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**Seismic anisotropy, dominant slip systems and phase transitions in the lowermost mantle**

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**SUMMARY**

The presence of seismic anisotropy at the base of the Earth’s mantle is well established, but there is no consensus on the deformation mechanisms in lower mantle minerals that could explain it. Strong anisotropy in magnesium post-perovskite (pPv) has been invoked, but different studies disagree on the dominant slip systems at play. Here, we aim to further constrain this by implementing the most recent results from atomistic models and high-pressure deformation experiments, coupled with a realistic composition and a 3-D geodynamic model, to compare the resulting deformation-induced anisotropy with seismic observations of the lowermost mantle. We account for forward and reverse phase transitions from bridgmanite (Pv) to pPv. We find that pPv with either dominant (001) or (010) slip can both explain the seismically observed anisotropy in colder regions where downwellings turn to horizontal flow, but only a model with dominant (001) slip matches seismic observations at the root of hotter large-scale upwellings. Allowing for partial melt does not change these conclusions, while it significantly increases the strength of anisotropy and reduces shear and compressional velocities at the base of upwellings.

**Key words:** Phase transitions; Plasticity, diffusion, and creep; Mantle processes; Seismic anisotropy; Rheology: mantle.

**1 INTRODUCTION**

The deepest 200–300 km of the Earth’s mantle form a complex thermal and mechanical boundary layer, D” (Bullen 1949), where the dynamics remain surprisingly elusive. Our current understanding of D” is guided by seismological observations which indicate the presence of significant laterally varying shear wave anisotropy in this region, in contrast to the bulk of the lower mantle which is largely isotropic (see review by Romanowicz & Wenk 2017). Indeed, it has been proposed that large strains during flow in the deep mantle could lead to crystal preferred orientation (CPO) of anisotropic minerals (also referred to as texture) such as the high-pressure magnesium post-perovskite (pPv), which could explain the seismic anisotropy observations (e.g. McNamara et al. 2002, 2003; Wenk et al. 2011).

Most seismological studies of D” anisotropy rely on splitting measurements of shear waves diffracted (Sdiff) or reflected (ScS) on the core–mantle boundary (CMB, Nowacki et al. 2011), as well as core phases SKS/SKKS (Long 2009; Nowacki et al. 2011). While such data sample the D” locally, the limited available earthquake source and receiver locations restrict azimuthal coverage. Their interpretation thus relies on simplified models of anisotropy, mainly vertically transverse isotropy (VTI, also referred to as radial anisotropy), in which the speeds of horizontally and vertically polarized waves are different ($V_{SH}$ and $V_{SV}$, respectively). In general, $V_{SH} > V_{SV}$ is found in regions of faster than average isotropic shear wave velocity ($V_{Siso}$), as imaged by seismic tomography, and attributed to the ‘graveyard’ of cold slabs. In contrast, $V_{SH} < V_{SV}$ or no significant splitting is found in regions of slower than average $V_{Siso}$ such as the large low shear velocity provinces (LLSVPs) beneath the central Pacific and Africa (e.g. Cottaar & Romanowicz 2013; Lynner & Long 2014, Fig. 1). There have also been some attempts at resolving a tilted fast axis of anisotropy (TTI, e.g. Garner et al. 2004; Pisconti et al. 2019).

While CPO could explain the observed anisotropy, consensus has yet to be reached on the underlying deformation mechanisms that could give rise to the observed bulk anisotropic signatures (Cottaar et al. 2014; Walker et al. 2018; Tommasi et al. 2018). Some studies propose that (010) is the preferred slip plane in pPv, as found from theoretical computations (Goryaeva et al. 2016; 2017), while

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in proportions consistent with a pyrolite composition; (2) we introduce a layer of intrinsically denser-than-average material at the base of the mantle, which is pushed around by the descending slab into thick thermochemical piles, from which upwellings initiate, which allows us to examine the character of the resulting seismic anisotropy and isotropic velocities ($V_{Siso}$), not only in the downwelling part of the slab but also in the region of onset of upwelling; (3) assuming pressure ($P$) as inferred from the Preliminary Reference Earth Model (PREM, Dziewonski & Anderson 1981) and considering temperature ($T$) variations throughout the geodynamic model, we take into account forward (Pv to PPv) and reverse (PPv to Pv) phase transitions in the lowermost mantle and the associated texture inheritance that may occur; and lastly 4) we introduce partial melting in the deepest portions of the slab at the base of upwelling. We then compare two scenarios, which differ by the choice of dominant slip systems for PPv, (001) slip for Model 001 (Miyagi et al. 2010; Wu et al. 2017), and (010) slip for Model 010 (Goryaeva et al. 2016, 2017; Tommasi et al. 2018). We extract maps of radial anisotropy described by the parameter $\xi = (V_{Sh}/V_{SV})^2$ and also compute wave splitting (SWS) directions and strength of splitting (as $100 \cdot (V_{Sh}-V_{SV})/(V_{Sh}+V_{SV})$) of a seismic wave that propagates horizontally in D"{o}, such as Sdiff or ScS.

