

The effects of pressure on crystal structure of δ -AlOOH up to 9.0 GPa

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Introduction

δ -AlOOH is a high-pressure polymorph of AlOOH. δ -AlOOH was synthesized by Suzuki et al. (2000) [1] at 1600°C and 21 GPa conditions using a Kawai type multi-anvil apparatus. According to some previous studies [2-3], δ -AlOOH is stable under wide PT conditions such as 18-130 GPa and <2300K, and is recognized as an important phase in the view of the carriers and reservoirs of hydrogen in the Earth's deep interior.

Crystal structure of δ -AlOOH is a distorted rutile type structure with space group $P2_1nm$ and has hydrogen bonding in its structure. It is considered that hydrogen bonding would be influenced on its thermal stability.

The previous powder X-ray diffraction study [4] implied the pressure induced phase transition of δ -AlOOH around 10 GPa, but it is not clear. Also Ab-initio calculations [5-6] suggested that the space group of δ -AlOOH would be changed from $P2_1nm$ to $Pnmm$ by rearrangements of hydrogen under high-pressure conditions. Hydrogen bonding, therefore, is the key to understand the mechanism of the pressure-induced phase transition.

We reported that some results of a high-pressure single crystal X-ray diffraction study on a δ -AlOOH at ambient, 0.6, 1.2, 4.0, 4.2, 6.2, 7.0, 8.7 and 9.0 GPa in order to investigate the effects of pressure on δ -AlOOH.

Experimental Procedure

The sample used for this study was synthesized at 18 GPa and 900-1000°C kept by 1 hour using a Kawai-type multi-anvil apparatus installed in Tohoku University. A single crystal of δ -AlOOH ($50 \times 50 \times 30 \mu\text{m}^3$ in size) was mounted in a modified Merrill-Bassett type diamond anvil cell. He gas was used for the pressure medium and a GIN6 stainless plate used for a gasket. Pressure was determined by the EOS of δ -AlOOH [4]. X-ray diffraction intensities were measured using an automated four-circle X-ray diffractometer installed at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization. The wavelength ($\lambda=0.6513\text{\AA}$) of synchrotron radiation was calibrated by the unit cell volume of the NIST ruby standard crystal at ambient temperature. Unit cell parameters of δ -AlOOH at each pressure point were determined from 15-34 centered reflections in the 2θ range between 11.9° and 34.9° . X-ray reflection intensity data sets were collected up to ($\sin \theta/\lambda < 0.99 \text{\AA}^{-1}$, $2\theta_{\text{max}}=80^\circ$) at 0.6, 4.2, 6.2 and 8.7 GPa. The $h0l$ and $0kl$ series reflections were used for the determination of space group.

Results

The unit cell parameters of δ -AlOOH at each pressure point were summarized in Table 1. No discontinuity was observed up to 9.0 GPa in the volume compression curve of δ -AlOOH (Fig 1). On the other hand, a new additional systematic absence ($k+l=2n+1$, in $0kl$ series) was observed in the X-ray diffraction reflection intensities up to 8.7 GPa. This observation suggested that the pressure induced phase transition of δ -AlOOH was occurred around 8.7 GPa and was a high-ordered transition. The candidate of the space group of the after transition phase was $Pnmm$ or $Pnn2$ based on the extinction rule.

Table 1. The lattice parameters of δ -AlOOH at each pressure point up to 9.0 GPa

P (GPa)	<i>a</i>	<i>b</i>	<i>c</i>	<i>V</i>
0.0001	4.7147(5)	4.2250(4)	2.8318(2)	56.408(9)
0.6	4.709(6)	4.216(1)	2.830(2)	56.18(8)
1.2	4.700(2)	4.211(1)	2.828(1)	55.97(3)
4.0	4.673(1)	4.177(1)	2.816(1)	54.96(3)
4.2	4.671(2)	4.175(1)	2.816(1)	54.91(3)
6.2	4.654(2)	4.153(1)	2.808(1)	54.27(3)
7.0	4.647(2)	4.145(1)	2.805(1)	54.03(3)
8.7	4.637(2)	4.129(1)	2.799(1)	53.60(4)
9.0	4.632(2)	4.129(1)	2.797(1)	53.49(3)

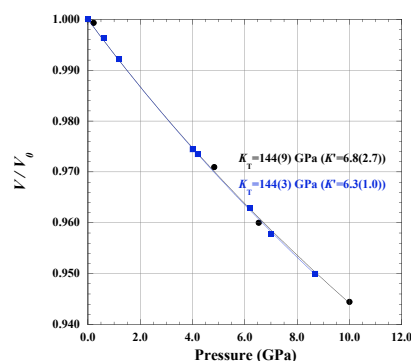


Figure 1. The compression curve of δ -AlOOH up to 9 GPa.

References

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