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Phase relation in Bismuth under high pressures

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1 Introduction

Bismuth (Bi) is one of the most investigated elements at high pressure because it has a number of pressure-induced transitions which have been widely used as pressure calibration points. Bi-I, which is stable at ambient condition, has rhombohedral structure. Bi-I undergoes three pressure-induced structural phase transitions to Bi-II with distorted simple cubic, Bi-III with host-guest composite structure, and Bi-V with body-centered cubic. At pressures of 3-5 GPa and temperatures higher than 450 K, Bi-IV has been identified. Two of the room-temperature transitions, I-II (2.55 GPa) and III-V (7.7 GPa), have been widely used as pressure calibration points because significant changes in resistance have been observed. In order to determine the phase boundary of III-V tightly, we performed experiments not only at room temperature but also at high temperatures.

2 Experiment

High-pressure experiments were carried out using multi-anvil high-pressure apparatus installed at NE-7A beamline, PF-AR, KEK. Experimental details were described elsewhere [e.g., 1,2]. A mixture of the powdered Bi and NaCl was used. Experimental pressures were determined from the unit cell volumes of NaCl.

3 Results and Discussion

The sample was first compressed at room temperature. After the pressure reached the target value, the temperature of the sample was increased and the X-ray diffraction data from the sample was acquired. The data were acquired at 300-440 K at fixed press loads.

Before heating at ~6 GPa, Bi-III with the bct structure was confirmed. After identifying the stable phase, the temperature was increased to 400 K. A significant change in the diffraction pattern was observed. The intensities of peaks from Bi-III decreased, and new peaks from Bi-V, with the bcc structure, appeared. This change indicated that the phase transition had started, and that this condition corresponded to a stable Bi-V. When the temperature decreased to 370 K, the back-transition from Bi-V to Bi-III was observed. We repeated the experiment with similar heating cycles to determine the phase boundary at high pressures and at high temperatures.

Fig. 1 shows the experimental conditions for the acquired X-ray diffraction data and the stable phase. The transition pressure at room temperature was 7.6 GPa. The dP/dT gradient of the phase boundary was negative [3]. The transition boundary, as shown in Fig. 1, is represented by the linear equation: $P\ (\mathrm{GPa}) = 12.4(2) - 0.016(2) \times T\ (\mathrm{K})$

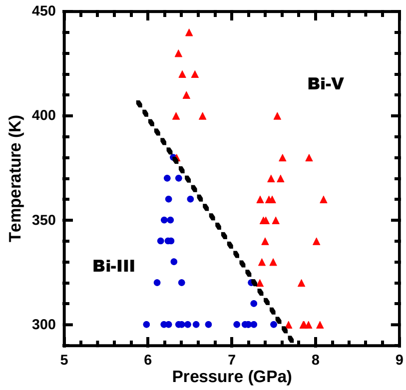

Fig. 1: Experimental results and the phase boundary between of Bi-III and Bi-V. Blue circles and red triangles denote the stability conditions for Bi-III with the host-guest composite structure and Bi-V with the bcc structure, respectively. The dashed line was experimentally determined based on our observations.

Fig. 2 shows the pressure-temperature phase diagram of Bi based on previous studies and our observations.

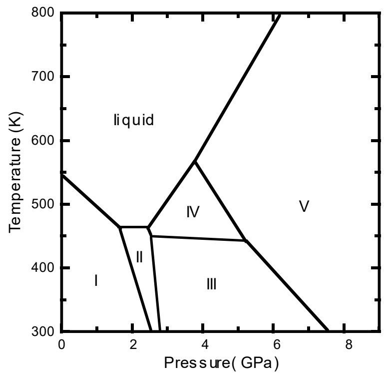

Fig. 2: Phase diagram of Bi.

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References

[1] Ono et al., *Phys. Chem. Minerals*, **40**, 811-816 (2013).
[2] Ono et al., *Phys. Earth Planet. Inter.*, **264**, 1-6 (2017).
[2] Ono, *High Press. Res.*, **38**, 414-421 (2018).

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