

Methods

1. Preparation of the starting material of bridgmanite aggregates

Well-sintered $(\text{Mg}_{0.97}\text{Fe}_{0.03})\text{SiO}_3$ -bridgmanite aggregates free from CPO were prepared by the following procedures. The composition is very close to the bridgmanite in the post-spinel assembly formed from San Carlos olivine $(\text{Mg}_{0.9}\text{Fe}_{0.1})_2\text{SiO}_4$ ³³. At first, orthopyroxene (Opx) powder with the composition of $(\text{Mg}_{0.97}\text{Fe}_{0.03})\text{SiO}_3$ was synthesized from a mixture of MgO, SiO₂ and Fe₂O₃ with the prescribed ratio at 1673 K and $f_{\text{O}_2} = \text{fayalite-magnetite-quartz (FMQ)} - 1 \text{ log unit}$ using a gas mixture (H₂ and CO₂) furnace. Then, the Opx powder was put in an iron inner capsule and sintered in piston-cylinder apparatus at 1 GPa and 1473 K. To avoid formation of cracks in the sintered Opx, we used PYREX glass as an outer capsule and decompressed the sample slowly at temperatures higher than 1073 K after sintering. Bridgmanite aggregates for the deformation experiments were synthesized from the sintered Opx at 25 GPa and 1873 K for 1 hours in the Kawai type apparatus. It is known that significant CPO develops in bridgmanite aggregate accompanied with conversion from Opx under high deviatoric stress conditions⁹. In syntheses of bridgmanite, therefore, we use NaCl capsule to reduce deviatoric stress³⁴. The obtained bridgmanite aggregates were examined by FE-SEM and by 2D X-ray diffraction patterns (see “3. sample characterization”). The backscattered electron image (Figure 1(a)) and the pole figures

(Figure 2(b)) of the sintered bridgmanite aggregate confirmed that the aggregate have random crystallographic orientation with grain-size of $\sim 15 \mu\text{m}$ and are suitable as starting material for shear deformation experiments and subsequent CPO analyses.

2. Deformation experiments

In the present study, shear deformation experiments at lower mantle conditions was conducted using the deformation-DIA type apparatus, which was named the Kawai-type Apparatus for Triaxial Deformation (KATD)³⁵, installed at Tokyo Institute of Technology. Extended Data Figure 1(a) schematically shows the cell assembly adopted in the present deformation experiments. A cylindrical LaCrO_3 was used as a heater. The upper and bottom pistons of well-sintered hard alumina are cut to make 45° surfaces to apply shear stress to the sample put between them when the differential rams are driven. A Pt foil ($50 \mu\text{m}$ thick) was placed at the ends of the 45° -cut alumina pistons to reduce the friction against the sideslip. A Ni foil ($30 \mu\text{m}$ thick) set at the middle of the ellipse sample served as a strain marker, which also kept the oxygen fugacity of the sample equal to or less than the Ni-NiO buffer. Temperature was determined from electric power based on calibration performed using similar cell assembly with thermocouple (Extended Data Figure 1b). Extended Data Figure 2 shows the relationship between generated temperature and the electric power obtained in two

calibration runs (K63 and K71). It should be noted that both curves almost overlapped each other up to 1873 K. Pressure calibration of the KAT-D apparatus was carried out by detecting the phase transformations of the α - β in Mg_2SiO_4 (15.1 GPa)³⁶, the β - γ in Mg_2SiO_4 (19.8 GPa)³⁷ and the dissociation of γ - Mg_2SiO_4 to MgSiO_3 -bridgmanite + MgO (periclase) (23.6 GPa)³⁸ at temperature of 1873 K.

The specimens were first compressed to the desired pressure (25 GPa) at room temperature, and then heated at 1873 K for 10 min to relax deviatoric stress in the specimens. In run K116, which is the undeformed experiment, the specimens were quenched by shutting off the electric power and recovered to observe the state of the sample just before deformation experiment. In the deformation experiment run (K122), the sample was also first annealed at 1873 K for 10 min and then deformed by advancing the upper and lower differential rams to 75 μm displacement each (i.e., 150 μm in total) for a duration of 1 hour at 1873 K (cf. Extended Data Figure 3). Throughout the heating and the deformation, load of the main ram was kept constant. The loads of differential rams were linearly increased to advance the differential rams at high temperature (1873 K). High pressure experiments were conducted under nominally dry condition. Since water solubility of Al-free bridgmanite is very low (< 1 ppm)³⁹, effect of water is considered to be negligible in the present study.

3. Sample characterization

In order to observe microstructure, the starting material and the recovered sample were polished with SiC sand papers and diamond paste in sequence, and then, were etched by colloidal silica to clarify the grain boundaries. The microstructures of samples were investigated by a field emission scanning electron microscope (FE-SEM, JSM-7001F) at ISEI, Okayama University as shown in Figure 1.

The ordinary electron backscattered diffraction technique to measure a crystallographic orientation does not work well due to the serious damage of bridgmanite crystals by electron beam. Therefore, we determined the crystallographic orientation of the bridgmanite by 2D monochromatic X-ray diffraction pattern method^{7,9,21} for both the starting and the deformed samples. In the present study, 2D monochromatic X-ray diffraction pattern was acquired by the imaging-plate (FUJIFILM Co., Ltd., 200 mm × 250 mm) at the synchrotron beam line, BL04B1, of SPring-8 at the Japan Synchrotron Radiation Research Institute (JASRI), Hyogo, Japan⁴⁰. The monochromatic X-ray of 61.388 keV ($\lambda = 0.20197 \text{ \AA}$) was employed. The beam size of X-ray is 100 μm × 200 μm with ~ 500 μm of deformed sample length of bridgmanite. As shown in Extended Data Figure 4, X-ray direction is parallel to shear plane and perpendicular to shear direction. 0 degree of azimuth angle ϕ means parallel to shear

