AR-NE5C/2018G023

P-V-T equation of state of β-CrOOH

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1 Introduction

Distorted rutile-type MOOH is characterized by O-H···O hydrogen bonds in *a*–*b* plane and an edge-sharing MO_6 octahedral chain along the *c*-axis (Fig. 1). In δ-AlOOH, with distorted rutile-type structure, pressure-induced hydrogen bond symmetrization occurs due to the shortening of the O-H···O bond [1].

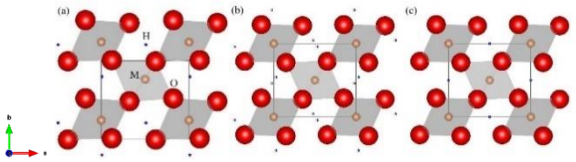

Fig. 1: Structures of distorted rutile-type MOOH. (a) H-asymmetric model ($P2_1nm$), (b) H-disorder model (*Pnnm*), (c) H-centered model (*Pnnm*).

Anisotropic stiffening behaviors, i.e., changes in compression behaviors related to hydrogen bond symmetrization, have been observed [1,2,3]. The stiffening behaviors result in an increase in the bulk modulus and a decrease in *a*- or *b*-axis compressibility because of the formation of strong hydrogen bonds in the *a*–*b* plane. Elastic parameters of β-CrOOH were determined by using X-ray diffraction in DAC [3]. However, *P-V-T* relationship of β-CrOOH has not yet been revealed.

2 Experiment

In situ X-ray diffraction experiments were performed at the beamline AR-NE5C of the Photon Factory, KEK. A cubic-type multi-anvil apparatus, MAX80, was used in the experiments. An MA 6-6 type cell assembly [4], which has six second-stage WC anvils, was used. The energy-dispersive method was adopted, and the diffracted X-rays were collected using a Ge-SSD set at 2θ = 6°. The X-ray diffraction experiments were conducted at pressures of up to 6.2 GPa and temperatures of up to 700 K.

3 Results and Discussion

P-V-T data were fitted to the second-order Birch-Murnaghan equation of state (Fig. 2). Thermoelastic parameters of β-CrOOH were determined as follows: bulk modulus K_{T0} = 191(4) GPa, temperature derivative $(\partial K/\partial T)_P$ = −0.04(2) GPa K^{-1}, and volumetric thermal expansion coefficient $\alpha = 3.3(2) \times 10^{-5}$ K^{-1}. The thermoelastic parameters have similar values to those of ε-FeOOH [5] and RhOOH [6].

Fig. 3 indicates that the pressure of the changes in the compression behaviors tends to increase as the temperature increases. At the higher temperature, the O-H···O distance may be the longer because of thermal expansion. Thus, this result implies that hydrogen bond symmetrization of distorted rutile-type MOOH can be dominated by the O-H···O distance. In the Earth's interior, hydrogen bond symmetrization could occur at above the pressure estimated under ambient temperature conditions. However, we do not know whether such temperature effects are universal with regard to distorted rutile-type MOOH. Further studies on distorted rutile-type MOOH at high pressures and high temperatures are required.

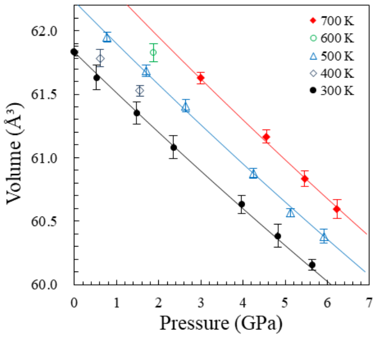

Fig. 2: *P-V* plot with isothermal compression curves.

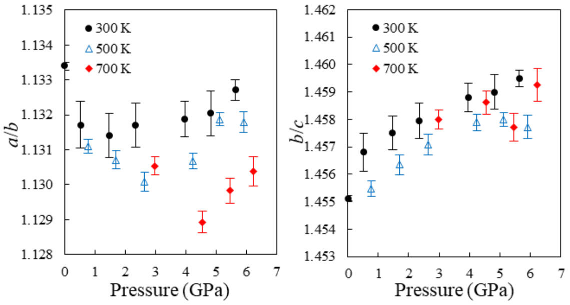

Fig. 3: Pressure evolution of axial ratio of β-CrOOH.

References

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