A Refined Approach to Model Anisotropy in the Lowermost Mantle

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Abstract.
Seismic anisotropy in the lowermost mantle has been attributed to texture development during mantle convection. This study models texture evolution in a subducting slab impinging on the core-mantle boundary. Using a 3-dimensional geodynamic model with tracers recording the deformation history, a visco-plastic self-consistent (VPSC) model for polycrystal deformation, and relying on experimentally determined slip systems, aggregate grains with volume fractions of 60\% orthorhombic silicate perovskite (MgSiO\textsubscript{3}), 20\% cubic calcium perovskite (CaSiO\textsubscript{3}), and 20\% cubic ferropericlase ((Mg,Fe)O) were deformed plastically and developed crystal preferred orientation. Forward and reverse perovskite (Pv)-post-perovskite (PPv) phase transitions were included by allowing for likely orientation variant selections. Grain orientations, P (compression) and S (shear) wave velocity pole figures were calculated for each phase as well as the aggregate. The results show that dominant (001) slip on PPv can produce strong texture and shear wave anisotropy of 0.01-3.07\% with $V_{SH} > V_{SV}$ which agrees with seismological observations in selected areas of the D'' layer.

1. Introduction
The presence of seismic anisotropy in the upper mantle has been attributed to preferred orientation of olivine [1-4]. With increasing depth in the mantle, uncertainties and speculations increase due to lack of seismic sampling as well as difficulties in performing experiments at relevant pressure and temperature conditions. Some reviews highlight the current state-of-the-art [5-7]. One specific area in the lower mantle, which Bullen (1950) called the D'' region [8], has intrigued scientists for quite some time. The D'' region acts as a thermomechanical boundary layer [9] between the Earth’s liquid outer core and the solid mantle. While the bulk of the lower mantle is mostly isotropic [10,11], seismic observations have revealed strong seismic anisotropy in D'' where upwelling and subduction occur [10,12-15]. With the discovery of the Mg-perovskite (Pv, also known as bridgmanite [16]) Mg-post-perovskite (PPv) phase transition [17,18] at deep mantle conditions, highly anisotropic PPv emerged as a likely candidate to explain the observed anisotropy in D''. It is expected that, for a pyrolytic mantle composition, Pv and PPv dominate in the lower mantle, with ferropericlase ((Mg,Fe)O) and calcium perovskite (CaSiO\textsubscript{3}) contributing
the rest in varying amounts (Fig. 1.a). Figure 1.b shows an enlarged depth/temperature phase diagram of the lowermost mantle with geotherms for a cold subducting slab and a warm upwelling plume.

![Phase diagram of the lower mantle assuming a pyrolytic composition](image)

![Depth/temperature phase diagram, plotting the Pv-PPv phase boundary and cold and warm geotherms](image)

**Figure 1:** (a) Phase diagram of the lower mantle assuming a pyrolytic composition [19]. (b) Depth/temperature phase diagram, plotting the Pv-PPv phase boundary and cold and warm geotherms. Black line separates Pv and PPv stability fields [20].

Modern geodynamic models predict significant plastic strain in areas of slab subduction into D″ as well as plume upwelling [21,22], with large variations in density, temperature and viscosity. Most geodynamic models assume an isotropic medium. In order to predict texture development, tracers are introduced into the convecting medium and record strain. From the strain history, texture evolution can be predicted based on deformation mechanisms. It is generally assumed that plastic deformation in the lower mantle occurs dominantly by dislocation creep leading to crystal rotations and resulting in systematic preferred orientation.

Since Mg-Pv, Mg-PPv and Ca-Pv are unstable at ambient conditions, potential deformation mechanisms must be studied in situ at high pressure and diamond anvil cell (DAC) experiments have become a favorite method, using diamonds not only to produce pressure but also as pistons to axially compress samples. With X-rays at synchrotrons the texture evolution in powders such as PPv can then be studied in situ by analyzing diffraction patterns [23-25]. Assuming a strain history from a geodynamic model and deformation mechanisms from ultrahigh pressure experiments, the evolution of texture in the lower mantle can then be modeled with polycrystal plasticity theory. This has been done before for 2D [26,27] and 3D geodynamic models [25,28,29]. Here we present an improved 3D modeling, including phase and texture transformations. We start with Pv at a relatively shallow depth. At greater depth Pv transforms to PPv and corresponding variant selection rules are applied. Slip systems are updated according to latest information and other mechanisms such as climb and grain boundary sliding are accounted for. Also, single crystal elastic properties are adjusted for temperature-pressure conditions. Results are shown for a single tracer that is representative for the system.