2 METHODS

2.1 3-D geodynamic model

Originally 2-D geodynamic models were applied to predict seismic anisotropy in the upper part of the lower mantle (Wenk et al. 2006) and the D"{o} zone (Wenk et al. 2011). Here, we focus on 3-D simulations. As the 3-D geodynamic model (Cottaar et al. 2014; Li & Zhong 2017) provides the framework for the macroscopic deformation, it will be described first. The geodynamic model used here was developed using a modified version of CitcomCU under the standard Boussinesq approximation for solving the non-dimensional equations of mass, momentum, and energy (eqs 1–3, e.g. Zhong 2006) along the same lines as previous works (Cottaar et al. 2014).

\[ \nabla \cdot \vec{u} = 0 \]  
\[ - \nabla P + \nabla \cdot (\eta \hat{e}) = Ra (T - BC) \hat{r} \]  
\[ \frac{\partial T}{\partial t} + (\vec{u} \cdot \nabla) T = \nabla^2 T + H, \]  

where $\vec{u}$ is the velocity, $P$ is the pressure, $\eta$ is the viscosity, $\hat{e}$ is the strain rate, $Ra$ is the Rayleigh number, $T$ is the temperature, $B$ is the buoyancy number, $C$ is the composition, $\hat{r}$ is a unit vector in radial direction, $t$ is the time and $H$ is the internal heating rate. The Rayleigh number is defined as:

\[ Ra = \frac{\rho g a \Delta T R^3}{\kappa \eta_0}, \]  

where $\rho$, $g$, $a$, $\kappa$ and $\eta_0$ are, respectively, the reference density, gravitational acceleration, thermal expansivity, thermal diffusivity and reference viscosity. The $\Delta T$ is the reference temperature which equals to the temperature different between the surface and the CMB. $R$ is the Earth’s radius. In this study, we use $Ra = 5.36 \times 10^8$. The buoyancy number is defined as:

\[ B = \frac{\Delta \rho}{\rho a \Delta T}. \]
Table 1. Geodynamic parameters used in this study.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Reference value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Earth’s radius, $R$</td>
<td>6371 km</td>
</tr>
<tr>
<td>Mantle thickness</td>
<td>2890 km</td>
</tr>
<tr>
<td>Mantle density, $\rho$</td>
<td>3300 kg m$^{-3}$</td>
</tr>
<tr>
<td>Thermal expansivity, $\alpha$</td>
<td>$3 \times 10^{-5}$ K$^{-1}$</td>
</tr>
<tr>
<td>Thermal diffusivity, $\kappa$</td>
<td>$1 \times 10^{-6}$ m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>Gravitational acceleration, $g$</td>
<td>9.8 m$^2$ s$^{-2}$</td>
</tr>
<tr>
<td>Temperature change across the mantle, $\Delta T$</td>
<td>3000 K</td>
</tr>
<tr>
<td>Reference viscosity, $\eta_0$</td>
<td>$1.4 \times 10^{11}$ Pa s</td>
</tr>
</tbody>
</table>

where $\Delta \rho$ is the density anomaly with respect to the background mantle. The physical parameters used in the geodynamic model are listed in Table 1.

The model domain has a longitude range of $-120^\circ$ to $120^\circ$, a latitude range of $-60^\circ$ to $60^\circ$, and a depth ranging from the surface to the CMB (Figs 2a and b). There are 128, 256 and 512 elements in the radial, latitudinal and longitudinal directions, respectively. All boundaries are free-slip except the surface which has a southward constant angular velocity of 3 cm yr$^{-1}$. The surface velocity is zero outside the subducting plate.

The viscosity is both temperature- and depth-dependent and is defined as:

$$\eta = \eta(r) \exp[A(0.6 − T)],$$

where $A$ is the dimensionless activation energy and we use $A = 9.21$, which corresponds to a dimensionless activation energy of $\sim 190$ kJ mol$^{-1}$. The $\eta(r)$ is the depth-dependent viscosity pre-factor as a function of the dimensionless radius $r$, and is given by:

$$\eta(r) = \begin{cases} 
1.0, & r > 0.8964 \\
30 \times (24.1 - 25.7r), & r \leq 0.8964 
\end{cases}$$

such that the $\eta(r)$ increases from 1.0 to 30.0 across the 660 km discontinuity, as suggested by (Hager 1984), and it continues to increase linearly by 10 times from 660 km to the CMB, similar to that in (Li & Zhong 2017).

Adding complexity to our previously presented models which focused only on slab impingement on the CMB (Cottaar et al. 2014), here, a global layer of intrinsically dense material is introduced initially at the bottom of the mantle, with a thickness of 300 km and a buoyancy number of $B = 0.8$ (i.e. $\Delta \rho/\rho = 2.4 \%$). This dense material is later pushed by a subducted slab into thermochemical piles in the lowermost mantle (green structure in Figs 3a–c).

Passive Lagrangian tracers are allowed to subduct with slab material and record the velocity gradient (and therefore strain rate as shown in Figs 3d and e) at each time step which are then used to calculate the resultant deformation within the aggregate. The position, temperature, and velocity gradient at each time-step is then extracted and combined with the radial pressure provided by PREM, which is interpolated to each passive tracer within the model. A surface temperature of 273.5 K and an average adiabatic temperature gradient of 0.35 K km$^{-1}$ are applied when converting non-dimensional temperatures to dimensional temperatures at passive Lagrangian tracers, and tracers at the CMB have a dimensional temperature of 4285 K. The path-lines of tracers used in this study were selected based on a spatial distribution to sample various deformation geometries present in the slab. Therefore, 25 individual path-lines were selected with multiple sampling from areas including (1) paths nearest to the CMB, (2) paths near the edge of the slab that may experience effects due to the spreading of the slab as it impacts the CMB, (3) areas within the bulk of the slab (away from edges) and (4) sections of the top layer of the slab that fail to meet the phase transition criteria depicted in Fig. 4(a). These path-lines all begin above 1000 km depth and end at various heights above the CMB in the upwelling area (radial depths of 1200–2000 km) and contain between 400 and 600 deformation steps. Note that this geodynamic model does not include any information about texture development which may alter the flow path. It treats the mantle as a homogeneous isotropic medium. We will address this issue later.