deformation direction. The distance between the sample and the imaging plate was about 601.8 mm, which was calibrated using CeO₂ standard. The typical acquisition time was 10 min. The imaging-plate data were digitized using a FUJI BAS2000 reader under the resolution of 100 μm × 100 μm. Extended Data Figure 5 represents 2D and 1D X-ray diffraction pattern converted from imaging-plate data. In CPO analysis of bridgmanite aggregates, the (111), (020), (120), (210), (022), (202), (113), (122), (212), (023) and (221) diffraction peaks were adopted. The software “ReciPro”²¹ was used for the CPO analysis. This software was previously used for analysis of CPO^{41,42}. Analysis was carried out adopting following parameters; number of crystallites: 2,000,000, size of crystallites: 1 μm, beam convergent angle: 0.02°, beam monochromaticity: 0.1%, number of step: 1%, and directional density: 60%. As shown in Extended Data Figure 6, observed intensities for all peaks are good agreement with simulated ones. In addition, results of CPO were reanalyzed by MAUD program. As shown in Extended Data Figure 7, orientations of CPO of deformed bridgmanite between ReciPro and MAUD software were confirmed to be same while intensities of the CPO are not perfectly identical because of the difference algorithms used in both software..

Extended data Table 1. Summary of dominant slip system of bridgmanite in the present and previous studies

	Dominant slip system	Composition	Pressure	Temperature	Methods
This study	[001](100)	(Mg _{0.97} Fe _{0.03})SiO ₃	25 GPa	1873 K	Shear deformation
Merkel et al. (2003) ⁷	Not observed	MgSiO ₃	< 32 GPa	300 K	Uniaxial deformation by DAC
Miyagi et al. (2016) ²²	[100],[010] and <110> on (001) below 55 GPa, (100) plane over 55 GPa	(Mg,Fe)SiO ₃ with (Mg,Fe)O	<65 GPa	300 K	Uniaxial deformation by DAC
Cordier et al. (2004) ⁸	[100]	MgSiO ₃	25 GPa	300 K - 1673 K	USRE*
Mainprice et al. (2008) ¹⁸	[010](100)	MgSiO ₃	30 GPa	0 K	FP ⁺ with VPSC ^{**}
Ferré et al. (2007) ²³	[100](010), [010](100)	MgSiO ₃	30 GPa	0 K	FP ⁺

*: Uniaxial stress relaxation experiments

⁺: First-principles calculation

^{**}: visco-plastic self-consistent (VPSC) model

Extended Data Table 2. Elasticity of deformed bridgmanite aggregate

i	$j = 1$	$j = 2$	$j = 3$	$j = 4$	$j = 5$	$j = 6$
1	557.6	218.1	219.9	-0.5	0.2	2.8
2		567.7	221.4	-0.4	-0.1	3.2
3			572.2	-0.6	0.3	0.5
4				174.4	1.3	0.1
5					171.7	0.2
6						171.8

Note: The C_{ij} (in GPa) was calculated from deformed bridgmanite sample (K122) at 25 GPa and 1873 K.

Reference axes defined as follows: 2- X (Shear direction), 1- Y (Shear plane normal) and 3- Z (perpendicular to both 1 and 2 directions) in Figure 2.

Extended Data Table 3. Elasticity of single crystal of bridgmanite aggregate¹⁹ used for calculation of elasticity of deformed bridgmanite aggregate

i	$j = 1$	$j = 2$	$j = 3$	$j = 4$	$j = 5$	$j = 6$
1	539	220	210	0	0	0
2		595	232	0	0	0
3			561	0	0	0
4				187	0	0
5					178	0
6						156

Reference axes defined as follows: 1- a axis, 1- b axis and 3- c axis in space group $Pbnm$.

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Extended Data Figure captions

Extended Data Figure 1. Schematic cross sections of cell assemblies for (a) shear deformation experiments and (b) temperature calibration experiment.

Extended Data Figure 2. The temperature and power relationship at 25 GPa using the cell assembly for temperature calibration experiments. Results of two runs are shown by black and red lines.

Extended Data Figure 3. Loads and strokes of the differential rams during the deformation experiment (run K122) are shown as functions of elapsed time. Green and pink lines almost overlapped are strokes of the top and the bottom differential rams, respectively. Black and red lines denote loads of the top and bottom rams, respectively. The sample was deformed by advancement of both the top and bottom differential rams linearly with time. During deformation, loads of differential rams also increased linearly.

Extended Data Figure 4. Schematic illustration showing 2D X-ray diffraction measurement. In this measurement, direct beam stopper arm was located from right side viewed from the front side.

Extended Data Figure 5. (a) 2D X-ray diffraction pattern where ϕ is an azimuthal angle and (b) 1D X-ray diffraction pattern of the deformed bridgmanite (K122) after

recovered. In (a), view direction to take 2D X-ray diffraction pattern by IP is from back side, which is opposite to polished plane. Direct beam stopper arm position becomes left side. Diffraction peaks of the (111), (020), (120), (210), (022), (202), (113), (122), (212), (023) and (221) were used in the analysis of CPO patterns.

Extended Data Figure 6. Normalized intensities of diffraction peaks of the deformed bridgmanite. Each diffraction peak intensity was normalized by its average value. (a): (111), (b): (020), (c): (120), (d): (210), (e): (022), (f): (202), (g): (113), (h): (122), (i): (212), (j): (023), and (k): (221) diffraction peaks. Black and red symbols represent normalized intensities of the raw and the simulated data, respectively.

Extended Data Figure 7. Pole figures of bridgmanite showing the variation of crystallographic orientation of the [100], [010] and [001] directions determined using the software “MAUD”.