Density of Liquid Se under High Temperature and High Pressure

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Liquid Se is a typical liquid semiconductor at atmospheric pressure. Main constituents of liquid Se are two-fold coordinated chain molecules. X-ray diffraction [1] and EXAFS [2] studies have revealed that the structure of liquid Se changes substantially under high pressure. Recently semiconductor-to-metal transition of liquid Se in the pressure region from 1 GPa to 4 GPa has been reported [2]. The study suggested that the transition had some features of first-order transition. Density is one of the most important values to study structural change. We have developed a new method for density measurements under high-pressure by means of x-ray absorption and measured density of liquid Se.

A large-volume Paris-Edinburgh press was used to generate pressure. A sapphire cylinder, 0.5mm i.d., 1.0 mm o.d. and 0.5 mm thick, was used as a sample container. An NaCl capsule surrounded it. Experiments were carried out at high-pressure station on BL10XU. The energy of the monochromatic x-ray was 36.6 keV. The size of the x-ray was reduced to less than 0.1 x 0.1 mm^2 by slits. The intensity of the incident and transmitted x-rays were measured by two photodiodes. They were measured as a function of sample position.

Figure 1 shows an example of the x-ray absorption profile. The shape of the sample was clearly observed. The density of the sample was obtained by a parameter fit. The solid line indicates the result of the fit. It well reproduced the experimental values. Figure 2 shows the density of Se at 2.5 GPa as a function of temperature. The density decreases with increasing temperature due to thermal expansion. The abrupt change at 800K corresponds to the melting of the sample. An abnormal increase of density with increasing temperature was observed around 1100 K. The temperature coincides with reported boundary for the semiconductor-to-metal transition. The result confirms that the transition is accompanied by a structural change.

[1]K.Tsuji, J.Non-Cryst. Solids, 117/118 (1990) 27. [2]Y. Katayama et al., J.Non-Cryst. Solids, 232-234 (1998) 93. [3]V.V.Brazhkin, et al., Phys. Lett. A166 (1992) 383.

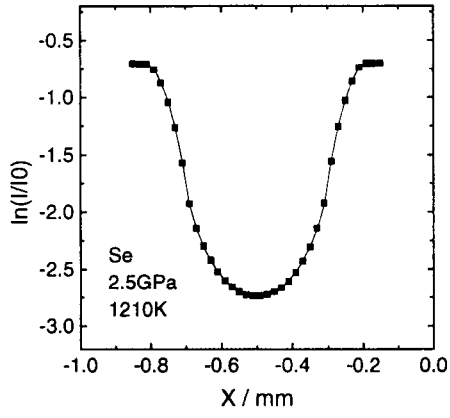

Fig.1 Absorption profile of selenium at 2.5 GPa and 1210 K

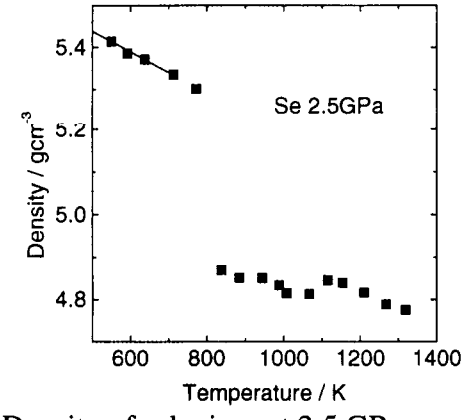

Fig.2 Density of selenium at 2.5 GPa