Crystallography

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Compressibility of fluorine end member super hydrous phase B, $Mg_{10}Si_3F_4O_{14}$, up to 7.4 GPa

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Introduction

Super hydrous phase B (sup B), $Mg_{10}{}^{VI}Si^{IV}Si_2H_4O_{18}$, is known as one of dense hydrous silicates minerals (DHMS). This phase is very important to understand the transportation of water in subduction zone. The stability fields of sup B phase have been studied some researchers (*ex.* [1], [2]). Also, in this phase, OH can be replaced by F and perfectly exchanged sample was synthesized at more higher PT conditions [3]. There is a much amount of fluorine in the subduction zone and F-bearing sup B might be more stable under high-pressure conditions. If so, hydrogen could be moved to deeper interior by partial replacements of OH⇆F. Moreover, in crystal chemistry, the effect of replacement of OH⇆F on the compression is little known and is needed to clarify.

In this paper, we conducted single crystal X-ray diffraction measurement of F end member sup B to investigate that effect and to determine the isothermal bulk modulus of this phase.

Experimental Procedure

The sample used for this study was synthesized at 21 GPa and 1300°C kept for 7 hours using a Kawai type multi anvil apparatus installed in Gakushu-in University. A single crystal of F end member sup B (0.04 × 0.04 × 0.03 mm^3 in size) was mounted on a modified Merrill-Bassett type diamond anvil cell with a small piece of a ruby crystal, which used for the pressure calibration. The 4:1 fluid mixture of methanol and ethanol was used for the pressure medium and a SUS301 stainless plate used for a gasket. Pressure was determined by the ruby fluorescence method [4]. The wavelength of X-ray radiation was calibrated by the unit cell volume of the ruby standard crystal at ambient temperature.

The X-ray diffraction intensities were measured using an automated four-circle X-ray diffractometer installed at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization. The cell parameters of F end member sup B were obtained at 1.5, 2.7, 4.0, 5.0, 6.4 and 7.4 GPa. Lattice constants were refined from over 25 centered reflections at each pressure point.

Results

The volume compression curve was shown in Fig. 1. The isothermal bulk modulus of F end member sup B, calculated using the Birch-Murnaghan equation of state with a pressure derivative $K' = 4$, was $K_T = 154$ (3) GPa. This value is slightly larger (7 %) than those of OH end member sup B (145±15 GPa from [5]; 142.6(8) GPa with K'=5.8(2) from [6]). This 7% difference is in good agreement with the estimated value in our paper [7]. The elastic property of super hydrous phase B became stiffer by replacing OH by F. This suggested that less compression property of F end member sup B may be caused by the loss of hydrogen bond.

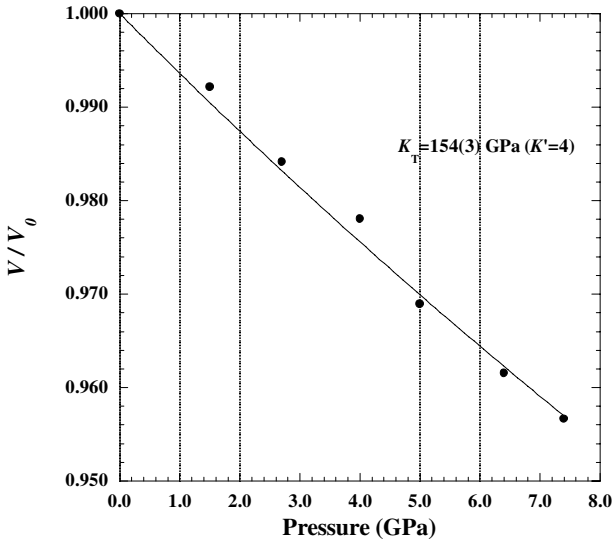

Figure 1. The volume compression curve of F end member super hydrous phase B up to 7.4 GPa.

References

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