2.2 Plastic deformation within the slab

Here we assume a pyrolite composition of 3 phases (17 % periclase (MgO), 9 % CaSiO$_3$ (CaPv) and 74 % bridgmanite (Pv) which transforms to post-perovskite (pPv) in D*). The aggregate entered into each path-line is represented by an initial set of 1000 randomly oriented spherical grains which are plastically deformed according to the recorded velocity gradient along the slab’s subduction using the viscoplastic self-consistent deformation code VPSC (Lebensohn & Tomé 1993). This approach allows us to simulate the plastic deformation of aggregate material by solving the constitutive equations under the Eshelby inclusion formalism in which an inclusion (here a grain) is imbedded in a fully anisotropic, yet homogenous, medium (Eshelby 1957). Each grain is subjected to external stresses and strains and the resulting deformation is caused by slip of dislocations on various slip systems. The strain rate $\dot{\varepsilon}$ is related to the applied stress $\sigma$ according to the power law $\dot{\varepsilon} \propto \sigma^m$. Here we
assume a stress exponent $n = 3$, corresponding to the dislocation creep regime. Although various deformation mechanisms have been proposed to take place in the lower mantle such as pure dislocation climb (Boioli et al. 2017) and diffusion (Ammann et al. 2010), these mechanisms, contrary to dislocation glide, are considered not to produce significant crystal rotations, and can act to weaken existing CPO. Contributions from such non-rotational mechanisms are incorporated here indirectly by assuming 50% of the accrued strain to contribute to plastic deformation by dislocation glide as was done in our previous studies (Wenk et al. 2011; Cottaar et al. 2014). It has also been argued that diffusion creep may preserve CPO (Wheeler 2009) and furthermore that anisotropic diffusion can lead to the development of CPO (Dobson et al. 2019). Here, we concentrate only on the slab material itself where dislocation creep is expected to dominate (McNamara et al. 2003).

Plastic deformation occurs on a specific slip system when the applied stress exceeds the critical resolved shear stress (CRSS). Values used in this model for each assumed active system are shown for each phase in Table 2. In reality CRSS changes with deformation and temperature but we keep it constant for the whole deformation path. We use values of Amodeo et al. (2011) for pure end member MgO, of Mainprice et al. (2008) for Pv, of Miyagi et al. (2009) for CaSiO3 and two variations of slip systems for the pPv phase. Model 001 contains systems based on high pressure experiments by Miyagi et al. (2011) while Model 010 is based on ab-initio calculations of Goryeva et al. (2016, 2017) also used by Tommasi et al. (2018). For all phases a lowest CRSS of 1 was assigned, even though there is some evidence that MgO may be weaker (e.g. Miyagi & Wenk 2016; Kasemer et al. 2020). We keep this at value at 1 to conform with Tommasi et al. (2018). Since MgO and CaPv
are minor phases, the impact on the macroscopic picture is not very significant. Also note that for Pv and pPv an artificial slip system \{111\}<010> had to be included with high CRSS to close the yield surface and prevent singularities in VPSC. VPSC proceeds by iterating between measuring the response of individual grains based on the input slip systems and the mean response of the bulk ‘effective’ medium and finds the consistent solution. Grains begin with an assumed spherical shape and are allowed to deform to a ratio of 3:1, after which only grain rigid rotation is allowed in agreement with previous models (Cottaar et al. 2014). Choosing a smaller ratio would lead to the texture developing earlier at the same strain rate, that is rigid rotation would occur sooner. This effect would increase the magnitude of anisotropy but not necessarily the signature of fast and slow directions. Furthermore, grains do not have the same shape, and the elongation varies due to the grain scale strain.

Also, no strain hardening is implemented. Although it is anticipated that the CRSS values would evolve with the P, T conditions in the lower mantle (Lin et al. 2019), we do not account for this in the present study because of lack of data. Furthermore, dynamic recrystallization is not taken into account in the current model even though it may be an important mechanism at lower mantle conditions. It can be incorporated in VPSC calculations (e.g. Wenk & Tomé 1999) but there is no experimental information to define controlling parameters.

From the resultant orientations after deformation along path-lines in steps, a 3-D orientation distribution (ODF) is calculated, and from it we obtain pole figures which are displayed in upper hemisphere projection (Figs 3d–e for a selected path-line), using the MTEX software package (Bachmann et al. 2010).

The pressure P (obtained through interpolation using PREM) and temperature T (obtained from the geodynamic model) are combined with a chosen Clapeyron slope for the Pv–pPv phase boundary of 11.2 MPa K\(^{-1}\) (Oganov & Ono 2004; Tsuchiya et al. 2004; Hirose et al. 2006) is applied to each path-line (illustrated for a single path-line in Fig. 4a) to find the location of forward and reverse phase transitions. If the transition conditions are met by a tracer crossing into the pPv stability zone, all Pv for that tracer transforms into pPv. During epitaxial phase transitions there are well-defined orientation relationships which are generally described by rotation matrices and there may be several variants which, especially under stress, are differently activated (e.g. Yue et al. 2019). Here we assume orientation relations described by Dobson et al. (2013) for the Pv–pPv transition where the crystal c-axis is maintained but there are two variants of a-axes. An original orientation \([\phi_1, \Phi, \phi_2]\) (Bunge convention) splits into two orientations \([\phi_1, \Phi, \phi_2 + \omega]\) and \([\phi_1, \Phi, \phi_2 - \omega]\) with \(\omega = 72.94^\circ\). After the phase transition, the new phase grains start from a spherical shape. We assume that both variants are equally active, regardless of orientation. Therefore, the number of orientations used in the VPSC calculations doubles during phase transitions, both P–pPv and pPv–Pv. To maintain the grain fractions of each phase, the number of MgO and CaPv grains are doubled again, resulting in 4000 grains at the end of the calculations.

