High-pressure Phase Transition of ZnSe

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1 Introduction

The II-VI and III-V compound semiconductors are well-known for their use in optoelectronic devices. Many of these semiconductors crystallize in the cubic zinc-blende structure. As pressure increases, this cubic phase transforms to a tetragonal metallic phase, which has the β-tin structure. The transition of ZnSe from semiconducting to the metallic phase around 13 GPa has been confirmed repeatedly by previous studies. Although the physical properties of ZnSe at high pressures have been investigated repeatedly, most studies have been performed at ambient temperature. It is known that the semiconducting-metallic transition induces a significant change in the electrical resistivity, which is easy to observe at extreme conditions. Therefore, the semiconducting-metallic transition has been used as a pressure calibration point at high-pressure experiments. Thus, the precise phase boundary of ZnSe needs to be determined in high-pressure science.

2 Experiment

The high-pressure and high-temperature X-ray diffraction experiments were performed using a hydrothermal diamond anvil cell (HDAC) high-pressure apparatus. The temperature was controlled by adjusting the power supply. After reaching the required temperature, we performed *in situ* measurements using the synchrotron X-rays and the temperature was maintained for 10-15 min. The ZnSe reagent (purity = 99.99%) was used as a starting material, which was ground in an agate mortar to grain sizes less than a few μm. The powdered material was loaded into a 80-100 μm diameter hole drilled into a rhenium gasket, which was pre-indented to a thickness of ~40 μm. The sample was sandwiched between pellets of NaCl powder. The sample was probed using angle-dispersive X-ray diffraction, employing the AR-NE1A synchrotron beamline at KEK, Japan. The angle-dispersive X-ray diffraction patterns were obtained on an image plate system (Rigaku R-AXIS, Japan).

3 Results and Discussion

Several experimental runs were carried out at pressures up to 20 GPa. In each run, the sample was compressed to roughly the desired pressure, which was confirmed by the pressure scale of Raman spectra from the diamond. After the desired pressure, the sample was then heated, and the X-ray diffraction data of the sample was acquired to identify the stable phase of ZnSe at high pressure and temperature. As the pressure scale of the Raman spectra from the diamond could not be used during the X-ray diffraction measurements, the sample pressure was estimated by the equation of state for B1-type NaCl. The stable phase could be identified using the X-ray diffraction data. The diffraction peaks of the semiconducting or the metallic phase can be indexed as the cubic or the tetragonal symmetry. After the identification of the stable phase, the temperature was changed to the desired value. The P-T conditions of the acquired X-ray diffraction data and the stable phases identified are shown in Fig. 1. The transition pressure at room temperature was 13.3 GPa [1]. The transition boundary shown in Fig. 1 is represented by the linear equation:
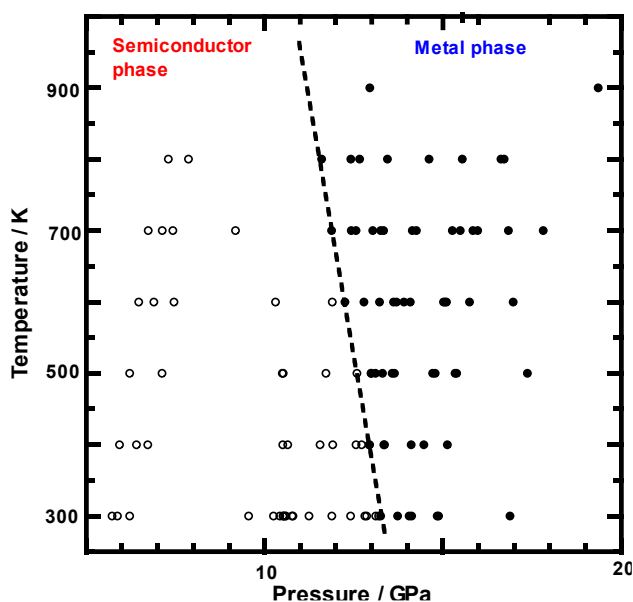
P (GPa) = 14.2(2) - 0.0033(2) x T (K).

Fig. 1: Experimental results and the boundary of the semiconducting-metallic transition in ZnSe. Open and black circles denote the stability conditions of the semiconducting and the metallic phases, respectively. The dashed line is the inferred phase boundary.

References

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