

## Pressure Induced Phase Transition of CdI<sub>2</sub>-type PbI<sub>2</sub>

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### Introduction

CdI<sub>2</sub>-type structure has a hexagonal symmetry with a layer structure. Pressure induced phase transitions of CdI<sub>2</sub>-type dihalides have only been reported for PbI<sub>2</sub>. Figure 1 summarizes the phase relation of PbI<sub>2</sub> under high pressure and temperature so far reported<sup>1-4</sup>. The structures of these high pressure forms have not been revealed yet. In the present study, x-ray in-situ observations were performed in order to investigate the possible pressure-induced phase transitions of PbI<sub>2</sub> and to elucidate their crystal structures.

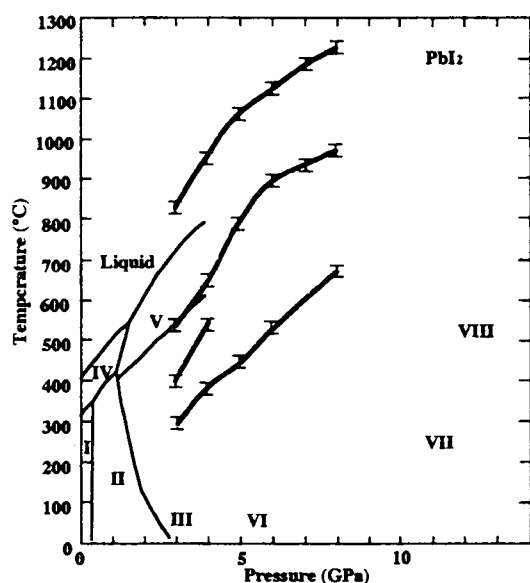


Fig.1

### Experimental

In-situ observation of PbI<sub>2</sub> under high pressure and temperature was performed by using a 1500ton large volume multi anvil type pressure system, which is installed at the BL04B1 in SPring8. Experiments were done with a Cr<sub>2</sub>O<sub>3</sub> doped MgO octahedron of 14mm edge length, WC cubes with 7 truncation edge length, a cylindrical graphite furnace positioned parallel to the x-ray beam, a K-type thermocouple, and a MgO sample capsule. Commercial PbI<sub>2</sub> powder with 95% purity and a mixture of MgO and Au powder for pressure markers were separately encased in a pressure medium. Because both Pb and I ions strongly absorb x-ray, the thickness of the sample chamber vertical to the incident x-ray beam

was reduced to 500  $\mu$ m. X-ray data were collected by an energy dispersive method using a pure Ge SSD.  $2\theta$  was 5 deg. The incident x-ray beam size was 0.1 mm in a vertical direction and 0.2 mm in a horizontal direction.

### Results and Discussion

The x-ray diffraction patterns obtained at several pressure and temperature conditions are shown in Fig.2. Further analysis of the x-ray data is being undertaken.

We suffered considerable pressure leak during heating. Because the cylindrical furnace was inserted parallel to the x-ray beam, the furnace itself was flowed with gasket. Present cell assembly has advantage for collecting x-ray data of good quality, however, it should be modified to prevent the pressure release during heating.

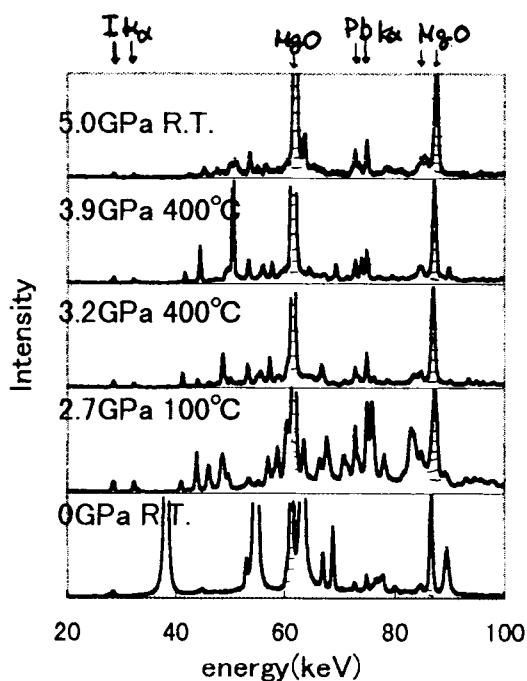


Fig.2

### References

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