Structure of Liquid Tellurium at High Temperatures

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Crystalline tellurium(c-Te) is a semi-conductor: the lone-pair states form top of the valence band and anti-bonding states form empty conduction band, while liquid Te(l-Te) is metallic. On the other hand, at atmospheric pressure both c- and l-Se are semiconductors. Semiconductor-to-metal transitions have been observed in l-Se at high temperatures and at high pressures. The similarity in the x-ray diffraction patterns and EXAFS spectra between l-Se under pressure and l-Te at atmospheric pressure suggests the similar structures for both liquids.

The electric conductivity of l-Te increases with increasing temperature, shows a maximum around 1000 °C and then decreases. To study the structural change of l-Te at high temperatures we have performed energy-dispersive x-ray diffraction measurements for l-Te on BL04B1. White x-rays ranging energy up to 150 keV from a bending magnet were used. The size of the incident x-ray beam was 0.2×0.2 mm^2. The beam was introduced into a high pressure vessel through a Be window. The specimen of Te was put in a specially designed sapphire cell. The sample thickness was 200 μ m. To prevent the evaporation of the l-Te at high temperatures, the vessel was pressurized to 100 bar. He gas was used as a pressure transmitting medium. The intensity of diffracted x-rays through Be windows was measured with a Ge solid state detector. The size of the receiving slits was 0.4×1.0 mm^2. When the l-Te was pushed into the sapphire cell after the measurements for the blank cell, the measured diffraction counts from the l-Te were too large for the detector. Therefore we used attenuator of stainless steel with thickness of 0.4 mm.

Measurements was done at 14 temperatures from 460°C to 1500°C, where densities of l-Te are from 5.74 to 5.03 g/cm^3. In Fig. 1 examples of the diffraction intensity for l-Te at high temperatures are shown. With increasing temperature, the peaks become broad and the position of the first peak around 2.2 A^{-1} shifts towards higher Q in spite of the thermal expansion. The changes in the peak positions of the second and third peaks are small. These results suggest that the weakening of the interchain interaction due to the increase of the mean atomic distance strengthens the intrachain interaction. Detailed analysis is in progress.

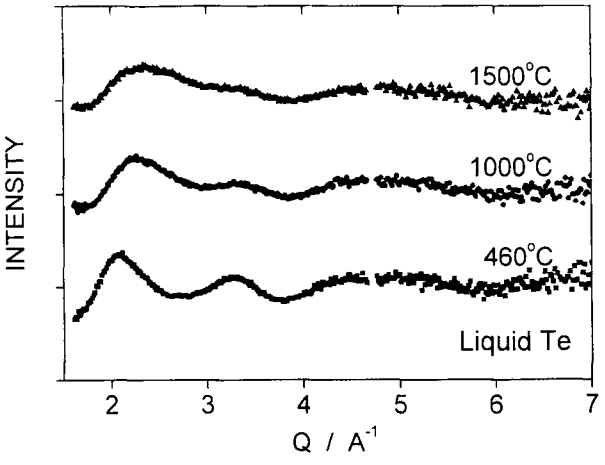

Fig.1 Example of the diffraction pattern for liquid tellurium at high temperatures up to 1500℃ measured at $2\theta=5.1^\circ$