Title:

Mantle dynamics inferred from the crystallographic-preferred-orientation of bridgmanite

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Bridgmanite, (perovskite-structured (Mg,Fe)SiO_3) is the dominant constituent mineral in the Earth's lower mantle but its rheological properties are largely unknown. Seismic shear wave anisotropies[1-6] are observed in the Earth's uppermost lower mantle around several subducted slabs. The anisotropy caused by deformation-induced crystallographic-preferred-orientation (CPO) of bridgmanite is the most plausible candidates of this feature. Uniaxial deformation experiments[7-9] have been carried out to determine the deformation texture of bridgmanite but the dominant slip system (slip direction and plane) has not been determined. Here we report the CPO pattern and dominant slip system of bridgmanite under uppermost lower mantle conditions (25 GPa and 1873 K) obtained for the first time through simple shear deformation experiments using the Kawai-type deformation-DIA apparatus[10]. The obtained fabrics are characterized by the a-axis perpendicular to the shear plane and the c-axis parallel to the shear direction, implying that the dominant slip system of bridgmanite is [001](100). The observed shear wave anisotropies near subducted slabs[1-4] (Tonga-Kermadec, Kurile, Peru and Java) are explained by the CPO of bridgmanite induced by flow directions along the strike on the plates. Flow direction in the lower mantle would be determined based on a combination of the CPO of bridgmanite and seismic observations[1-6].

Recent P-wave seismic tomography[11] revealed four types of geometry of subducted slabs in the mantle: I - slab stagnant above the 660 km discontinuity; II - slab penetrating the 660 km discontinuity (e.g. Kuril); III - slab lying in the uppermost lower mantle between a depth of 660–1000 km (e.g. Tonga-Kermadec, Sumatra and South America); and IV - slab continuously descending into the mid lower mantle. Seismic tomography[11-13] provides morphological images of the subducted slabs in the Earth's mantle, but does not give any insight into the dynamic features of the slab. However, seismic anisotropy observed in the mantle provides information on the flow direction of the slabs in the deep mantle because the anisotropy may be the reflection of the crystallographic–preferred-orientation (CPO) of the constituent minerals yielded by dislocation creep deformation.

As shown in previous reports, a significant anisotropy demonstrating clear shear wave splitting was observed in the uppermost lower mantle of the Tonga-Kermadec slab region[1,2]. Recently, such anisotropies were also observed in the uppermost lower mantle of slab regions[3-5]. In these observations, shear wave splitting shows fast polarization generally parallel to the plane of the subducted plate (e.g. Tonga-Kermadec, Java, Peru and Kurile)[1-4] while other observed slab regions do not show a consistent splitting pattern[3]. Therefore, it is interesting to examine how the observed shear-wave anisotropy could be interpreted by the CPO of the lower mantle minerals. It is generally accepted that in pyrolitic mantle model, the constituents of the lower mantle are bridgmanite (77 vol. %), (Mg,Fe)SiO_3-perovskite of space group *Pbnm*, ferropericlase (16 vol. %), and $CaSiO_3$-perovskite (7 vol. %)[14]. The contribution of the CPO of ferropericlase is negligible because of its nearly isotropic elasticity at the uppermost lower mantle conditions[15]. $CaSiO_3$-perovskite is elastically anisotropic[16] but the contribution of this phase to seismic anisotropy will not be significant because of the small amount of $CaSiO_3$ in the lower mantle. In contrast, it is anticipated that the significant seismic anisotropy can be produced by the CPO of bridgmanite[17,18], based on its high elastic anisotropy[19,20] and overwhelming presence in the lower mantle. Thus, we focused on the deformation-induced CPO of bridgmanite as the most important factor of the plausible lower mantle seismic anisotropy.

We performed shear deformation experiments of bridgmanite with controlled strain rate under lower mantle conditions employing the deformation-DIA (D-DIA) type multi-anvil press with the Kawai-type cell assembly (6-8 type)[10]. Dense sintered $(Mg_{0.97}Fe_{0.03})SiO_3$ bridgmanite aggregates synthesized at 25 GPa and 1873 K were used as samples for the deformation experiments. A backscattered electron image (Figure

1(a)) and pole figures (Figure 2(a)) of sintered bridgmanite revealed that the sample was an equigranular aggregate with a typical grain size of 15 μm and a random crystallographic orientation, which was determined by 2D monochromatic X-ray diffraction pattern method (see Methods). In the deformation experiments, a thin ellipse of bridgmanite aggregate with a strain marker of Ni foil, which was initially set at the middle of the sample perpendicular to the cut surfaces of the alumina pistons, was sandwiched between 45º-cut polycrystalline dense alumina pistons at the centre of the cell assembly. Corresponding to the advancement of the differential rams of the D-DIA press, the alumina pistons apply simple shear to the thin bridgmanite sample.