2.3 Estimations of elastic properties and absolute velocities

To obtain elastic constants and seismic velocities of the 3-phase aggregate, we need to know elastic constants of single crystals. Here we use constants for pure end-members: MgO (Karki et al. 2000), CaPv (Kawai & Tsuchiya 2009) and Pv and pPv (Zhang et al. 2016) due to the availability of data at various P–T conditions. Where in previous models the evolution of the elastic constants with increasing P–T were not considered and a constant reference value was used (Cottaar et al. 2014; Wenk et al. 2011), in this study the elastic tensor components of each phase were interpolated to each P–T condition along the path-lines at every deformation step using the first and second derivatives in P and T. After each deformation step (which occurs at every recorded point along each path-line),

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Table 2. Deformation mechanisms (slip systems) and relative CRSS values used for each model in this study. Relative CRSS values are provided for each system. (a) Mainprice et al. (2008), (b) Amodeo et al. (2011), (c) Miyagi et al. (2009), (d) Miyagi et al. (2011), (e) Goryaeva et al. (2016, 2017). Slip system activity (per cent) which represents the sum of relative amounts of shear contributed by each phase is given at two locations along a selected path-line at 200 steps after initiation and then 100 steps after the Pv–pPv transition.

| Phase % | Slip system | CRSS | Act. % Step 200 | Act. % 100 steps after transition | Phase % | Slip system | CRSS | Act. % Step 200 | Act. % 100 steps after transition**
<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pv(^{\ast}) 74 %</td>
<td>(010)[100]</td>
<td>1.8</td>
<td>2.6</td>
<td>*</td>
<td>MgO(^{\ast\ast})</td>
<td>{110}&lt;110&gt;</td>
<td>1</td>
<td>14.4</td>
<td>16.4</td>
</tr>
<tr>
<td>(001)[100]</td>
<td>2.5</td>
<td>5.6</td>
<td>*</td>
<td>17 %</td>
<td>(010)&lt;110&gt;</td>
<td>1</td>
<td>10.2</td>
<td>10.9</td>
<td></td>
</tr>
<tr>
<td>(100)[010]</td>
<td>1</td>
<td>15.4</td>
<td>*</td>
<td>1</td>
<td>(111)&lt;110&gt;</td>
<td>g</td>
<td>4.7</td>
<td>5.2</td>
<td></td>
</tr>
<tr>
<td>(001)[010]</td>
<td>2.6</td>
<td>*</td>
<td></td>
<td>29.3</td>
<td>32.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(100)[001]</td>
<td>3.8</td>
<td>1.6</td>
<td>*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(010)[001]</td>
<td>1.6</td>
<td>5.1</td>
<td>*</td>
<td>CaPv(^{\ast\ast})</td>
<td>{110}&lt;110&gt;</td>
<td>1</td>
<td>5.7</td>
<td>6.4</td>
<td></td>
</tr>
<tr>
<td>[110]&lt;010&gt;</td>
<td>1.9</td>
<td>7.6</td>
<td>*</td>
<td>9 %</td>
<td>(100)&lt;110&gt;</td>
<td>1.5</td>
<td>4.5</td>
<td>5.4</td>
<td></td>
</tr>
<tr>
<td>(001)&lt;100&gt;</td>
<td>1.8</td>
<td>8.1</td>
<td>*</td>
<td></td>
<td></td>
<td>(110)&lt;110&gt;</td>
<td>3.0</td>
<td>0.7</td>
<td>0.9</td>
</tr>
<tr>
<td>[110]&lt;110&gt;</td>
<td>2.0</td>
<td>11.2</td>
<td>*</td>
<td>Total (%)</td>
<td>10.9</td>
<td>12.7</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| Total (%) | 59.8 |

| pPv\(^{\ast}\) 001 74 % | (010)[100] | 4 | * | 1.1 | pPv\(^{\ast}\) | (010)[100] | 1 | * | 22.4 |
| (001)[001] | 4 | * | 9.8 | 010 | (010)[001] | 1 | * | 19.5 |
| (100)[010] | 2 | * | 18.2 | 74 % | (011)[100] | 10 | * | 2.9 |
| (100)[001] | 2 | * | 8.9 | (001)[100] | 20 | * | 0.0 |
| (001)[100] | 1 | * | 20.3 | \{110\}<110> | 3 | * | 10.0 |
| (001)[010] | 1.5 | * | 1.0 | \{111\}<110> | 50 | * | 0.0 |
| [110]<110> | 3 | * | 0.0 | \{111\}<011> | 50 | * | 0.0 |
| [110]<001> | 4 | * | 0.8 | Total (%) | 54.8 |

| Total (%) | 60.1 |

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*Indicates phase not present.
**MgO and CaPv activities taken from 010 model.
the resulting crystal orientations were combined with the respective elastic tensor through the self-consistent formalism used in VPSC to determine the elastic properties of the aggregate (Lebensohn et al. 2007). The self-consistent approach used here provides estimates of the aggregate elastic tensor with values that fall between the Voigt upper bound, which assumes the local strain in the aggregate is constant everywhere (i.e. iso strain) and the Reuss lower bound, formulated under the assumption that the local stress is constant everywhere (e.g. Kocks et al. 2000, pp. 303–305). At each time step along a path-line, the self-consistent aggregate elastic tensor is represented in a 6×6 matrix (21 independent values, $C_{ij}$), in Voigt notation, so that each data point in the model space is described by a set of 27 values ($\theta$, $\varphi$, $r$, $T$, $P$, $C_{ij}$, $\rho$). The number of data points in each of the 25 path-lines varies depending on the length of each path-line with values ranging from 350 to 580 data points per path-line resulting in over 10 000 data points throughout the model space. The radial anisotropy parameter $\xi$ which compares the ratio of speeds of horizontally and vertically polarized shear waves was calculated from each aggregate elastic tensor at all points for both models using the following equation (Browaays & Chevrot 2004).

$$\xi = \frac{V_{SH}^2}{V_{SV}^2} = \frac{V_{SH}^2}{V_{SV}^2} = \frac{\frac{1}{2} (C_{11} + C_{22}) - \left(\frac{1}{6} C_{12}\right) + \left(\frac{1}{2} C_{44}\right)}{\frac{1}{2} (C_{55} + C_{66})}. \quad (8)$$

Determining the aggregate isotropic velocities requires estimations of the density of the individual phases. We obtain the density of each phase at several pressures and temperatures from the literature also used to determine the elastic properties and it was then interpolated to all points within the model, together with each elastic tensor, based on pressure and temperature. As directly constraining the isotropic velocities, composition, and density are beyond the scope of this investigation, we compare the calculated isotropic velocities with PREM as a guide to the applicability of our model to observations, for example areas of faster and slower $V_{Siso}$ than the 1-D average. The calculated absolute velocities from the model were compared to PREM and the change of $V_S$ (d$V_S$) was calculated at each point along each path-line while the shear wave splitting (SWS) and radial anisotropy was compared to seismic observations of the lower mantle. SWS and $V_{Siso}$ were computed using the MSAT software package (Walker & Wookey 2012) at selected points that sample different deformation geometries/flow patterns along each path-line.

