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Crystal structure of hydrous ringwoodite,γ-$Mg_{1.97}SiH_{0.03}O_4$ at 7.9 GPa

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The specimen used in this study was a single crystal of hydrous ringwoodite synthesized by Ohtani and Mizobata (1998)[1] using a multi-anvil apparatus at conditions of 1680˚C and 22 GPa. Electron microprobe analysis showed a chemical composition of 42.83wt% SiO_2, 56.42 wt% MgO, yielding a total wt% of 99.25 (H_2O excluded) with Mg/Si being 1.97. The H_2O content measured by SIMS was 0.2(0.004) wt %. The unit cell content is calculated to be $Mg_{1.97}SiH_{0.03}O_4$. Sets of X-ray diffraction intensities up to 7.9 GPa were measured with a single crystal of 35x35x24 μm using synchrotron radiation at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The wave lengths were calibrated by the unit cell constants of a ruby standard crystal. The modified Merrill-Bassett type diamond anvil pressure cell [2] was used. The 4:1 fluid mixture of methanol and ethanol was used for pressure medium and SUS301 plate was used for gasket. The pressure was calibrated using the ruby fluorescence method. The crystallographic data and the final atomic parameters at ambient condition and at 7.9 GPa are given in Table 1. The atomic parameters were refined by SHELEX-93. Interatomic distances and angles are given in Table 2. The compression of T-O distance was 0.25 % while the compression of M-O was 1.8 %. The compression of the unit cell axial length was 1.3 %. The compressibility of the unit cell is close to the compressibility of the MO_6 octahedron. This fact indicate that the compression of the crystal structure of hydrous ringwoodite is governed by the compression of MO_6 octahedron.

Table 1 Crystallographic data and final atomic parameters

P(GPa)	0.00	7.9
Lattice parameters		
a(Å)	8.065(1)	7.962(1)
V(Å^3)	524.6(1)	504.8(3)
Wave length (Å)	0.6998	0.7019
Space group	*Fd*3*m*	*Fd*3*m*
Maximum 2θ (˚)	70.6	88.5
No. of |Io| measured	390	1077
No. of unique |Io|	87	125
No. of |Io| used	74(>1.5σ|Io|)	55(>1.5 σ|Io|)
R (%)	5.3	4.8
Atomic parameters		
M site ($Mg_{0.98}$⁄$_{0.02}$)		
x	1/2	1/2
B(eq)	0.353(1)	0.710(1)
T site ($Si_{1.00}$)	1/8	1/8
x	1/8	1/8
B(eq)	0.421(1)	0.586(1)
Oxygen		
x	0.2431(3)	0.2444(4)
B(eq)	0.650(1)	0.616(1)

Table 2. Interatomic distances (Å) and angles (˚)

P(GPa)	0.00	7.9
TO_4 tetrahedron		
T-O	1.650(2)[x4]	1.646(3)[x4]
O-O	2.694(4)[x6]	2.688(7)[x6]
O-T-O	109.5(1)[x6]	109.5(2)[x6]
MO_6 octahedron		
M-O	2.074(2)[x6]	2.036(3)[x6]
O-O(hared edge)	3.009(4)[x6]	2.942(7)[x6]
O-O(unshared)	2.8536(2)[x6]	2.8164(3)[x6]
<O-O>	2.927	2.879
O-M-O	93.04(8)[x6]	92.5(1)[x6]
O-M-O	86.96(8)[x6]	87.5(1)[x6]
<O-M-O>	90.0	90.0

References

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