Figures 1(b) and (c) show the microstructures of the recovered samples from the undeformed (only annealing) experiment (run K116) and from the deformation experiment (run K122), respectively, both performed at identical *P*/*T* conditions (25 GPa, 1873 K). In the former, the strain marker was almost normal to the cut surfaces of the alumina pistons, showing that the shear strain of the bridgmanite sample was very close to zero. Thus the sample was almost free from deformation through all the processes; i.e., compression, heating, annealing, and subsequent decompression. As shown in Figure 1(c), the strain marker definitely tilted in the deformed sample. From the tilting angle of the strain marker (~38°) and the deformation time (1 h), the total strain and average strain rate were determined to be γ ~0.8 and $\dot{\gamma}$ ~2 × 10^{-4} /s, respectively. Thickness of the deformed sample was reduced by about 20% in comparison with the original, suggesting the presence of some amount of uniaxial component of the deformation. The microstructural observation in Figure 1(d) shows that the elongated bridgmanite grains of sizes up to 30-40 μm declined along the shear direction and are surrounded by small grains of less than a few micrometres. The structural features indicate that dynamic recrystallization occurred, and hence, CPO of bridgmanite could be induced by deformation involving dislocations.

The crystallographic orientation of the bridgmanite was determined using the 2D monochromatic X-ray diffraction pattern method[7,9,21] for both the starting and deformed samples. The sheared bridgmanite aggregate demonstrated strong fabric (Figure 2b), whereas the starting material did not show significant CPO pattern (Figure 2a). In the sheared bridgmanite, the [100] axis was oriented perpendicular to the shear plane. Although weak girdle patterns of the [001] and [010] axes corresponding to uniaxial compressive strain were observed, the [001] and [010] axes were mostly aligned parallel and normal to the shear direction on the shear plane, respectively. Experimental textures are compatible with an orientation-producing deformation mechanisms such as dominant slip on [001](100) under conditions of 25 GPa and 1873 K, corresponding to the uppermost lower mantle conditions.

The dominant slip system of bridgmanite at a high deviatoric stress condition was reported through high pressure experiments[7,8,22] and theoretical calculations[18,23], as shown in Extended data Table 1. Using a diamond anvil cell, uniaxial deformation experiments of bridgmanite were conducted at room temperature[7,22]. No clear CPO pattern was observed[7], probably due to insufficient strain while dominant slip systems were reported as [100], [010] and <110> on (001) below 55 GPa and (100) plane over 55 GPa[22]. Uniaxial stress relaxation experiments (USRE) of bridgmanite were carried out using the Kawai-type multianvil press at 25 GPa and 1673 K[8]. Analysis of the recovered samples using the X-ray peak broadening technique suggested that the dominant slip direction is the [100] in contradiction to the present results. Dense deformation bands across the pre-existing twin boundaries observed in the USRE[8] suggested that the bridgmanite aggregate was deformed under very high deviatoric stress. Such an extremely high deviatoric stress, up to several GPa by compression at room temperature, was directly measured during in-situ USRE of olivine polymorphs[24.25]. The [100] slip direction observed by USRE of bridgmanite[8] might be the result under very high deviatoric stress condition.

The [100](001) slip system was reported to be one of the most easily activated slip systems of bridgmanite in the dislocation glide region by a first principles calculation[23], supporting that the observed slip direction by USRE results from dislocation glide, whereas other study by first principles calculations with visco-plastic self-consistent model[18] suggested that the most easily activated slip system is [010](100) at 0 K and a pressure range between 0 to 100 GPa in the dislocation glide region. Both calculations and previous experimental results are inconsistent with the present results. This could be due to the differences of dominant slip mechanisms or dominant deformation mechanisms by variation of experimental conditions (e.g. stress, temperature and pressure) such as in the case of olivine[26].