### 2.4 Addition of partial melting

In order to gain insight into the effects of partial melting that may occur at the base of upwellings, we compared the experimental data of Nomura et al. (2014) which looked at the melting conditions of a pyrolytic sample across the whole range of lower mantle conditions with the $P$-$T$ conditions within our model to determine model locations where partial melting may occur along each path-line. A rough approximation of the properties of a silicate-based partial melt were implemented by incorporating a phase making up a volume fraction of 1–15% of the aggregate that has the rough elastic properties of a silicate melt (Williams & Garnero 1996) and a shear modulus of 0. This phase was given the slip systems of a symmetric cubic crystal with critically resolved shear stress (CRSS) values of 0.01 (relatively no resistance compared to the other phases present) and an initial aspect ratio of 0.1 to simulate an equilibrium melt texture. The elastic properties were approximated under the assumption of isotropic elasticity (Babuska & Cara 1991).

The volume fraction of melt was tested at 1, 5, 10 and 15%. An equivalent volume fraction was then removed from the $Pv$/$Psv$ phase to accommodate the added 1–15% of partial melt. Because the model space where partial melting is observed only varies in $T$ by at most 50 K and roughly 20 GPa, and due to a lack of $P$ and $T$ derivatives at lower mantle conditions for a partial melt, we do not impose $P$–$T$ variations in the elastic properties of the melt phase or the $P$–$T$ effects to the density but rather directly impose the experimental values. As the volume fraction of melt increases the melt density contribution to the aggregate density would increase and would have to be taken into account.

Here we do not intend to constrain precise effects but instead we aim to observe a first order approximation of the effect from the addition of melt. Moreover, at low percentages of partial melting, the choice of volume percent partitioning was found to have little effect on the calculated signature of anisotropy from the aggregate. This is to be expected since the signature is dominated by the $Pv$/$Psv$ phase where an expected loss of at most 15% volume fraction still makes it 40% more abundant than the second most prevalent phase, MgO. We are aware that this implementation is a rough approximation but argue that it provides insight into the effects on anisotropy at the onset of melting for low volume fractions. It also provides first order insight on the trends in isotropic velocities that could be expected in these high temperature areas, on the corresponding anisotropic signature of the aggregate, and also on the complicated signatures of anisotropy and velocities that may arise due to the presence of layering of phases atop a partial melt layer near the CMB.

### 3 RESULTS

#### 3.1 CPO evolution within the slab

The CPO evolution within the slab is dictated by the evolving strain rate as the slab moves into different flow regimes. For instance, during downwelling we find an average equivalent strain rate of $\sim1.15 \times 10^{-13} \text{ s}^{-1}$ and increasing by $\sim1.6 \times$ as the slab turns along the CMB (Fig. 3c), which leads to a rapid evolution of the CPO within the aggregate. The strain rate reaches a minimum once the slab material meets the pile but is then forced into upwelling flow and the rate of strain dramatically increases to $\sim8 \times 10^{-13} \text{ s}^{-1}$ (38× increase at a depth of 2296 km, $\sim500$ km above the CMB compared to the minimum value as the slab meets the pile) and then decreases as the material travels upward away from the CMB. Fig. 5 shows the crystal preferred orientation (CPO) developed along a selected path-line for both tested models at three important locations within the slab: (1) just before the $Pv$–$Psv$ transition (first row), (2) during horizontal flow along the CMB (rows 2–3) and (3) during upwelling (post reverse $Pv$–$Psv$ transition in rows 4–5). Both models are identical except for the dominant slip systems in the $Psv$ phase. The initial $Pv$ texture shows a strong (100) texture just prior to the phase transition $\sim8$ m.r.d. which is immediately dispersed once the phase transition is initiated. After the phase transition occurs (signified by horizontal black lines in Fig. 5), Model 001 develops a steady increase of an (001) maximum orthogonal to the material flow direction due to ‘textural inheritance’ from the (001) maximum developed in the parent $Pv$ phase. While Model 010 shares an (010) distribution similar to that of Model 001, albeit weaker, the normals to the (001) and (100) lattice planes are nearly orthogonal between the two models. The secondary cubic phases MgO and CaPv both develop CPO in a girdled fashion with maxima nearly aligned with the flow direction attaining a maximum of $\sim5$ m.r.d. during downwelling,
that is maintained throughout the simulation. Table 2 shows the slip system activity for each phase as a percent which defines the relative contribution of each slip system to the total shear. The minor phases are found to be slightly more active in Model 010 making up 45.2% of the slip activity compared to 39.9% in Model 001 (Table 2). After the reverse pPv–Pv phase transition, the (001) texture is again inherited into the daughter Pv phase and continues to increase in strength as well as rotate with the flow direction for Model 001, reaching a maximum of ∼10 m.r.d. By contrast Model 010 sees an initial dispersion of CPO just after the reverse phase transition and only reaches a maximum of ∼4–5 m.r.d for any slip system in the volumetrically dominant Pv phase during upwelling.

