

## High-pressure phase transitions of Zn(OH)<sub>2</sub>

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### Introduction

High-pressure and high-temperature behavior of hydroxides is very important to consider an origin and a cycle of water of the earth. There have been some investigations of M(OH)<sub>2</sub>-type hydroxides under high-pressure as a simple model of general hydroxides. Almost M(OH)<sub>2</sub>-type hydroxides except for Zn(OH)<sub>2</sub> and Be(OH)<sub>2</sub> have the Cd(OH)<sub>2</sub>-type structure at ambient condition. Zn(OH)<sub>2</sub> and Be(OH)<sub>2</sub> have a peculiar orthorhombic structure, in which a cation is in a tetrahedral coordination site. The detail of high-pressure and high-temperature behavior of Zn(OH)<sub>2</sub> has not been observed yet, however a high-pressure phase with the Cd(OH)<sub>2</sub>-type structure was reported [1].

The aims of the present study are to search new phase transitions, and to investigate the Cd(OH)<sub>2</sub>-type phase in detail.

### Experiment

The starting material of  $\epsilon$ -phase with the peculiar orthorhombic structure was synthesised by an aqua-solution reaction.

*In-situ* X-ray observation under high-pressure and high-temperature conditions was carried out by the energy-dispersive type X-ray powder diffraction method with the MAX80 system at AR-NE5C and the MAXIII system at BL-14C2. The details of the *in-situ* observation method were described in our report [2].

### Result and discussion

Figure 1 shows typical X-ray diffraction patterns of Zn(OH)<sub>2</sub>. In the present study, we observe three phases except for the orthorhombic phase (Fig. 1-a), in the pressure and temperature range up to 15GPa and 400°C.

A new phase (High Pressure Phase I; HPPI) is observed in the pressure range higher than 2GPa. The X-ray diffraction pattern of the HPPI at 14.5GPa and 27°C is too broadening to be indexed (Fig. 1-b).

In the elevating-temperature process at about 14GPa, the X-ray diffraction pattern is drastically changed at 200°C. Figure 1-c) shows the X-ray diffraction pattern for the single phase of the HPP-II. The crystal system has not been determined yet.

The HPP-II furthermore transforms to the HPP-III in the elevating-temperature process (Fig. 1-d). The X-ray diffraction pattern of the HPP-III can be explained as the Cd(OH)<sub>2</sub>-type structure. The hexagonal cell parameters of the HPP-III at 14.2GPa and 400°C are determined to be  $a=3.075(1)\text{\AA}$  and  $c=4.318(3)\text{\AA}$ .

The HPP-III is quenchable at ambient condition. An anisotropic behavior of the HPP-III is observed in the decompression process at room temperature; the  $c$ -direction is more compressive than the  $a$ -direction. It can be explained by a large compressibility of a van der Waals bond between layers in the Cd(OH)<sub>2</sub>-type structure.

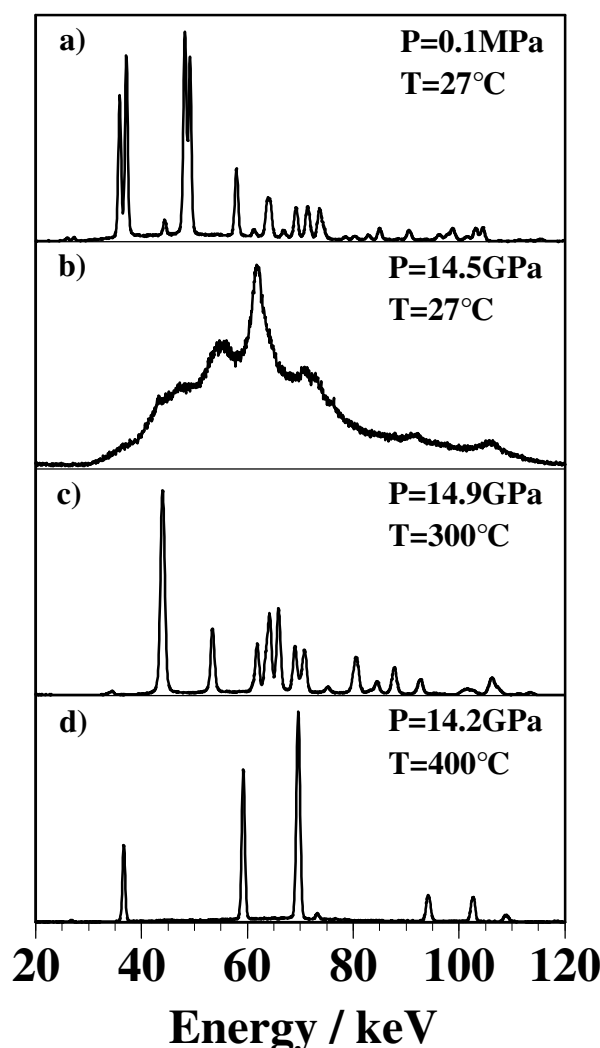


Fig. 1 X-ray diffraction patterns of Zn(OH)<sub>2</sub> taken  $2\theta=4.51^\circ$ . a) the  $\epsilon$ -phase with orthorhombic structure, b) the HPPI, c) the HPP-II and d) the HPP-III with the Cd(OH)<sub>2</sub>-type structure.

### References

- [1] Baneyeva *et al.*, *Geochem. Int.* 6, 807 (1969).
- [2] Kusaba *et al.*, *J. Phys. Chem. Solids* 63, 651 (2002).

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