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

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Crystalline Te consists of helical chains arranged parallel in a hexagonal array. Each atom covalently bonded to two neighbors within a chain at distance *r* of 2.835 A. There are four second nearest neighbors in adjacent chains. The second nearest neighbor distance, *R*, is 3.495 A. This distance is considerably closer than 4.40A, twice the van der Waals radius, indicating that there exists covalent-like bonding between the chains. Crystalline Te is a semiconductor at atmospheric pressure. At 4 GPa, crystalline Te transforms to a metallic high-pressure phase in which each atom has four nearest neighbors. Liquid Te at atmospheric pressure is also metallic. In order to study pressure dependence of local atomic arrangements we measured XAFS of crystalline and liquid Te under high pressure and temperature up to 6 GPa and 1000 K.

A large-volume Paris-Edinburgh press was used to generate high-pressure high-temperature conditions. Mixture of Te 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 Te K-edge (31.8keV) 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 filled with Kr gas.

Figure 1 shows x-ray absorption spectra of crystalline and liquid Te under various temperatures and pressures. The EXAFS oscillations were observed in spite of small beam size and high-temperature high-pressure condition. The change of the spectrum between 2 GPa and 6 GPa corresponds to the structural phase transition. The EXAFS oscillation for liquid Te under high pressure is very small, which is typical of liquid metal. In order to get structural information such as bond lengths and coordination numbers, further data analysis is currently under way.

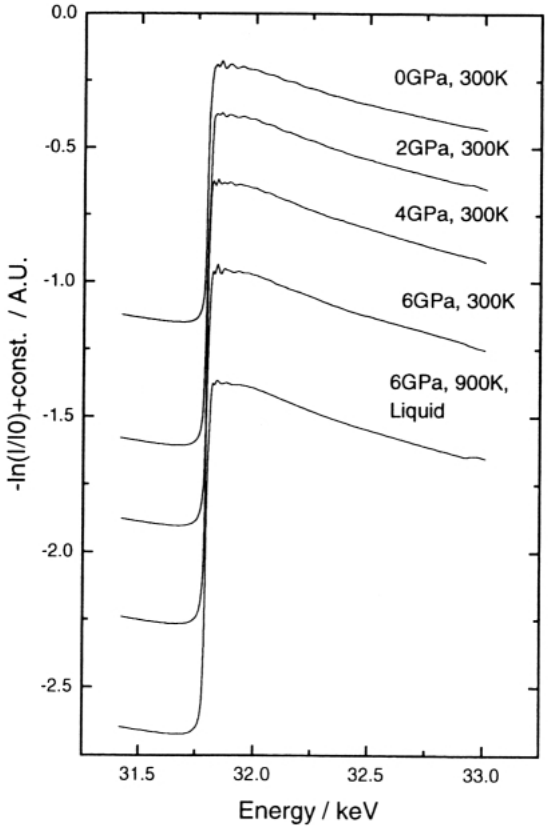

Fig.1 X-ray absorption spectra of crystalline and liquid Te under various temperatures and pressures.