10A/2001G037

Structural behavior of hydrous ringwoodite at high pressure and its estimated maximum hydrogen content

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Sets of X-ray diffraction intensities up to 7.9 GPa of a single crystal of 35x35x24 micron hydrous ringwoodite $Mg_{1.97}SiH_{0.06}O_4$, synthesized by Ohtani and Mizobata (1998) using a multi-anvil apparatus at conditions of 1680 °C and 22 GPa were measured using synchrotron radiation at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The modified Merrill-Bassett type diamond anvil pressure cell was used. The 4:1 fluid mixture of methanol and ethanol was used for pressure medium. The compressibility of the unit cell is close to the compressibility of the MO_6 octahedron. The mean Si-O distance stay almost constant up to 7.9 GPa (Fig. 1). The compression of the crystal structure is governed by the compression of MO_6 octahedron, being consistent to the fact that the bulk modulus is affected significantly by the substitution of Mg by 2H. The octahedral shared edges are compressed more than the unshared edges, keeping the edge lengths of SiO_4 tetrahedron almost constant. Based on the assumption that the vacant octahedral sites are separated each other with equal distances, the maximum H_2O content was obtained from the configuration with minimum separation distances (Fig. 2). The maximum H_2O contents were thus estimated to be 3.3 wt%.

Table 1. Crystallographic data and final atomic parameters

P (GPa)	0.00	3.2	5.0	6.2	7.9
Lattice parameters					
a (Å)	8.065(1)	8.014(1)	7.996(2)	7.993(2)	7.962(1)
V (Å^3)	524.6(1)	514.6(3)	511.2(3)	510.6(4)	504.8(3)
Wavelength (Å)	0.6998	0.7017	0.6958	0.6961	0.7019
Radiation	Synchrotron	Synchrotron	Synchrotron	Synchrotron	Synchrotron
Maximum 2θ (°)	70.6	85.9	86.2	89.5	88.5
No. of I_o measured	390	928	1071	1067	1077
Independent I_o used	74[a]	64[b]	50[b]	53[b]	55[b]
R (%)	5.3	8.5	5.5	7.4	4.8
Atomic parameters					
M site ($Mg_{0.98}\square_{0.02}$)					
x	1/2	1/2	1/2	1/2	1/2
B(eq)	0.353(1)	0.655(1)	0.727(2)	1.174(2)	0.710(1)
T site ($Si_{1.00}$)					
x	1/8	1/8	1/8	1/8	1/8
B(eq)	0.421(1)	0.559(1)	0.686(1)	0.959(1)	0.586(1)
Oxygen site					
x	0.2431(3)	0.2428(5)	0.2437(7)	0.2441(6)	0.2444(4)
B(eq)	0.650(1)	0.594(1)	0.601(2)	0.793(2)	0.616(1)

[a] $I_o > 1.5\,\sigma I_o$, [b] $I_o > 3.0\,\sigma I_o$

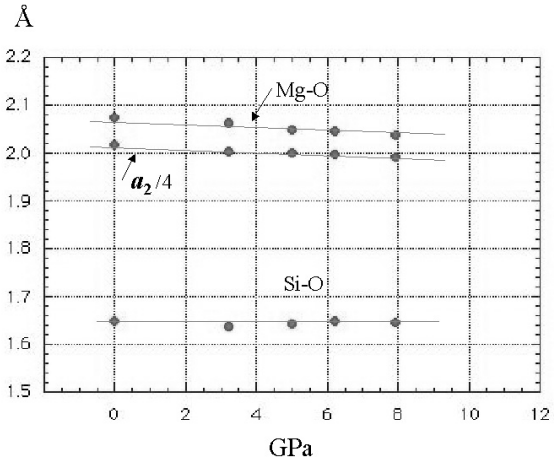
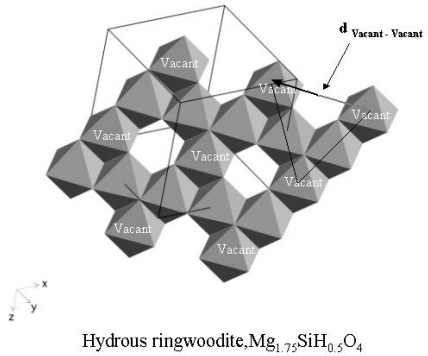


Fig. 1. Mean Mg-O distance, lattice constant and mean Si-O distance versus pressure.



Hydrous ringwoodite, $Mg_{1.75}SiH_{0.5}O_4$

Fig. 2. Minimum separation distance d (= 5.703 Å) of vacant octahedra.

References

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