2. Methods

2.1. Geodynamic model

As slabs subduct to the deep mantle, large-strain deformation occurs. In this study, the convection-induced deformation within subducted slabs is calculated in a 3D regional spherical geodynamical model. The governing equations for conservation of mass, momentum, and energy are solved using a modified version of code CitcomCU [31] under Boussinesq approximation. The geodynamic model includes tracers that follow the flow, defining location, pressure, temperature and velocity gradient tensors for each step to define the incremental deformation. Figure 2 shows
a tracer as function of depth projected onto the core-mantle boundary, indicating top and bottom of D′′. The depth, temperature, and pressure along the streamline at selected steps are included for reference. Grey colors along the streamline represent the presence of perovskite while red represents the presence of post-perovskite. The forward transition from Pv to PPv occurs at a shallower depth than the reverse transition during upwelling. This can be explained by increasing temperatures in the upwelling section decreasing the PPv stability field (Fig. 1.b).

**Figure 2:** Spatial representation of selected tracer projected on the core-mantle boundary. Grey represents Pv and red represents presence of PPv. Blue layer represents D′′ at 2550 km and green the core mantle boundary.

2.2. Deformation mechanisms
Information about deformation mechanisms were largely derived from DAC experiments, observing texture development at ultrahigh pressure (>30 GPa) and interpreting patterns with plasticity theory, e.g. for Pv [32,33], PPv [23–25], Ca-Pv [34], ferropericlase [35–38]. Additional information may be obtained from low-pressure analogs, although bonding characteristics are different [39,40], and from atomic force calculations over a wide range of pressure-temperature conditions [41–44]. Slip systems used in the simulations are shown in Table 1. Since other deformation mechanisms that do not produce texture may be active, such as climb and grain boundary sliding [45,46,47], it is assumed that only 50% of the deformation is accommodated by dislocation glide.
Table 1: Proposed dominant slip systems (hkl)[uvw] and critical resolved shear stress coefficients of deep Earth minerals.

|       | (100) (001) | (100) (010) | (110) (110) | (010) (100) | (001) (100) | (001) (010) | (010) (001) |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| PPv   | 2           | 2           | 3           | 4           | 1           | 1.5         | 4           |
| [32,33] | 2           | 4           | 3           | 4           | 1           | 1           | 1.5         |
| Ca-Pv | (111) (10-1) | (110) (-110) | (000) (011) | -           | -           | -           | -           |
| [34]   | 3           | 1           | 1.5         | -           | -           | -           | -           |
| Periclase | {111} (10-1) | {110} (-110) | {100} (011) | -           | -           | -           | -           |
| [35,36,37] | 1.5         | 0.5         | 0.5         | -           | -           | -           | -           |

2.3. Visco-plastic self consistent model

Based on velocity gradients from the geodynamic model and slip systems derived from diamond anvil cell (DAC) experiments, a polycrystal plasticity model can simulate texture evolution. Here the Visco-Plastic Self-Consistent (VPSC6) method [48] is used, starting with 500 grains for each phase that are randomly oriented. In this method, known as the Eshelby inclusion approach, each grain is treated as a finite inclusion that is under constant strain. The inclusion is interacting with a homogenous but anisotropic medium with the averaged properties over all single crystals. Grain reorientation within this medium is a result of deformation by slip along specified lattice planes resulting in rotations. At each step the properties of the effective medium are updated by fitting the constitutive equations between stress and strain within the grain to that of the aggregate. The behavior of the individual grains in the anisotropic medium is obtained by iteratively fitting the behavior of individual grains as well as the averaged response of the medium, leading to a self-consistent solution. Each grain is initialized as spherical in shape but becomes elongated into an ellipsoid due to deformation.

Three phases are deformed simultaneously with slip systems for each phase defined by slip planes, slip directions and critical resolved shear stresses (Table 1). The stress exponent n, given by (ε~σ^n), was set to 3 that appears appropriate for high temperature/slow strain rate creep conditions. Four phases are included in accordance with a pyrolite composition (Fig. 1.a), Mg-perovskite (Pv), Ca-perovskite (Ca-Pv), ferropericlase, and at high pressure Mg-post-perovskite (PPv). Each streamline follows a trajectory beginning with downward flow followed by transversal flow parallel to the core-mantle boundary, and ending with near vertical upwelling in the back-arc region. CitcomCU 3D uses a coordinate system colatitude, longitude and depth to define the location of a tracer and velocity gradients. This is converted to Cartesian coordinates with Z=S/N and X=E/W to convert velocity gradients as input for VPSC. After computation, orientation distribution functions (ODF) as well as elastic tensors for each step are rotated such that the core-mantle boundary is the horizontal (x,y) plane in each image.

