Structure of Ga_2Se_3 and GaSe under High Pressure

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In the Gallium(Ga)-Selenium(Se) binary system, two kinds of stable forms exist. One is Ga_2Se_3 and the other is GaSe. Ga_2Se_3 has a defect zinc-blende structure, in which one third of the Ga cation sites are vacant. GaSe has a layer structure. In this beam time, pressure induced structural phase transition have been investigated for both Ga_2Se_3 and GaSe at pressure up to 52.0GPa and 63.7GPa, respectively.

Vacancy ordered β–type Ga_2Se_3 and GaSe grown by Bridgman method were used as the samples. The diamond anvil cell technique was used for the high pressure experiments. Pressure was determined by the ruby fluorescence method. The X-ray beam monochromatized to a wave length of 0.4373Å was collimated to 50μm square and was directed to the sample. Angle dispersive powder X-ray diffraction patterns were recorded with imaging plate detector.

1. β-Ga_2Se_3

The structural phase transition is observed at 13.5GPa. This pressure agrees with the phase transition pressure obtained for α-Ga_2Se_3 previously by electrical resistance and thermoelectric power measurements[1]. Fig. 1 shows the X-ray diffraction patterns of β-Ga_2Se_3 at 0.8GPa and at 30.9GPa. A number of small diffraction lines are observed at lower pressure region. These lines originate from the superstructure which consists of three zinc-blende subcells. On the other hand, the diffraction pattern of the high pressure phase is simple. This shows that the high pressure phase of β-Ga_2Se_3 has small unit cell. However the structure has not yet been determined. With further increasing pressure, no phase transition is observed up to 52.0GPa.

2. GaSe

The structural phase transition is observed at 20.3GPa. This pressure agrees with the phase transition pressure obtained previously by electrical resistance measurement[2]. Fig. 2 shows the X-ray diffraction patterns of GaSe at 0.2GPa and at 31.2GPa. The diffraction peak at 31° is due to diamond. Although the concentrations of the alloy in atomic percent are different between Ga_2Se_3 and GaSe at atmospheric pressure, the diffraction pattern of the high pressure phase in GaSe is much similar to that in Ga_2Se_3. With further increasing pressure, no phase transition is observed up to 63.7GPa.

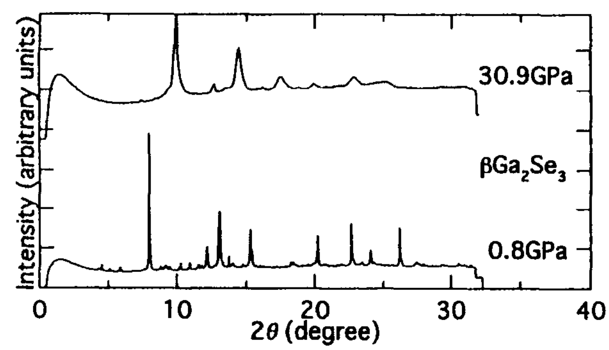

Fig. 1. The X-ray diffraction patterns of β-Ga_2Se_3 at 0.8GPa and at 30.9GPa.

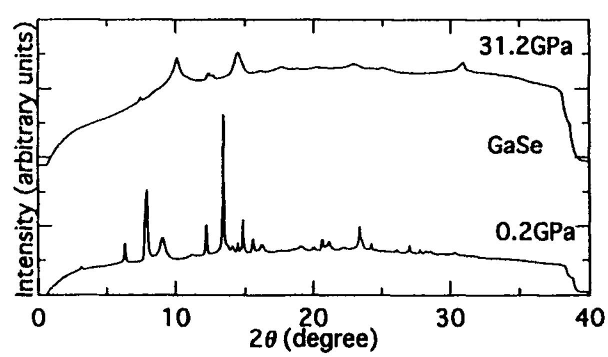

Fig. 2. The X-ray diffraction patterns of GaSe at 0.2GPa and at 31.2GPa.

References

[1] K. V. Savchenko and V. V. Shchennikov, Can. J. Phys. 72 681 (1994).
[2] K. J. Dunn and F. P. Bundy, Appl. Phys. Lett. 36 709 (1980).