$CaTiO_3$-perovskite is often used as an analogue material for bridgmanite because of their similar rotation angles of the SiO_6 or TiO_6 octahedron. Uniaxial deformation experiments were performed on $CaTiO_3$-perovskite[27], in which dislocation creep is expected due to high temperature (up to 1973 K) and low deviatoric stress (25-120 MPa). TEM observations of the recovered sample revealed that screw dislocation with Burgers vectors $[100]_{pc}$ and $[011]_{pc}$ on the $(01\text{-}1)_{pc}$ plane, where indexing is based on the pseudo-cubic (pc) system, formed rectangular networks. The $[100]_{pc}$ and $[011]_{pc}$ directions on the $(01\text{-}1)_{pc}$ plane in pseudo-cubic indexation of perovskite include the 1/2[001] and [010] directions on the (100) plane in the orthorhombic system. The

[001](100) slip system in the present study does not contradict with that of $CaTiO_3$-perovskite.

The seismic wave anisotropy formed by the CPO of deformed bridgmanite in the present study was calculated based on the elastic constant[19] as shown in Figure 3. For the shear wave anisotropy of deformed bridgmanite, the velocity of horizontally polarized shear waves, V_{SH}, is ~ 1% higher than that of vertically polarized shear waves, V_{SV}, in horizontal flow as shown in Figure 3(b), whereas V_{SV} is 0.03-1.10% higher in vertical flow in Figure 3(d). As shown in Figure 4(a), shear wave splitting with $V_{SH}>V_{SV}$ are observed in the uppermost lower mantle from the Tonga-Kermadec subduction zone to the Australian continental seismic stations, where the ray path is nearly parallel to the section[1,2]. The delay time ranges from 0.7 to 6.2 s[1,2], which corresponds to average (V_{SH} - V_{SV})/V_{SV} ~ 0.1–1% assuming a 3000–6000 km ray path including 1000-2000 km subducted plate region[11] on the uppermost lower mantle. The magnitude of the shear wave anisotropy is consistent with deformed bridgmanite in the present study as shown in Figure 3(b). In contrast, opposite shear wave anisotropy ($V_{SV} > V_{SH}$) was observed from the Tonga-Kermadec subduction zone to the western North America stations, where the ray path is nearly perpendicular to the section[4]. It is thus concluded, that both of the observed shear-wave anisotropies around the Tonga-Kermadec subduction zone, which are type III in the P-wave tomography[11], are well explained by the CPO of bridgmanite yielded by the penetration of subducted slabs down to 1000 km by vertical motion and by the stagnation at around 1000 km depth with a horizontal flow in the pyrolitic mantle as shown in Figure 4(a). This flow pattern could be caused by the viscosity hill[28-30] at depths between 1000 and 1500 km, and the viscosity reduction of the slab by interconnection of ferropericlase in the post-spinel phase[31]. Shear wave anisotropies at the top of the lower mantle beneath Java (type III), Peru (type III), and Kuril subducted slabs (type II) were observed along the seismic ray path nearly parallel to the subducted plate surface[3] (Figure 4 b-d). In these observations, the fast polarization in shear wave splitting appear to be arranged generally parallel to the plane of the plate[3], which is explained by the deformation-induced CPO of bridgmanite formed by the parallel flow to the subducting direction. Therefore, the present results on CPO of bridgmanite coupled with the observation of seismic anisotropy provides a strong evidence to understand the direction of the mantle flow, which can be often expected from seismic tomography.

Figure captions

Figure 1. Backscattered electron images of the bridgmanite aggregates. (a): sample sintered, (b): sample annealed at 25 GPa and 1873 K for 10 min (run K116), (c) and (d): sample deformed at 25 GPa and 1873 K for 1 h (run K122). In (a) and (d), polished surfaces were etched with colloidal silica to clarify grain boundaries. In (b) and (c), black arrows indicate Ni foil strain markers. The strain marker in the annealed sample in (b) remains perpendicular to the 45°-cut surfaces of alumina pistons, indicating almost no deformation during compression and annealing. In (c), tilting of the Ni strain marker to 38 ° in the deformed sample indicating a strain of γ~0.8. Elongated grains, indicating dynamic recrystallization, were only observed in the deformed sample indicated by the gray arrow in (d). X, Y, and Z coordinates correspond to the shear direction, shear plane normal, and perpendicular to both “X” and “Y” directions, respectively. This definition of coordinates is used in Figures 2 and 3 and in extended data Figure 7.

Figure 2. Pole figures of bridgmanite showing the variation of crystallographic orientation of the [100], [010] and [001] directions in the coordinate system defined with respect to the deformation geometry of bridgmanite (a) sintered and (b) deformed

(K122) at γ~0.8 and $\dot{\gamma}$ ~2 × 10^{-4} /s. Black dashed lines represent the long axis of the ellipsoid strain of the deformed bridgmanite.

