Elastic anisotropy of experimental analogs of perovskite and post-perovskite by means of inelastic X-ray scattering

Recent studies have shown that the D" layer, just above the Earth's core-mantle boundary, is composed of $MgSiO_3$ post-perovskite and has a significant lateral inhomogeneity. Here we consider the D" diversity as related to the single crystal elasticity of the post-perovskite phase. We measured the single-crystal elasticity of the perovskite *Pbnm*-$CaIrO_3$ and post-perovskite *Cmcm*-$CaIrO_3$ using inelastic X-ray scattering (IXS) at beamline **BL35XU** [1]. These materials are structural analogs to same phases of $MgSiO_3$. Our results show that *Cmcm*-$CaIrO_3$ is much more elastically anisotropic than *Pbnm*-$CaIrO_3$, which gives an explanation for enigmatic seismic wave velocity jump at the D" discontinuity. Considering a relation between lattice preferred orientation and seismic anisotropy in the D" layer, we suggest that the *c*-axis of post-perovskite $MgSiO_3$ aligns vertically beneath the Circum-Pacific Rim, and the *b*-axis vertically aligns beneath the Central Pacific.

Since the discovery of the transition from perovskite (Pv) to post-perovskite (pPv) in $MgSiO_3$ [2], pPv-$MgSiO_3$ has been considered to be a major component of the D" layer just above the core-mantle boundary (CMB). Seismological observations of the D" layer are difficult to interpret as they suggest both non-uniform response at the layer boundary and non-uniform anisotropy inside the layer [3]. With this background, elastic anisotropy, or single-crystal elasticity, of pPv-$MgSiO_3$ has been the focus of theoretical calculations [4]. However, no experimental data are available on the single-crystal elasticity of pPv-$MgSiO_3$, because it is unstable at ambient pressure.

Cmcm-$CaIrO_3$, or pPv-$CaIrO_3$, has been frequently selected as a representative analog of pPv-$MgSiO_3$. According to the phase diagram, pPv-$CaIrO_3$ is the stable phase at ambient conditions and Pv-$CaIrO_3$ is the high-temperature and low-pressure phase. Here we report the first experimental data on single crystal elasticity of Pv and pPv structures in a homogeneous chemical composition of $CaIrO_3$.

Figures 1(A) and 1(B) show single crystals of Pv-$CaIrO_3$ and pPv-$CaIrO_3$ used in the present study. The Pv-$CaIrO_3$ sample was synthesized at 2 GPa and 1450°C for 15 h in a piston cylinder apparatus at Okayama University. We produced many grains on the order of a few tens of microns, but most of them turned out to have multiple domains. We examined more than 20 grains using a four-circle X-ray diffractometer at Yamaguchi University and selected a quasi-single domain crystal with a size of ~20 μm.

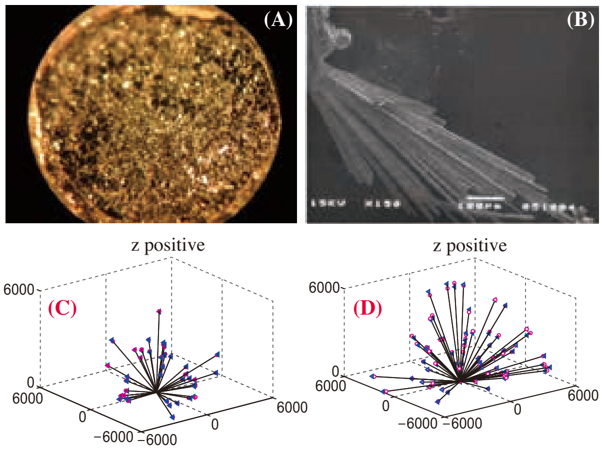

Fig. 1. Specimen and measurement data. Left and right columns refer to *Pbnm*- and *Cmcm*-$CaIrO_3$, respectively. **(A, B)** Photographs of the single crystals used. Horizontal edge lengths are ~5 mm and ~800 mm for **A** and **B**, respectively. **(C, D)** Overall picture for the experimental data and analytical fitting. Black lines indicate the direction of wave propagation in the crystal. Blue triangles and red circles are experimental velocities and recalculated values after the least-squares analysis, respectively. Vertical direction is the positive z direction, while horizontal leftward and rightward directions are positive x and y directions, respectively. Note that the difference between experimental and recalculated velocities is less than 5%. Uniformly distributed misfit indicates untwined crystal specimens.

Its lattice constants were determined as $a = 5.3527(1)$, $b = 5.5969(5)$, and $c = 7.6804(6)$ Å, which yields a density (ρ) of 8091 kg/m³. The pPv-$CaIrO_3$ sample was synthesized by slowly cooling from 1000°C in $CaCl_2$ flux. Figures 1(C) and 1(D) compare the experimental velocities obtained from the IXS spectra with velocities calculated from the optimized elastic constants.

According to seismological studies, the region of the Circum-Pacific Rim is interpreted having a vertically transverse isotropy (VTI) with $V_{SH} > V_{SV}$, while the region of the Central Pacific has a complicated VTI with many relations between V_{SH} and V_{SV} [3]. Either polarization anisotropy is not recognized beneath the Atlantic Ocean, or the region is considered as having VTI with $V_{SH} \approx V_{SV}$. On the other hand, from the polarization pattern in the *a*-*b* plane of the faster V_S plot (Fig. 2(B)), we can expect that $V_{SH} > V_{SV}$ in the D" layer if the *c*-axis of pPv is aligned vertically. Similarly, if the *b*-axis aligns vertically, the magnitude relation between V_{SH} and V_{SV} can be complicated.

