

Reversible phase transition of Zn(OH)₂ under hydrostatic condition

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Introduction

There have been some investigations of M(OH)₂-type hydroxides under high-pressure condition as a simple model of general hydroxides from the viewpoint of earth science and crystal chemistry. Almost M(OH)₂-type hydroxides except for Zn(OH)₂ and Be(OH)₂ have the Cd(OH)₂-type structure at ambient condition, in which cations are in a octahedral site. Zn(OH)₂ and Be(OH)₂ have a peculiar orthorhombic structure, in which the cation is in a tetrahedral coordination site. The detail of high-pressure behavior of Zn(OH)₂ has not been observed yet, however a high-pressure phase with the Cd(OH)₂-type structure was reported [1-2].

The aims of the present study are to search new phase transitions of Zn(OH)₂ under hydrostatic condition and to consider the high-pressure behavior based on crystal chemistry.

Experiment

The starting material of the ε-phase with the peculiar orthorhombic structure was synthesised by an aqua-solution reaction from ZnO [2-3].

Powdered specimen and NaCl as a pressure marker were separately sealed in a teflon capsule with a 4:1 methanol/ethanol mixture. The capsule was encased in a solid state pressure medium. *In-situ* X-ray observation under hydrostatic condition was carried out by the energy-dispersive type X-ray powder diffraction method with the MAX80 system at AR-NE5C. The details of the *in-situ* observation method under hydrostatic condition were described in our report [3].

Result and discussion

Figure 1 shows typical X-ray diffraction patterns of Zn(OH)₂. We observed two High Pressure Phases (HPPs) in the present study.

In the pressure increasing process, the ε-phase (Fig. 1-a) was stable up to 1GPa. A drastic change of X-ray powder diffraction was observed at 1GPa (Fig. 1-b). This X-ray powder pattern of HPP1 could be indexed on a tetragonal cell. It was worth while to notice that the diffraction lines of the HPP1 was very sharp. The phase transition was reversible with a hysteresis as large as 0.4GPa and the HPP1 completely reverted to the ε-phase at ambient condition. The present result shows that the phase transition is a typical first order transition. It also suggests that the transition may occur by a displacive type mechanism.

Another pressure-induced transition was observed at 2GPa (Fig. 1-c). The volume fraction of the HPP2

continuously increased with pressure increasing. The phase transition was irreversible and the HPP2 was quenchable at ambient condition (Fig. 1-d).

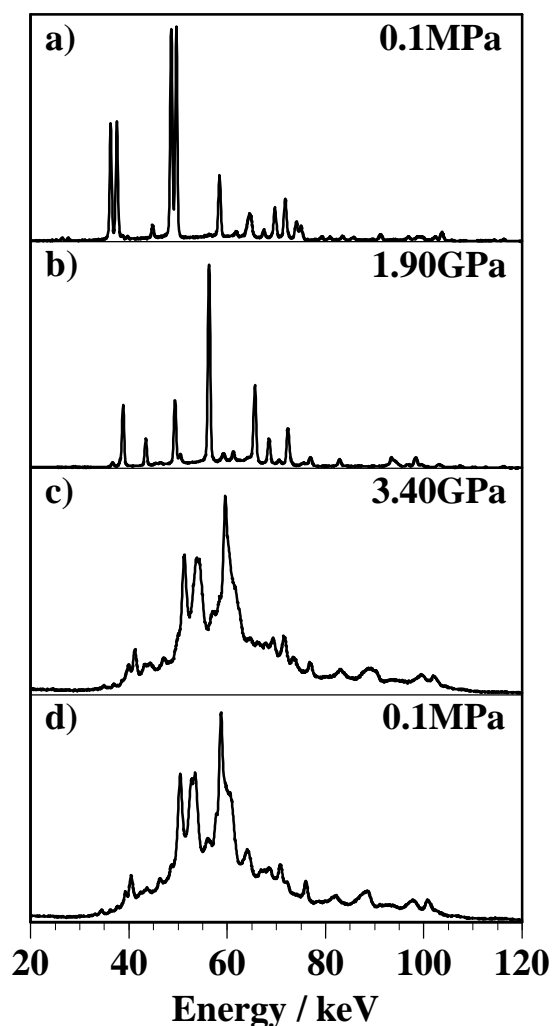


Fig. 1 X-ray diffraction patterns of Zn(OH)₂ taken $2\theta=4.50^\circ$. a) the ε-phase with the orthorhombic structure, b) the HPP 1 with a tetragonal cell, c) the HPP2 and d) the HPP2 quenched to ambient condition.

References

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