2.4. Accounting for phase transitions

During subduction Pv transforms to PPv and during upwelling PPv reverts to Pv. This transition from the Pv Pbnn structure to the PPv Cmcm structure has been studied on the analog system NaNiF$_3$ [40]. Each Pv grain transforms to two PPv orientations, keeping the c-axis unchanged (Fig. 3). In terms of Euler angles it corresponds to a $\pm 16.75^\circ$deg rotation of $\Phi$ around [001] keeping ($\Psi$, $\Theta$) constant.
During the simulation, at the forward phase transition the number of Pv grains is doubled from 500 to 1000 to account for both possible orientations of each PPv grain. The new 1000 grains have PPv slip system information and elastic properties. To maintain the correct volume fraction, the other phases are also doubled from 500 to 1000 grains. VPSC is reinitiated and continues deforming the aggregate until the reverse phase transition point is reached, again doubling grains (1000 to 2000). The PPv grain then transitions back to Pv crystals by the reversal of the same symmetry operation and the deformation continues through the upwelling section of the streamline.

2.5. Elastic properties and seismic velocities
We computed single crystal elastic properties at different pressure and temperature based on a linear approximation to the second derivative. Pressure information was determined by the Preliminary Reference Earth Model (PREM) [50]. Temperature was recorded by the geodynamic model at each timestep. Table 2 provides the densities and single crystal stiffness coefficients (GPa) for each phase based on first principle calculations and figure 4 shows images for P and dS velocity surfaces for single crystals of Pv and PPv. Single crystal elastic tensors for each phase were averaged over the crystal orientation distributions in VPSC and from aggregate elastic properties corresponding P and dS wave velocities were calculated.

Figure 3: Orientation relation between Pv (center) and PPv (left and right) during phase transition [41].

Figure 4: Equal area projection P-wave and dS wave velocities (where dS-wave velocites (S1-S2 and ticks are orientation of fast S-wave polarizations) of perovskite (A,C) and post-perovskite (B,D) single crystals from values in Table 2.
Table 2: Phase density (gm/cm$^3$) and elastic stiffness (GPa) of deep Earth materials at 3000 K and 125 GPa.

| Phase                  | density | $C_{11}$ | $C_{12}$ | $C_{13}$ | $C_{22}$ | $C_{23}$ | $C_{33}$ | $C_{44}$ | $C_{55}$ | $C_{66}$ |
|------------------------|---------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Post-perovskite [51]   | 5.35    | 1107.0   | 429.0    | 318.0    | 847.0    | 441.0    | 1131.0   | 251.0    | 221.0    | 361.0    |
| Perovskite [52]        | 5.25    | 860.0    | 535.5    | 437.0    | 1067.5   | 467.5    | 1053.0   | 294.0    | 249.5    | 284.5    |
| Calcium perovskite [53]| 5.6     | 970.0    | 505.0    | 505.0    | 970.0    | 505.0    | 970.0    | 305.0    | 305.0    | 305.0    |
| Periclase [54]         | 5.0     | 1008.6   | 233.4    | 233.4    | 1008.6   | 233.4    | 1008.6   | 191.5    | 191.5    | 191.5    |

3. Results

Figure 5 shows (001) pole figures for texture, P-wave velocities and dS-wave ($S_1$-$S_2$) in km/s for each phase at step increments marked in Figure 2 while Figure 6 displays velocities for the aggregate. Depth, pressure, and temperature for each row is indicated in Figure 2. All projections are plotted with the core-mantle boundary horizontal for reference. PPv is present from rows 3-5, while Pv is present in rows 1, 2, and 6.

The strongest texture developed in PPv reaching a maximum of 15 multiples of random (m.r.d.) shortly after the PPv-Pv phase transition during upwelling (step 5 in Fig. 5.A). Textures of Pv are weaker since Pv is much stronger than Ca-Pv and ferropericlase. Minimal texturing is seen in cubic Ca-Pv (Fig 5.B) and ferropericlase (Fig. 5.C) throughout the entire streamline with maxima of 3.5 m.r.d. at 2500 km and 115 GPa. During high temperature upwelling, the PPv and Pv textures remained stable while both Ca-Pv and ferropericlase textures were reduced. (001) planes of PPv preferentially align parallel to the core mantle boundary. Rotation of the aggregate material is observed in the final steps of the simulation, during upwelling of slab material.

