BL-10A/2013G127

Structural properties of (Al, H)-bearing bridgmanite, $MgSi_{0.9}Al_{0.1}H_{0.1}O_3$

T. Kuribayashi[1,*], T. Inoue[2], K. Fujino[2] and T. Nagase[3]
[1]Department of Earth Science, Graduate School of Science, Tohoku University, Sendai 980-8578
[2]GRC, Ehime University, Matsuyama 790-8577
[3]The Tohoku University Museum, Tohoku University, Sendai 980-8578

1. Introduction

Perovskite structured $MgSiO_3$ was recently approved by IMA-CNMNC as bridgmanite [1], although the phase has been confirmed in a Tenham meteorite in 1997 [2]. Bridgmanite is regarded as one of main component minerals in earth's lower mantle, and would control its various physical properties such as elasticity and electromagnetism

Crystal structure of Mg-Pv belongs to the orthorhombic system with space group of *Pbnm* (#62), and deviates from the ideal cubic perovskite structure. The Mg-Pv structure can include various minor components such as Ca, Fe, Al, H and so on. Mg-Pv including a larger amount of Al and H was synthesized at the conditions of 25-26 GPa and ~1600ºC, and its incorporation mechanism ($Si^{4+} \Leftrightarrow Al^{3+} + H^{+}$) is suggested [3]. However, structural detail on (Al, H)-bearing Mg-Pv is unknown, and is needed to investigate the behaviors of Al and H in Mg-Pv structure.

Single-crystal X-ray diffraction measurements on (Al, H)-bearing Mg-Pv was conducted to obtain its structural information. In this report, we showed the brief results of structural refinement, and compared the polyhedral properties of our sample with the previously reported values of the perovskite structure with various chemical formula.

2. Experimental Procedure

Although experimental details were already shown in our last year report [4], we showed them again. The sample used for this study was synthesized by [3] at 25-26 GPa and ~1600ºC. The run product included (Al, H)-bearing $MgSiO_3$ phase, phase D, stishovite and quenched dendritic phase, which was liquid under high pressure and temperature conditions. The chemical formula, $Mg_{0.976}Si_{0.925}Al_{0.094}H_{0.089}O_3$, of (Al, H)-bearing Mg-Pv was verified by [3] with EDS-SEM and SIMS. After checking the quality of crystals by taking oscillation photographs, a single crystal of Al, H-bearing Mg-Pv (56 μm × 48 μm × 40 μm in size) was selected for synchrotron X-ray diffraction experiments. Single crystal 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 = 0.7129 Å) of synchrotron radiation was calibrated by the unit cell volume of the NIST ruby standard crystal at ambient temperature. The unit cell parameters of Al, H-bearing MgPv at room temperature were determined from 52 centered reflections in the 2θ range between 11° and 35°. The X-ray diffraction intensity data were collected up to $\sin\theta/\lambda < 0.71$ ($2\theta_{max}$ = 60º) by using ω-scan method. Structural refinement was conducted by using SHELXL with WIN_GX software [5, 6]. The latest R and wR2 values are 3.8 % and 10.4 %, respectively.

3. Results and Discussion

The obtained lattice parameters of (Al, H)-bearing Mg-Pv are as follows: a = 4.7890(18) Å, b = 4.954(2) Å and c = 6.924(6) Å. Table 1 shows several information of BO_6 octahedron in Mg-Pv with various minor components.

The averaged B-O distances is 1.8010(17) Å, while that of A-O is 2.210(2) Å for 8-coordinates in (Al, H)-bearing Mg-Pv. The mean distance of BO_6 octahedron is expanded 0.4% comparing with those of pure Mg-Pv[7]. It suggested that the B site should be occupied by Al and Si. Also, the distance of 1.8010Å is the same as that of [8]. In the reference [8], the B-site is occupied by 92%Si and 8% Al. This result is in good agreement with our structure refinement and chemical analysis. The octahedral site is a key to understand its incorporation mechanism.

Table 1.Information on lattice constant and BO_6 octahedron of our (Al, H)-bearing Mg-Pv and the reference data

	This study (sample #1)	Horiuchi et al. (1987)	Dobson & Jacobsen (2004)	Vanpeteghem et al. (2006)
Composition	$Mg_{0.98}Si_{0.92}Al_{0.09}H_{0.09}O_3$	$MgSiO_3$	$MgSiO_3$	$Mg_{0.88}Si_{0.92}Al_{0.11}Fe_{0.09}O_3$
Unit Cell Parameters				
a	4.7890 (18)	4.7754 (3)*	4.7780 (2)	4.7820 (1)
b	4.954 (2)	4.9292 (4)*	4.9298 (3)	4.9422 (2)
c	6.924 (6)	6.8969 (5)*	6.8990 (3)	6.9207 (3)
V [Å^3]	164.25 (7)	162.35 (2)*	162.50 (1)	163.561 (1)
BO_6 Octahedron				
B-O(2) [2]	1.7922 (18)	1.7827 (7)	1.7952 (8)	1.794 (1)
B-O(2) [2]	1.8023 (17)	1.7960 (7)	1.7998 (4)	1.799 (1)
B-O(1) [2]	1.8086 (15)	1.8005 (3)	1.7829 (8)	1.8126 (7)
Mean [6]	1.8010 (17)	1.7931 (6)	1.7930 (7)	1.802 (1)

*derived from [9]
** lattice constants derived from [4]

4. References

[1] Tschauner et al., *Science*, **346**, 1100-1102 (2014) [2] Tomioka and Fujino, *Science,* **277**, 1084-1086 (1997) [3] Inoue *et al*., *in prep*. (2015). [4] Kuribayashi et al., PFAR, **31**, 299, (2014) .[5] Sheldrick (1997) [6] Farrugia LJ *J. Appl. Crystallogr*., **32**, 837-838 (1999) [7] Horiuchi *et al*., *Am. Mineral*., **72**, 357-360 (1987) [8] Vanpeteghem *et al*., *Phys. Ear. Planet. Interior*., **155**, 96-103 (2006) [9] Ito and Matsui, *Ear. Planet. Sci. Lett*., **38**, 443-450 (1978) [10] Dobson and Jacobsen, *Am. Mineral*., **89**, 807-811 (2004).

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