

## Pressure-induced phase transition of $\text{Zn}(\text{OH})_2$ with a large volume change

Keiji KUSABA<sup>1</sup>, Takehiko YAGI<sup>2</sup>, Jun-ichi YAMAURA<sup>2</sup>,  
Nobuyoshi MIYAJIMA<sup>2</sup>, Takumi KIKEGAWA<sup>3</sup>

<sup>1</sup>IMR, Tohoku Univ., Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan

<sup>2</sup>ISSP, University of Tokyo, Kashiwa 277-8581, Japan

<sup>3</sup>KEK-PF, Tsukuba 305-0801, Japan

### Introduction

We have found two pressure-induced phase transition of  $\text{Zn}(\text{OH})_2$  at room temperature under hydrostatic condition [1]. The first transition was reversible and the second transition was irreversible. We investigated amply the first reversible transition using both powdered and single crystalline specimens [2]. In the present report, we focused on the experimental result using the powdered specimen.

### Experiment

Starting material with an orthorhombic structure was synthesised by an aqua-solution reaction [1, 2].

High-pressure behavior of  $\text{Zn}(\text{OH})_2$  under hydrostatic condition were observed by energy-dispersive type X-ray powder diffraction method using the MAX80 system at AR-NE5C. The detail of the *in-situ* observation method was described in our article [2].

### Result and discussion

The low-pressure phase (LPP) with the orthorhombic cell suddenly transformed to a high-pressure phase (HPP) at 1.1GPa in a compression process, as shown in Fig. 1.

The X-ray powder diffraction pattern of the HPP could be indexed on a tetragonal cell. Its cell parameters at 1.9GPa were calculated to be  $a = 5.190(2)\text{\AA}$  and  $c = 6.734(3)\text{\AA}$  from 24 observed  $d$ -values by least-square method. The selection rule ( $00l; l = 4n$  and  $h00; h = 2n$ ) demonstrated that a possible space group was  $P4_2,2_1$  (92) or  $P4_3,2_1$  (96). The possible space group and the  $c/a$  ratio (1.297) suggested that the crystal structure of the HPP was similar to that of  $\alpha$ -cristobalite ( $\text{SiO}_2$ ).

In a decompression process, the HPP was stable at around 0.7GPa, where the HPP reverted to the LPP completely. Compression curves of both the LPP and the HPP under hydrostatic condition were shown in Fig. 2. It is clear that the phase transition has about -10% volume change and that the transition is reversible with a hysteresis of about 0.4GPa. These two facts show that the phase transition is a typical first-order transition.

It is worth while to notice that the diffraction lines of the HPP is very sharp. The fact demonstrates that the grain size of the HPP is larger than  $1000\text{\AA}$ ; however the transition occurs at room temperature condition. The phase transition was also observed using a single crystalline specimen in order to examine the transition mechanism. The detail of the result is described in Highlights of this volume.

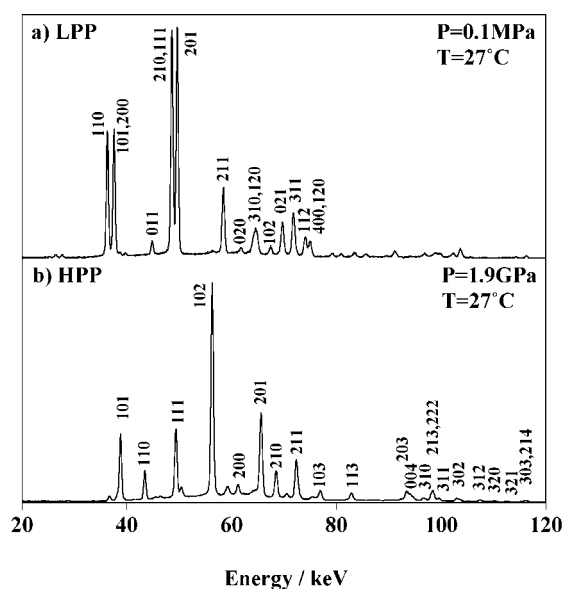


Fig. 1 X-ray powder diffraction patterns of  $\text{Zn}(\text{OH})_2$  [2].

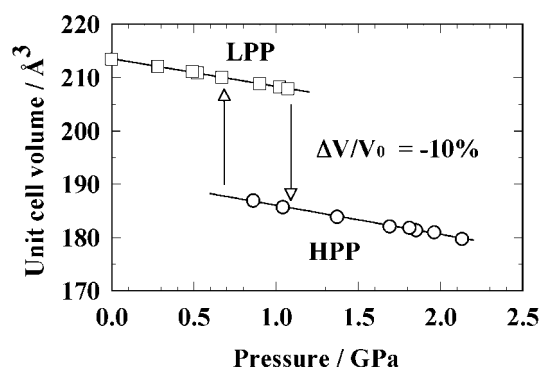


Fig. 2 High-pressure behavior of  $\text{Zn}(\text{OH})_2$  [2].

(Figs. 1 and 2 were redrawn based on original figures in ref. 2 with permission of Elsevier on 16 May 2007.)

### References

- [1] K. Kusaba et al., PF Act. Rep. B21, 200 (2004).
- [2] K. Kusaba et al., Chem. Phys. Lett. 437, 61 (2007).

\* kusaba@imr.tohoku.ac.jp