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The effects of pressure on the δ-AlOOH and post-transition phase up to 14 GPa

Takahiro KURIBAYASHI[1*], Asami Sano-Furukawa[2] , Toshiro Nagase[3]
[1]Department of Earth Science, Graduate School of Science, Tohoku Univ., Sendai 980-8578, Japan
[2]JAEA, Tokai, Ibaraki 305-, Japan
[3]The Tohoku University Museum, Tohoku Univ., Sendai 980-8578, Japan

Introduction

δ-AlOOH is a high-pressure polymorph of AlOOH. δ-AlOOH was first synthesized by Suzuki et al. (2000) [1] at 1600°C and 21 GPa conditions using a Kawai type multi-anvil apparatus. Crystal structure of δ-AlOOH is a distorted rutile type structure with space group $P2_1nm$ and has hydrogen bonding in its structure. Previous reseachers were reported that δ-AlOOH is stable under wide PT conditions such as 18-130 GPa and < 2300 K [2, 3]. The phase is recognized as an important phase in the view of the carriers and reservoirs of hydrogen in the Earth′s deep interior. However, 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 $Pnnm$ by re-arrangements of hydrogen, yielding symmetric hydrogen bonding under high-pressure conditions. Recently, the phase transition of δ-AlOOH around 8.2 GPa has been confirmed by our experiments [7]. They also suggested that hydrogen bond in the post-phase should not be symmetrized but be located disorderly at the crystallographic equivalent sites near inversion center.

In this report, we showed that some results of a high-pressure single-crystal X-ray diffraction measurements on δ-AlOOH and post-transition phase up to 14 GPa in order to investigate the pressure effects on each axial length of δ-AlOOH and the post-transition phase.

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 (30 μm × 30μm ×20 μm in size) was mounted in a modified Merrille-Bassett type diamond anvil cell. A fluid mixture of 4:1 Methanol and Ethanol was used for the pressure medium and a SUS301 stainless plate was used for a gasket. Pressure was determined by using the EOS of δ-AlOOH [4]. X-ray diffraction experiments were performed using the automated four-circle X-ray diffractometer installed at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization. The wavelength (λ=0.6513 Å and 0.8010 Å) 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° and were determined up to around 14 GPa.

Results and Discussion

The pressure evolution of the a/b and b/c ratios of δ-AlOOH at each pressure point were shown in Fig 1. The b-axis is stacking direction of oxygen layer. As the results from the analysis of X-ray diffraction intensity dataset, δ-AlOOH with space group $P2_1nm$ changed to the post-phase with space group $Pnnm$ around 8.2 GPa. No discontinuity was observed in the volume change around 8.2 GPa. These plots suggested that the compression mechanism was changed after transition.

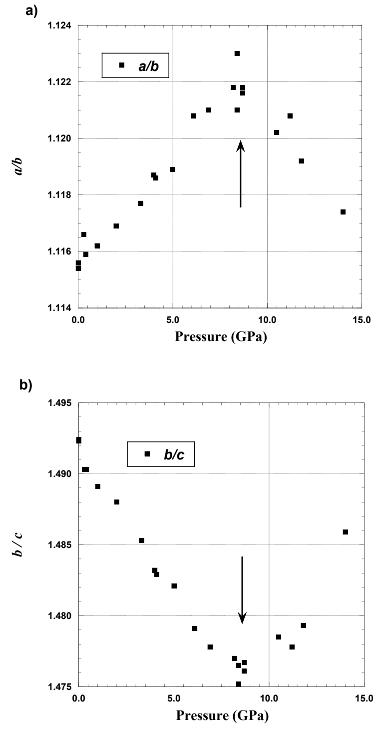

Figure 1. Pressure evolutions of the axial ratios of δ-AlOOH and the post-transition phase, a) a/b and b) b/c.

References

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* t-kuri@m.tohoku.ac.jp