P-waves are fast perpendicular to the core-mantle boundary (Fig. 5.D and Fig. 6). Anisotropy of P-wave velocities remains fairly stable throughout the streamline with intensities that align with the texture developed in both Pv and PPv. S-wave anisotropy, however, shows strong variability due to phase transitions. The forward Pv-PPv transition (steps 2-3, Fig. 5.E) leads to an immediate change in S-wave polarization, becoming dominantly horizontal and a S-wave anisotropy of 4.48% with $V_{SH} > V_{SV}$. With further deformation, anisotropy in PPv decreases to 4% with $V_{SH} > V_{SV}$ in sections where the slab is traveling parallel to the core mantle boundary at a depth of 2690 km. Velocity pole figures for the aggregate (Fig. 6) show that anisotropy from PPv texture development dominate at deep mantle conditions. At the Pv-PPv phase transition (steps 2-3) S-wave anisotropy increases immediately by over 1% and reaches a maximum of 3.07% (step 4). After the PPv-Pv transition fast S-wave polarization is no longer predominantly horizontal but maintains shear wave anisotropy of 3.0% just after the reverse phase transition. P wave anisotropy also reaches a maximum of 2% at step 4.
Figure 5: (001) Pole figures (A) Pv and PPV, (B) ferropericlase, and (C) Ca-Pv (scale in multiples of random distribution), (D) P-wave, (E) dS wave velocities ($S_1$-$S_2$) (ticks are orientation of fast S-wave polarization) along streamline intervals shown in Figure 2. Equal area projection. Core-mantle boundary is horizontal. Black lines indicate Pv-PPv and PPv-Pv phase transitions, respectively.
Figure 6: P-wave velocities (A), dS-wave velocities (S₁-S₂ where ticks are orientation of fast S-wave polarizations) (B) of 3 phase aggregate along streamline intervals shown in Figure 2. Equal area projection. Core-mantle boundary is horizontal. Black lines indicate Pv-PPv and PPv-Pv phase transitions, respectively.

4. Discussion
The goal of this study has been to link anisotropy in the deep mantle that has been observed by seismologists [10,12-16] to the evolution of mineral texture during convective deformations by combining geodynamic flow models with polycrystal plasticity. Earlier models [24-27] were refined by including variant selections during phase transitions and adjusting elastic properties to actual PT conditions. The model predicts strong texture patterns in Pv and PPv that develop rapidly during slab subduction. Texture is inherited across the Pv-PPv phase transition and remains stable as the slab travels along the core-mantle boundary. The deformation texture is further inherited and strengthened across the PPv-Pv phase transition. VPSC simulations also provide information about activity of slip systems as displayed in Figure 7. Ferropericlase is assumed to be the weakest phase (Table 1) and particularly 100<011> slip accounts for most of the strain, even though this phase only contributes 20% of the volume. (001) slip dominates in both Pv and PPv and is responsible for the (001) pole figure maximum. The c-axis orientations do not change during the phase transition, assuming a texture memory (Fig. 3). During strong texture development in PPv in Leg 2 there are significant changes in relative activities. Deformation of Ca-Pv is minimal. In this model only half of the deformation is achieved by dislocation glide with the rest accommodated by non-texture contributing mechanisms such as climb and grain boundary sliding.

The shear wave anisotropy of 0.01 to 3.07% predicted by the aggregate grain with \( V_{SH} > V_{SV} \) is consistent with seismic observations in the D layer in areas such as the circum-Pacific rim, Caribbean and Antarctic Ocean [10,13,14] and further corroborates that dominant (001) slip on PPv is a plausible cause for seismic anisotropy observed in the lower mantle. The low anisotropy in the upper part of the lower mantle can be attributed to relatively low single crystal anisotropy of Pv.
Figure 7: Slip system activity plotted against simulation time step along the tracer streamline. Legs 1 and 3 include Pv,MgO, CaPv (vertical columns 1 and 3) while Leg 2 includes PPV, MgO, CaPv (vertical column 2).

5. Conclusions
This study models texture development in a subducting slab traveling through the lower mantle of the Earth, combining a 3D geodynamic model with the visco-plastic self-consistent approach to polycrystal plasticity. The results portray a characteristic seismological pattern of anisotropy that is consistent with observations demonstrating the importance of an interdisciplinary approach using material science, mineral physics, and seismology to better understand deep Earth processes. Here a single tracer was used. Moving forward, the model will be extended to many tracers traversing the lower mantle and obtaining a topological map with seismic properties of areas consisting of subducted slabs as well as initiation of deep mantle plumes.

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