
Fig.1(a): courtesy of IUCr [2].

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References

[1] D. G. Stearns, *Philos. Mag.* **49** (1984) 541.
[2] Y. Nishihata *et al., J. Synchrotron Rad.* **5** (1998) 1007.