

High-pressure Phase Transition of ZnSe

Shigeaki ONO^{1,*}

¹ Research Institute for Marine Geodynamics, Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Yokosuka 237-0061, Japan

The abstract is optional; if your report is long and an abstract is necessary, please include it here. If an abstract is not necessary, please delete this sentence.

1 Introduction

The semiconducting II-VI and III-V compounds are of great industrial interests due to their wide band gaps. Pressure-induced phase transitions from the semiconductors to the metal states are also of interest in the high-pressure science, since they are used as the fixed-points for the static pressure calibration curves. Zinc chalcogenides, such as zinc selenide (ZnSe) and zinc sulfide (ZnS), have cubic zinc-blende-type structures under ambient conditions. The phase transition from the zinc-blende type (fourfold-coordinated) to the rock-salt type (sixfold-coordinated) phase transition is accompanied by a drastic drop in the electrical resistivity. The behavior of ZnSe under high pressure has been the subject of many experimental and theoretical studies. The phase transition of ZnSe from the zinc-blende structure to the rock-salt structure has been reported as occurring at around 13 GPa. Theoretical studies have confirmed that the phase transition from the zinc-blende to the rock-salt structure occurs at pressures of 10-15 GPa. Since most previous experiments have been performed at room temperature, these observations might be related to the transition kinetics and the differential stress in the sample. Taking into account these factors, our aim in this work is to investigate the phase transition from the zinc-blende to the rock-salt structure at high temperatures, as it is known that the influences of the transition kinetics and the differential stress on the phase transition decrease with an increase in temperature.

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 15–30 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 100-150 μm diameter hole drilled into a rhenium gasket, which was pre-indented to a thickness of ~ 50 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 between 5 and 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 zinc-blende or the rock-salt structure. 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:

$$P \text{ (GPa)} = 14.2(2) - 0.0032(2) \times T \text{ (K)}.$$

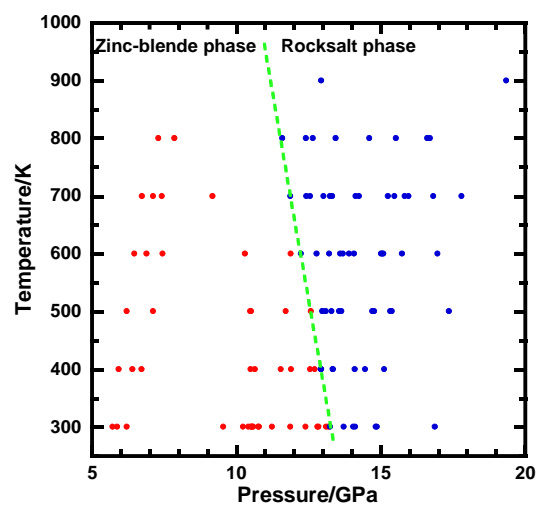


Fig. 1: Experimental results for the transition boundary of ZnSe. Red and blue circles denote the stability conditions for the zinc-blende and rock-salt phases, respectively. The

green dashed line was experimentally determined phase boundary.

Acknowledgement

We thank the PF staffs for their helps in carrying out the experiments.

References

[1] S. Ono, Phase transition in ZnSe at high pressures and high temperatures, *J. Phys. Chem. Solids* **141**, 109409 (2020).

* sono@jamstec.go.jp