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Effect of hydrogen on the density and compressibility of hydrous ringwoodite

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With a single crystal of 35x35x24 micron hydrous ringwoodite $Mg_{1.97}SiH_{0.06}O_4$, synthesized at conditions of 1680 °C and 22 GPa, sets of X-ray intensities were measured up to 7.9 GPa with the modified Merrill-Bassett type diamond anvil pressure cell [1], using synchrotron radiation at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The calculated isothermal bulk modulus using the unit cell volumes at ambient pressure, 3.2 GPa, 5.0 GPa, 6.2GPa and 7.9 GPa with the third-order Birch-Murnaghan equation of state assuming K'=4 was K_0=184(6) GPa. The results of structural analyses up to 7.9 GPa indicate that 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. This is considered to be due to the fact that the ratio of (M-O)/(T-O) in the silicate spinel is larger than the ideal value of the closest packing of oxygen atoms. With increasing pressure, the ratio of (M-O)/(T-O) decreases and approaches to the ideal value. The Mg/Si ratio versus H_2O content diagram for hydrous ringwoodite [2][3][4] indicate the existence of Si↔4H substitution in ringwoodite together with Mg↔2H substitution. This is considered to be due to the fact that the substitution of Si↔4H has less effect on the reduction of density than the substitution of 2Mg↔4H because the molecular weight of SiO_2 (=60) is smaller than the molecular weight of 2MgO (=80). The Si↔4H substitution is favorable at high pressure. The partial disorder of Mg-Si found from the crystal structure analysis of hydrous ringwoodite, γ-$Mg_{1.89}Si_{0.98}H_{0.30}O_4$ with 2.0 wt% H_2O [5] may reduce the number of vacancies at the tetrahedral site. The bulk modulus versus number of Mg atoms diagram (Fig. 1) indicates that the bulk modulus of hydrous ringwoodite is inversely proportional to the number of Mg atoms. Incorporation of hydrogen in the ringwoodite structure has more effect on the bulk modulus than on the density (20% decrease of bulk modulus and 4 % decrease of density with 2.8 wt%H_2O [10]).

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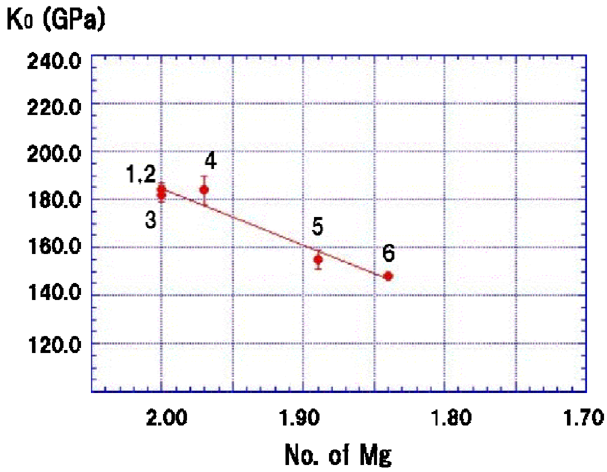

Fig. 1. Bulk modulus (K_0) versus number of Mg atoms for ringwoodite. 1; Weidner et al. (1984)[6]. 2; Hazen (1993)[7]. 3; Meng et al. (1994)[8]. 4; This study. 5; Inoue et al. (1998)[9]. 6; Yusa et al. (2000)[10]

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