Crystallography

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Bulk modulus and linear compressibilities of phase G, $Mg_{1.24}Si_{1.76}H_{2.48}O_6$

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X-ray diffraction data of phase G at high pressures were measured with the modified Merrill-Bassett type diamond anvil cell [1]. The data at 4.1 GPa were measured using synchrotron radiation (λ=0.6992Å) at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The data at 5.7 and 6.8 GPa were measured using MoKα radiation (50kV,40mA).

The single crystal (47x35x12μm) used in this study is phase G, $Mg_{1.24}Si_{1.76}H_{2.48}O_6$ synthesized at 1050˚C and 22 GPa [2] which was previously used for the structure determination at ambient pressure (Kudoh et al., 1997)[3]. The fluid pressure medium was a 4:1 mixture of methanol:ethanol. The pressure was calibrated with the ruby fluorescence method.

Using the unit cell data (Table 1; Fig. 1) and a Birch-Murnaghan equation of state, the isothermal bulk modulus was calculated as K_{0T} =150(4) GPa assuming K'_{0T} =4. The linear compressibilities of the *a* and *c* axes are $1.70(3)\times10^{-3}$ GPa^{-1} and $2.56(7)\times10^{-3}$ GPa^{-1}, respectively. The *c*-axis is more compressible than the *a*-axis. The present bulk modulus value of phase G is 10% smaller than the 166 GPa value of phase D, $Mg_{1.11}Si_{1.89}H_{2.22}O_6$ (=phase G) reported by Frost and Fei (1999)[4]. The results of structural analyses with space group *P*31*m* (No.162) at high pressures (*R*w=6.1% for 47 *F*o at 4.1 GPa,, *R*w=8.0% for 23 *F*o at 5.7 GPa and *R*w=7.0% for 18 *F*o at 6.8 GPa) showed that the (Si,Mg)-O distance at the S-site approaches to the Si-O distance of stishovite at corresponding pressures.

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Table 1. Crystallographic data for phase G

P (GPa)	Ambient*	4.1	5.7	6.8
a (Å)	4.790(3)	4.752(1)	4.739(1)	4.725(3)
c(Å)	4.344(3)	4.299(3)	4.284(2)	4.266(5)
V(Å^3)	86.3(2)	84.07(9)	83.32(5)	82.5(1)

*Kudoh et al. (1997).

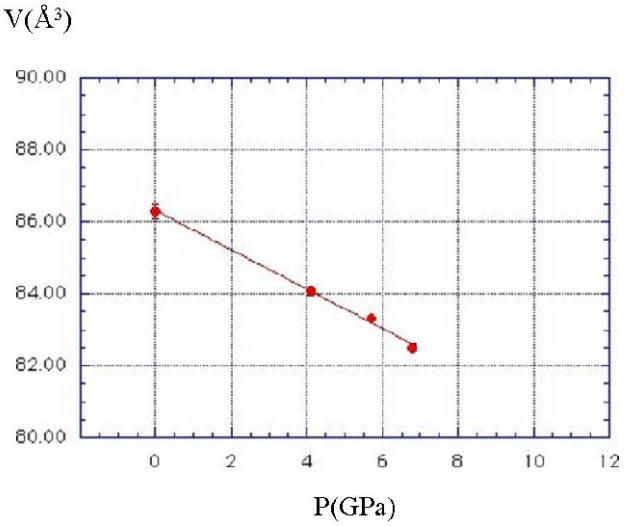

Fig. 1. Unit cell volume (V) versus pressure (P) for phase G. The unit cell volume at ambient pressure is from Kudoh et al. (1997)[3].

References

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