We can summarize the above conclusion in alternative way: for the *c*-axis vertical case, the horizontal wave propagation directions lie in the *a*-*b* plane, which the in-plane shear mode (SH) has consistently higher wave speeds (Fig. 2(B)). However, if instead the *b*-axis is vertical, the horizontal wave propagation directions lie in the *a-c* plane, which neither the in-plane (SH) nor the out-of-plane (SV) is consistently faster for all such propagation directions (Fig. 2(B)).

The dominant slip system of pPv-$CaIrO_3$ was determined as [100](010) from the shear deformation experiments. Since the slip system of pPv-$MgSiO_3$ has not yet been determined, we assumed that it is similar to that of pPv-$CaIrO_3$. This assumption leads to LPO of pPv-$MgSiO_3$ in which the *b*-axis aligns vertically along the lateral flow in the D" layer. The LPO pattern is consistent with the complicated polarization S-wave anisotropy beneath the Central Pacific (Fig. 2(B)).

Although the textural development during Pv-pPv transition in $MgSiO_3$ has not yet been clarified, we expect the *c*-axis alignment of pPv-$MgSiO_3$ immediately after the phase transition from Pv-$MgSiO_3$ from analogy with the case for $MgGeO_3$. If the *c*-axis aligns vertically, we expect VTI with $V_{SH} > V_{SV,}$ which is consistent with the seismic feature beneath the Circum-Pacific Rim.

Figure 3 summarizes the present idea for the seismic anisotropy and LPO structure in the D" layer. The VTI of the vertical *c*-axis and that of the vertical *b*-axis can be interpreted as transformation LPO and deformation LPO, respectively. It is noted that isotropic pPv-$MgSiO_3$ is a reasonable interpretation for the seismic feature beneath the Atlantic Ocean; an alternative interpretation may be the VTI of the vertical *a*-axis because of less lateral polarization anisotropy than in other cases. The difference between beneath the Pacific and Atlantic may be attributed to differences in temperature, chemical composition, and strain rate. The proposed LPO behavior for pPv-$MgSiO_3$ obtained from the present mineral physics perspective is consistent with seismic observation.

In this study, we presented a new data set of Pv and pPv-$CaIrO_3$ single-crystal elasticity by means of IXS at BL35XU. We used the present results to interpret the seismic wave anisotropy in the D" layer and proposed a model of pPv LPO in the D" layer consistent with seismic observations and the mineral physics experiments on analog materials. The present model may allow a sophisticated discussion about global mantle convection, which is triggered by heating at the CMB and modulated by lateral flow in the D" layer.

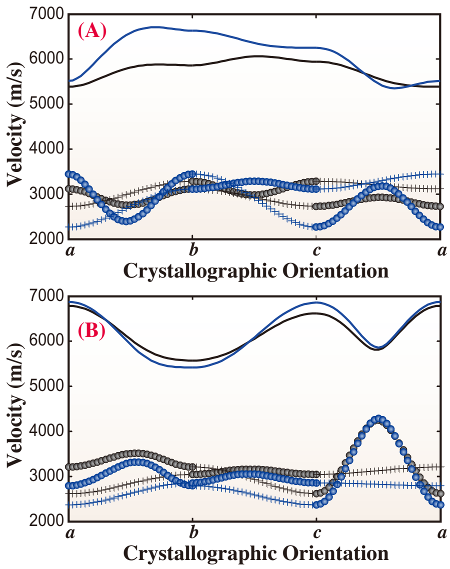

Fig. 2. Velocity surface of *Pbnm*- and *Cmcm*-$CaIrO_3$. **(A)** Upper and **(B)** lower plots correspond to *Pbnm*- and *Cmcm*-$CaIrO_3$, respectively. Black lines are drawn for the present results, while blue lines are drawn for the results obtained in Ref. 5. Upper lines correspond to the P-wave velocity, and lower lines to the S-wave velocity. Solid circles and crosses correspond to V_S specify in-plane and out-of-plane particle motions.

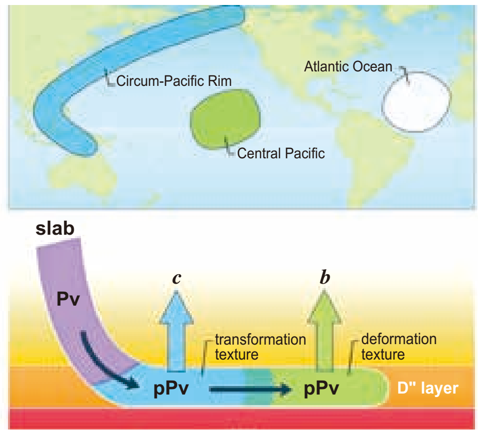

Fig. 3. Schematic illustration of the LPO of pPv-$MgSiO_3$ in the D" layer. From a mineral physics viewpoint, the Pv slab (pink region) transforms into pPv (light blue region) and then the pPv slab moves along the path of mantle convection with deformation (light-green region). In contrast, from seismic observations, the region of the Circum-Pacific Rim has VTI anisotropy of $V_{SH} > V_{SV}$, while the region of the Central Pacific has complicated VTI with an undetermined magnitude relation, i.e., $V_{SH} > V_{SV}$, $V_{SH} < V_{SV}$ or $V_{SH} \approx V_{SV}$. Region of the Atlantic Ocean (white circle) has VTI with $V_{SH} \approx V_{SV}$, suggesting isotropy or negligible LPO of pPv $MgSiO_3$. The speculated aligned axes of pPv LPO are shown by arrows for each region; the vertical *c*-axis is beneath the Circum Pacific Rim and the vertical *b*-axis is beneath the Central Pacific.

Akira Yoneda

Institute for Study of the Earth's Interior,
Okayama University

E-mail: yoneda@misasa.okayama-u.ac.jp

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