Figure 3. Seismic wave anisotropy of bridgmanite aggregates deformed in shear under the uppermost lower mantle pressures and temperatures (25 GPa and 1873 K) (run K122) calculated using a software[32]. (a) and (c) P-wave seismic velocity at horizontal and vertical flow, respectively. (b) and (d) Trace of the V_{S1} polarization plane at horizontal and vertical flow, respectively.

Figure 4. Schematic cross-sections of subducted slabs of (a) the Tonga-Kermadec arc (b) Java arc, (c) Peru arc, and (d) Kuril arc based on P-wave tomography[11]. Blue and orange lines represent shear seismic ray paths nearly parallel and perpendicular to the section for the observation of shear wave anisotropies at the Tonga-Kermadec slab[1-2,4] and Kuril, Peru and Java slabs[3], respectively. Blue and orange polar histograms show polarization of the fast shear wave perpendicular to blue and orange seismic ray paths of the Tonga-Kermadec slab[1,2,4] Kuril, Peru and Java slabs[3], respectively. The fast polarization arrangement is almost parallel to the plane of the subducted plates. Yellow dashed lines correspond to flow directions of the subducted slab. Black double arrows

represent shear directions. The uppermost lower mantle near the subducted slab is deformed by the flow directions parallel to the subducted slab, which align the *a*- and *c*-axis of bridgmanite from normal to shear deformation plane and parallel to shear direction, respectively.

Reference

1 Wookey, J., Kendall, J.-M., Barruol, G., 2002. Mid-mantle deformation inferred from seismic anisotropy. Nature 415: 777-780

2 Wookey, J., Kendall, J.-M., 2004. Evidence of midmantle anisotropy from shear wave splitting and the influence of shear-coupled *P* wave. J. Geophys. Res. 109: doi: 10.1029/2003JB002871

3 Nowacki, A., Kendall, J,M., Wookey, J., Pemberton, A., 2015. Mid-mantle anisotropy in subduction zones and deep water transport. Geochem. Geophys. Geosys., doi: 10.1002/2014GC005667

4 Foley, B.J., Long M,D., 2011, Upper and mid‐mantle anisotropy beneath the Tonga slab. Geophys. Res. Lett., VOL. 38, L02303, doi:10.1029/2010GL046021

5 Lynner, C., Long M,D., 2014, Sub-slab anisotropy beneath the Sumatra and circum-Pacific subduction zones from source-side shear wave splitting observations. Geochem. Geophys. Geosys. doi: 10.1002/2014GC005239

6 Heintz, M., 2006, Midmantle deformation between the Australian continent and the Fiji-Tonga subduction zone? J. Geophys Res., VOL. 111, B09303, doi:10.1029/2005JB004058,

7 Merkel, S., Wenk, H.R., Badro, J., Montagnac, G., Gillet, P., Mao, H., Hemley, R.J., 2003. Deformation of $(Mg_{0.9},Fe_{0.1})SiO_3$ perovskite aggregates up to 32 GPa. Earth Planet. Sci. Lett. 209: 351-360

8 Cordier, P., Ungár, T., Zsoldos, L., Tichy, G., 2004. Dislocation creep in $MgSiO_3$ perovskite at conditions of the Earth's uppermost lower mantle. Nature 428: 837-840

9 Wenk, H-R., Lonardelli, I., Merkel, S., Miyagi, L., Pehl, J., Speziale, S., and Tommaseo, C. E., 2006 . Deformation textures produced in diamond anvil experiments, analysed in radial diffraction geometry. J. Phys.: Condens. Matter 18. S933–S947

10 N. Tsujino: Experimental study on rheology of the Earth's lower mantle, doctoral thesis, Tokyo Institute of Technology, 2012.

11 Fukao, Y., Obayashi, M., 2013. Subducted slabs stagnant above, penetrating through, and trapped below the 660 km discontinuity. J. Geophys. Res. 118, 5920–5938, doi:10.1002/2013JB010466

12 van der Hilst, R.D., Widiyantoro, R.D.S., Engdahl, E.R.E., 1997 Evidence for deep mantle circulation from global tomography. Nature, 386, 578-584

13 Zhao, D., 2004, Global tomographic images of mantle plumes and subducting

slabs: Insight into deep Earth dynamics, Phys. Earth Planet. Inter., 146, 3–34.