3.2 Shear wave anisotropy

Given the weakly anisotropic elastic structure of the dominant Pv phase, we find that the initial downwelling part of the slab appears largely isotropic. The forward Pv–pPv transformation occurs over a range of 50 km (2550–2600 km) and leads to an abrupt jump in magnitude of both shear (∼1.5% on average, 3.5% max) and compressional (1.5–4.0%) wave velocities (Fig. 6). This recorded jump in isotropic velocities is accompanied by the appearance of a lower symmetry anisotropy than the generally assumed vertical transverse anisotropy (VTI, Fig. 7) with $V_{SH} > V_{SV}$ (i.e. $\xi > 1$, Figs 8a and b), with $\xi$ steadily increasing as the slab proceeds along the CMB, in both models, from a value of 1–3% (i.e. $\xi = 1.01 - 1.03$) to a maximum of ∼6% in the deepest parts of the slab, as it impinges on the CMB. Horizontal fast axis orientation (also region highlighted in red for presence of pPv in Figs 8(c) and (d)) continues throughout the region of horizontal flow along the CMB, in agreement with seismic observations in regions of slab graveyards (Panning & Romanowicz 2006; Sturgeon et al. 2019). Due to the 3-dimensional nature of the geodynamic model, we are able to investigate deformation arising from the heterogeneous strains imparted along different paths through the thickness of the slab such as edges, where spreading and rolling occur as the slab impacts and traverses the CMB near the edges of the simulated LLSVP resulting in varying depth and azimuthal anisotropic signatures. Here we find the plane of highest shear wave anisotropy has a tilted axis of symmetry (tilted transverse anisotropy (TTI)) with an inclination of up to ∼20–30° from the radial direction (vertical, Fig. 9, #3) similar to that observed at D” depths beneath the Caribbean (Garnero et al. 2004). Included in Fig. 8(b) is also a path-line (1) that fails to meet the phase transition conversion criteria and therefore retains the Pv phase. The Pv layer atop the slab exhibits a vertically oriented fast S-wave propagation.
direction orthogonal to the horizontally oriented fast S-wave of the underlying pPv.

Several studies (Williams & Garnero 1996; Simmons & Grand 2002; Yuan & Romanowicz 2017) have suggested that a small percentage of partial melt could explain the strongly decreased velocity signatures of ultra-low velocity zones (ULVZs). We investigated these effects in our model through the methods described in Section 2.4. Rough estimates on the elastic parameters of a silicate-based melt are incorporated to the aggregate at the determined locations. The onset of partial melting in the model was found to occur in the deepest portion of the slab near locations with the reverse pPv–Pv phase transition. We find the presence of as little as 1 % melt results in a ∼2.5 % decrease in P-wave velocity and ∼4 % decrease in S-wave velocity compared to the same path-lines without partial melting added. Increasing the melt per cent to 15 % leads to reductions in $F_S$ and $V_p$ of ∼18 and 7 %, respectively at the base of the upwelling (Figs 10 and 11). We observe a very small deviation in the direction of fast polarization in either model, but a strong increase in the amplitude of anisotropy (Fig. 12).

As slab material approaches the edge of the dense hot pile, the increase in $T$ initiates the reverse pPv–Pv transformation, which occurs at a range of depths depending on location in the model, but generally deeper (2595–2835 km) than for the forward transition, as anticipated due to the larger $T$ near the edge of the hot pile. This is where significant differences between the two pPv models emerge in both texture development as well as anisotropy (Figs 5–7): for Model 010, the fast axis direction with relatively larger SWS strength (∼1.0–3.0 %) remains horizontal after the reverse transition and the trend continues during the upwelling; Model 001, on the other hand, shows a complex pattern of mixed horizontal and vertical fast axis directions after the reverse pPv to P transition with ∼2.0 % of SWS strength, and a tilted fast axis with 1.0–2.0 % SWS strength in the upwelling segment (Fig. 7). Interestingly, a triple layering (Fig. 7) of varying shear wave polarization as well as isotropic velocities due to double crossing of the pPv phase boundary occurs over a 300 km depth range in Model 001. While the same triple layering of phases occurs in Model 010, the extreme reversal in fast propagation directions between layers is not as apparent. Also, Model 010 only presents small patches of $V_{SH} < V_{SV}$ at the base of the upwelling (red areas in a prevailing pattern of $V_{SH} > V_{SV}$ (blue areas) in the upwelling region). The latter is inconsistent with available seismic observations (e.g. Long 2009; Romanowicz & Wenk 2017).

4 DISCUSSION

4.1 Distribution of Pv and pPv in the lowermost mantle

By including cubic MgO and CaPv as well as both direct and reverse phase transition from Pv to pPv, we gain a more realistic representation of the complex aggregate thought to exist in the lowermost mantle. Furthermore, an interesting observation that arises due to the temperature variations in the model is the depth dependence of the Pv–pPv and pPv–Pv phase transitions. While the forward transition is found to only vary over ∼40 km in this model, the changes in elevation of the reverse transformation are much larger, ranging over a ∼200 km depth and 15° of colatitude along the slab’s path (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab (Fig. 13). This results in a situation where we find a ∼100–250 km wedge of lower-than-average isotropic velocity Pv on top of the CMB at the edge of the simulated pile located beneath the faster wedge of lower-than-average isotropic velocity Pv on top of the slab.
path-lines (depicted by path-line 1 in Fig. 9) show the effect of absence of the pPv transition and lead to very weak but vertically polarized shear waves being the fastest. This is at odds with previous studies (Cottaar et al. 2014) but this discrepancy is understandable due to the choice of dominant slip systems in the Pv phase with (001) dominant (Wenk et al. 2011) compared to a mix of (001) and (100) in this study based on Mainprice et al. (2008). Furthermore, in Cottaar et al. (2014) the intrinsically dense layer used in the current model was not present. This addition leads a drastic change in the local dynamics between models near the CMB. For instance, once the slab meets the CMB, without the thermochemical pile acting as an initiating point for upwelling the slab would have been able to spread further along the CMB. The lack of the pile would also affect the extent and location of the reverse pPv–Pv transition we observe in this model.

