

X-ray diffraction study of Bi₂Te₃ under high pressure

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Introduction

Bismuth telluride (Bi₂Te₃) crystallizes with a rhombohedral structure (space group *R*-3*m*, denoted by phase I); the hexagonal unit-cell parameters are $a = 4.395$ Å and $c = 30.44$ Å. As pressure increases, the high-pressure phases of Bi₂Te₃ appear at pressures of 8 and 14 GPa, denoted by phase II and III, respectively [1]. Both phases coexist in the wide pressure range. Additionally, we observed pressure-induced superconducting transition in the high-pressure phases; a transition temperature (T_C) is 2.7 K at 9 GPa [2]. T_C decreases in phase II on compression, whereas it increases in phase III and reaches a value of 5.0 K at 13 GPa. A further increase in T_C is expected in phase III and another high-pressure phase. Here we report x-ray diffraction measurements of Bi₂Te₃ to reveal the crystal structure at higher pressures. This study is published in Physical Review B [3].

Experiments

High-pressure x-ray diffraction studies of Bi₂Te₃ were performed using a diamond anvil cell (DAC) up to 30 GPa at room temperature. A powder sample was placed into a hole 160 μm diameter drilled in the rhenium (Re) gasket of 45 μm thick and loaded into the DAC with 0.3 mm culet anvils. A few ruby chips 5–10 μm diameter were put in the hole together with the sample to determine the pressure by the ruby fluorescence method. The sample chamber was filled with high-density helium gas as the pressure-transmitting medium. The incident beams were monochromatized to the energy of 25.6 keV ($\lambda = 0.04840$ nm) and collimated to 40 μm in diameter. An imaging plate was used as a detector. Each exposure time was set between 120 and 540 min.

Results and Discussion

Figure 1 shows x-ray diffraction patterns of Bi₂Te₃ with increasing pressure at room temperature. All the reflections obtained at 0.61 GPa are explained by space group *R*-3*m* with lattice parameters of $a = 4.366(0)$ Å and $c = 30.11(0)$ Å. The reflections from phase II and III are observed above 8.4 and 14 GPa, respectively, which is consistent with the previous report [1, 3]. After the transition from phase I to phase II and III, we observed small reflections above 14 GPa, which are not assigned to phase II or III reflections. The diffraction pattern becomes simple at 25 GPa; a single phase assigned to a body-

centered cubic (bcc-phase, denoted by phase IV) is obtained as shown in the top of Fig. 1. Except for the bcc-phase peaks, extra reflections are not present. It suggests the structural model of phase IV is analogous to substitutional binary alloys; the Bi and Te atoms with their original concentrations are arranged in the bcc-sites.

Zhu *et al.* recently reported similar results of pressure-induced structural change and the crystal structure of phase IV in Bi₂Te₃ [4].

References

- [1] A. Nakayama *et al.*, High Pressure Res. **29**, 245 (2009).
- [2] M. Einaga *et al.*, J. Phys.: Conf. Ser. **215**, 012036 (2010).
- [3] M. Einaga *et al.*, Phys. Rev. B **83**, 092102 (2011).
- [4] Li Zhu *et al.*, Phys. Rev. Lett. **106**, 145501 (2011).

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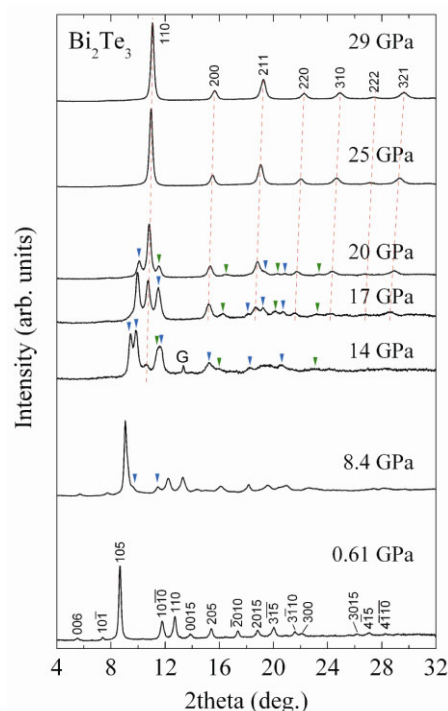


Figure 1 X-ray diffraction patterns with increasing pressure from 0.61 to 29 GPa at room temperature. G indicates a reflection from a Re gasket. Blue and green symbols indicate the reflections from phase II and III, respectively. Red broken lines show the reflections from phase IV and pressure dependence of them.