14 Hirose, K., 2002. Phase transitions in pyrolitic mantle around 670-km depth: Implications for upwelling of plumes from the lower mantle. J. Geophys. Res., 107, B4, 2078.

15 Yamazaki, D., Karato, S., 2002. Fabric development in (Mg,Fe)O during large strain, shear deformation: implications for seismic anisotropy in Earth's lower mantle. Phys. Earth Planet. Int., 131, 251–267

16 Karki B.B., Crain, J., 1998. First-principles determination of elastic properties of $CaSiO_3$ perovskite at lower mantle pressures. Geophys, Res, Lett., 25, 2741-2744

17 Wenk, H.-R., Speziale, S., MacNamara, A.K., Garnero, E.J., 2006. Modeling lower mantle anisotropy development in a subducting slab. Earth Planet. Sci. Lett. 245, 302–314

18 Mainprice, D., Tommasi, A., Ferré, D., Carres, P., Cordier, P., 2008. Predicted glide systems and crystal preferred orientations of polycrystalline silicate Mg-Perovskite at high pressure: Implications for the seismic anisotropy in the lower mantle. Earth Planet. Sci. Lett. 271, 135–14414

19 Wentzcovitch, R.M., Karki, B.B., Cococcioni, M., de Gironcoli, S., 2004. Thermoelastic properties of $MgSiO_3$-perovskite: Insights on the nature of the earth's lower mantle. Phys. Rev. Lett. 92: DOI: 10.1103/PhysRevLett.92.018501

20 Oganov, A.R., Brodholt, J.P., Price, G.D., 2001. The elastic constants of MgSiO3 perovskite at pressures and temperatures of the earth's mantle. Nature, 411, 934–937.

21 Seto, Y., 2012. Whole Pattern Fitting for Two-Dimensional Diffraction Patterns from Polycrystalline Materials Rev. High Press. Sci. Tech. 22, 2, 144-152

22 Miyagi, L., Wenk, H.-R., 2016. Texture development and slip systems in bridgmanite and bridgmanite + ferropericlase aggregates. Phys Chem Minerals DOI 10.1007/s00269-016-0820-y

23 Ferré, D., Carrez, P., Cordier, P., 2007. First principles determination of dislocations properties of $MgSiO_3$ perovskite at 30 GPa based on the Peierls-Nabarro model. Phys. Earth Planet. Int. 163: 283-291

24 Chen, J., Inoue, T., Weidner, D.J., Wu, Y., Vaughan, M.T., 1998, Strength and water weakening of mantle minerals olivine, wadsleyite and ringwoodite. Geophys. Res. Lett., 25, 4, 575-578

25 Nishihara Y., Funakoshi, K., Higo, Y., Tsujino, N., Kawazoe, T., Kubo, T., Shimojuku, A., Terasaki, H., Nishiyama, N., 2010. Stress relaxation experiments

of olivine under conditions of subducted slab in Earth's deep upper mantle. Phys. Earth Planet. Int., 183, 164-174

26 Jung, H., Karato, S., 2001 Water-induced fabric transitions in olivine. Science 293, 1460-1463

27 Besson, P., Poirier, J.P., Price, G.D., 1996, Dislocations in $CaTiO_3$ perovskite deformed at high-temperature: a transmission electron microscopy study. Phys Chem Minerals 23, 337-344

28 Forte, M.A., Mitrovica, J.X., 2001. Deep-mantle high-viscosity flow and thermochemical structure inferred from seismic and geodynamic data. Nature, 410, 1049-1056

29 Morra, G., Yuen, D.A., Boschi, L., Chatelain, P., Koumoutsakos, P., Tackley, P.J., 2010. The fate of the slabs interacting with a density/viscosity hill in the mid-mantle. Phys. Earth Plants. Int., 180, 271-282

30 Marquardt, H., Miyagi, L., 2015. Slab stagnation in the shallow lower mantle linked to an increase in mantle viscosity. Nature Geoscience, DOI: 10.1038/NGEO2393

31 Yamazaki, D., Yoshino, T., Nakakuki, T., 2014. Interconnection of ferro-periclase controls subducted slab morphology at the top of the lower mantle. Earth Plants. Sci. Lett., 403, 352-357

32 Mainprice, D., 1990. A FORTRAN program to calculate seismic anisotropy from the lattice preferred orientation of minerals. Comput. Geosci., 16,385–393.

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