The viscosity of the pPv phase has also been debated, and a viscosity either greater (Karato 2010, 2011) or weaker (Ammann et al. 2010) than that of Pv has been proposed, which may have opposite effects on the dynamics in the D” and CMB regions. In the case of ‘weak’ pPv, Li et al. (2014) and Nakagawa & Tackley (2011), showed that slab material that reaches the CMB would spread more easily. In our model, the incorporation of a ‘weak’ pPv could potentially lead to a higher strain rate which would allow for a more rapid texture development of the local minerals. The weak pPv would also lead to a thinner thermal boundary layer beneath subduction regions above the CMB, which would widen the region of pPv stability in our model, since we include the reverse pPv–Pv transition and the amount of Pv along the CMB would possibly decrease. As mentioned above, we find that the newly formed Pv at the CMB has an anisotropic signature with $V_{SV} >$
4.2 Effect of phase transitions and partial melting on deformation and shear wave anisotropy

Along the lines of previous studies, we aim to identify models that are consistent with the long wavelength seismic anisotropy structure observed in D\". In previous studies (Wenk et al. 2011; Cottaar et al. 2014), we were able to provide evidence that dominant slip on 001 or 010 in a pPv+MgO+CaPv aggregate caused by convection-driven shear deformation could provide an explanation for the anisotropic signatures of D\". Those same studies showed that Pv alone as well as...
as dominant slip in (100) in the pPv phase could not reconcile the bulk seismic anisotropy signatures in the lowermost mantle and therefore we do not include those systems here. A more recent study performed by Tommasi et al. (2018) provided further evidence for (010) dominant slip by utilizing 2-D corner flow models similar to those of Wenk et al. (2011). They were able to show that an (010) dominant pPv phase was capable of explaining both a horizontal (to sub horizontal) fast shear wave polarization in D'' as well as a flow-directed fast direction in upwelling areas. A key aspect of the current study is the temperature dependence on the spatial presence of the pPv phase, and the corresponding phase transition which was not taken into account by Tommasi et al. (2018). In our model, pPv cannot exist thermodynamically in the hotter regions near the edges of the simulated LLSVPs, and therefore we conclude alternate explanations are needed to describe the observed anisotropy at the base of upwellings.

The current model corroborates the findings of Tommasi et al. (2018) and Ford & Long (2015) that dominant (010) slip in the pPv phase (our Model 010) can explain the anisotropic signature during the transition from downwellings to horizontal flow along the CMB but cannot reconcile signatures seen in areas of upwelling. Nowacki et al. (2010) also tested (001) and (010) dominant slip in pPv through comparison of the orientation of shear planes and slip directions of the two models and the measured differential shear wave splitting of S and ScS phases passing through D'' beneath the Caribbean. There they found the strongest correlation between (001) dominant slip in pPv but could not rule out (010) without further investigation. By incorporating the three flow regimes here (downwelling, horizontal flow, and upwelling) we are able to draw a clear distinction between (001) and (010) dominant slip. The difference between the two models tested here is due to the textural (001) inheritance across the pPv–Pv phase transition (Dobson et al. 2013) that occurs at the base of the upwelling section in Model 001, which leads to an increase in 001 texture intensity during upwelling flow (up to >10 m.r.d), aligning the aggregate fast direction of anisotropy, on average, near the material flow direction (Figs 7 and 8c). In contrast, in Model 010 there are two abrupt partitions of slip activity (Fig. 14b). At the forward Pv–pPv transition we see a
Figure 13. Spatial variation of forward (red dots) and reverse (black dots) phase transitions in the slab. 3-D visualization in a with 2-D in (b) and (c). When viewed from above (b) the spread of the reverse pPv–Pv transition is clearly identified. Grey area in c shows the pPv stability field within the slab highlighting the deeper penetrating path-lines reverting to Pv (near 90° Co latitude) compared to shallower paths (black dots at 75–80° Co latitude). Slab flow direction is shown by black arrows in all images.

Figure 14. Strain partitioning between Pv/pPv (blue) and MgO (red) and CaPv (black) measured as slip system activity (%) which represents the sum of relative amounts of shear contributed by each phase per simulation step for path-line 3 in Fig. 7 for (a) Model 001 and (b) Model 010. Shaded blue area represents the section of the path-line the pPv phase. Step 0 represents the start of the simulation and step 525 is at the end. Interestingly, in Model 010, there is sudden transfer of slip activity from Pv/pPv to MgO and CaPv at the phase transition points. This feature is also present in Model 001 but is suppressed due to the textural inheritance in the pPv phase.

Partition of ~15% of slip activity to the weaker MgO and CaPv phases due to the fact that pPv in Model 010, is in an unfavourable geometry for slip on its dominant mode (010) but in two directions [100] and [001]. But it is clearly seen that after the transition the (001) texture from the original Pv remains (Fig. 5 columns 3 and 8). A second partition happens after the reverse pPv–Pv transition, this time in the opposite direction and the newly formed Pv phase abruptly absorbs ~8% of the slip activity from the minor phases which is understandable seeing as the Pv in this study can accommodate slip on the three major planes (100) (010) or (001) in various directions. Ultimately, this leads to a substantially weaker preferred orientation in the Pv phase in Model 010 as well as to (010) and
(001) distributions orthogonal to those seen in Model 001 (Fig. 5), ultimately leading to the fast direction in PpV remaining near parallel to the CMB. This results in the dominantly horizontal fast direction of anisotropy, that is orthogonal to the flow direction during upwelling, at odds with seismic observations in the LLSPVs (e.g. Nowacki et al. 2011; Romanowicz & Wenk 2017). This is further illustrated by visualizing the lateral and depth dependent anisotropic structure in D” produced by the model as a whole similar to that done in 2-D by Wenk et al. (2011). If the effect of textural inheritance we find in Model 001 does occur in the lower mantle, then it would follow that the strength of anisotropy in D” due to PpV would be modulated by the amount of (001) texture that occurs in the precursor PpV phase, that is strong (001) texture in PpV would lead to a strong (001) starting texture in PpV, and therefore a strong anisotropic signature emanating from a PpV dominated aggregate. This scenario could explain the variation in strength of anisotropy in areas of suspected PpV. Also, including the P–T dependent phase transition, we find a complicated mix of vertically and horizontally polarized shear waves dominating in the hottest regions at the base of the slab (bottom of Fig. 8), where lateral temperature variations induce reversion to PpV in some locations but not others, a feature not seen in our previous studies but consistent with seismic observations (Romanowicz & Wenk 2017; Nowacki et al. 2011). Beyond these differences however, and although we introduce more realistic complexity, even when including the PpV–PpV–PpV transition pathway, our Model 001 correlates to the PpV C model proposed in Cottaar et al. (2014), with fast shear propagation directions aligning near the flow direction through all three flow types of the model (downwelling, horizontal flow, upwelling).

