High-pressure phase I of sulfur

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Introduction

We reported three high-pressure phases (HPPs) of sulfur in our previous study [1]. Their stable pressure ranges were 3-8GPa, 8-15GPa and higher than 15GPa, respectively. All HPPs were formed at high-temperature condition and were unquenchable at ambient condition. The HPP II was found to have a hexagonal cell containing 18 atoms and to be built up of S_6 molecules. However, the unit cells of the HPPI and HPPIII have not been determined yet.

The aim of the present study is to determine the unit cell of the HPPI under high-pressure condition using synchrotron X-ray source.

Experiment

In-situ X-ray observation of sulfur was carried out by the energy-dispersive type X-ray powder diffraction method with the MAX80 system at PF-AR-NE5C. The details of the *in-situ* observations under high-pressure and high-temperature were described in our report [1].

The compression behavior of the low-pressure phase (LPP) of sulfur was observed under hydrostatic condition at room temperature. For the hydrostatic experiment, powdered sulfur and NaCl as a pressure marker were encased in a teflon capsule with a mixture of methanol and ethanol (4:1). The teflon capsule was put in a pressure medium.

Result and discussion

Figure 1 shows typical X-ray diffraction patterns of the HPPI at 4.17GPa and 27°C with several 2θ angles. An automatic indexing computer code, 'DICVOL' shows a possible hexagonal unit cell (a = 6.976±0.001Å and c = 4.291±0.002Å) from 24 diffraction lines. The unit cell volume of the HPPI is calculated to be 180.86 ± 0.007 Å.

The HPPI is expected to have 9 atoms of sulfur in the unit cell from an assumption; the volume per atom of the HPPI is smaller than that of the LPP and larger than that of the HPPII at 4.17GPa and 27°C, as shown in Fig. 2.

The determined unit cell of the HPPI shows that the crystal structure is related to those of hexagonal selenium and tellurium [2]. The cell parameters of selenium (space group; $P3_121$) are a_{Se} = 4.35517Å, c_{Se} = 4.94945Å and Z_{Se} = 3 at 0.1MPa and 20°C. Selenium atoms form endless zigzag chains along the c-axis in the hexagonal cell. The cell parameters of the HPPI may be described as $a = \sqrt{3} * a_{Se}$, $c = c_{Se}$ and $Z = 3 * Z_{Se}$, by taking a difference of atomic radius and a compression effect. The fact shows that the high-pressure behavior of sulfur is related to those of selenium and tellurium.

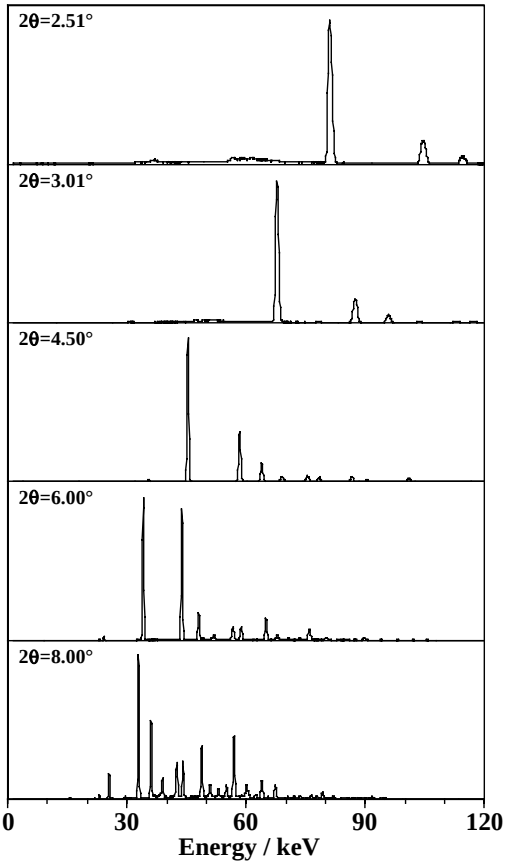

Fig. 1 X-ray diffraction patterns of the HPPI of sulfur with MgO at 4.17 GPa and 27 °C

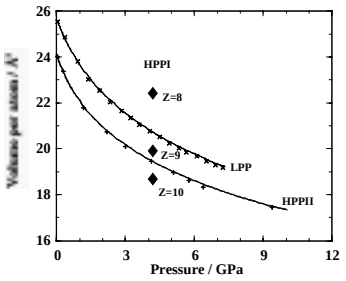

Fig. 2 Compression behaviors of the LPP and HPPII at room temperature. Solid circle marks show calculated atomic volume of the HPPI.

Reference

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