We also tested a case in which the phase transition does not follow the toptothermal relationship of Dobson et al. (2013) but instead its occurrence results in randomization of the newly introduced grains in the PpV (or PpV). Because PpV (or PpV) heavily dominates the volume fraction of the aggregate, this has the overall effect of decreasing the magnitude of the calculated anisotropy to near isotropic, with the anisotropy increasing near the end of horizontal flow, which is then removed by the randomization once again at the reverse PpV–PpV transformation at the base up upwelling. Both results are in disagreement with the magnitudes of anisotropy observed in D”.

We not only investigate the anisotropy developed along individual path-lines, but also collapse each deformed aggregate elastic tensor into its scalar $\xi = (\xi_{SH})^2$ value at over 10,000 points within the model which allows for a volumetric mapping of the radially anisotropic structure of the slab in Model 001 and Model 010 (Fig. 15). This approach provides a volumetric image of the anisotropic structure of the slab with clear demarcations in the change from $V_{SH} > V_{SV}$ (blue) during horizontal flow along the CMB to areas of $V_{SV} > V_{SH}$ (red) during upwelling flow for Model 001 (a–d) while Model 001 only shows small patches of $V_{SV} > V_{SH}$ in those areas (Fig. 15h).

As for the secondary phases, although MgO exhibits strong shear wave anisotropy (Marquardt et al. 2009), and at 19% volume fraction accommodates between 25 and 35% of the strain in this model, while the overall signature of anisotropy is dictated by the abundance of the PpV/pPpV phase, which makes up 73% of the aggregate and the fact that in cubic MgO, velocity values are spread in three vertically identical directions. The resulting patterns of shear wave anisotropy we find here in D” are very similar to those calculated in previous models (Wu et al. 2017; Zhang et al. 2016) when accounting for 001 slip in the pPpV phase. The addition of the also cubic CaPv appears to reduce the amplitude of anisotropy, compared to the case where only a combination of PpV and MgO was considered (Cottaar et al. 2014) but has a minimal effect otherwise.

In our model, thermal variations at the base of the pile meet the conditions necessary for partial melting to occur, which then acts to decrease the absolute velocities for both P and S waves (Fig. 10) while increasing the magnitude of anisotropy of the plastically deformed aggregate. This is consistent with seismic observations near the edges of LLSPVs at D” depths (Lynner & Long 2014) using SK/IDK/S observations along the edge of the African LLSPV. While splitting was observed near the edges, that study found little or no splitting for phases that pass through the LLSPV, also in agreement with Cottaar & Romanowicz (2013). This led the authors to infer that deformation may only occur along the LLSPV edge while the interior possibly remains relatively undeformed. While in our model, we do not sample the interior of the simulated LLSPV but instead concentrate only on the slab material near the edge of the pile, that is deflected upward by its presence, future models should incorporate anisotropic signatures from material surrounding the slab. This will allow further investigation and comparison between the upwelling slab material and the signature arising from the pile interior.

4.3 Limitations

While this revised model incorporates many new features, still, our model relies on several simplifications and assumptions. The geodynamic model assumes a homogeneous isotropic viscous medium and does not take texture evolution into account nor does the geodynamic model include effects of partial melting or hydrous phases. CPO is introduced a posteriori based on the recorded velocity gradients. In one of the first studies of texture evolution in a convecting mantle with finite element methods (Blackman et al. 1996; Dawson & Wenk 2000) it was illustrated that plastic anisotropy can have a large effect on convection, causing local curling and stagnation. In the future one should consider introducing plastic anisotropy into the geodynamic model. Even if PpV in the lower mantle is elastically fairly isotropic, our modelling shows that it is plastically very anisotropic, with strong texture development (e.g. Fig. 4 top).

We assume that the mantle is a homogeneous medium of PREM composition. This is clearly a simplification as recent geochemical investigations suggest, with regions of peridotitic composition but others of eclogitic composition (e.g. Gleeson & Gibbons 2019; Gleeson et al. 2020) and also a mixed composition of high-density mid-ocean ridge basalts (MORB) and lower density harzburgite which causes slab rotation, placing the MORB layer along the CMB (Tackley 2011). Some studies have mentioned evidence for minor phases in the deep Earth such as the hexagonal H-phase (Zhang et al. 2014) resulting from the Fe disproportionation in iron bearing PpV to an iron depleted PpV + iron rich H-phase, or seifertite (Zhang et al. 2016) coexisting with PpV. Our model incorporates only pure end-member and dry, phases, while Nomura et al. (2014) conducted their study on a sample containing iron as well as 400 ppm H2O. The partitioning of water could affect the ease of deformation in the dominant PpV and PpV phases, although investigations into hydrolytic weakening of mantle minerals (Muir & Brodholt 2018) found that at low ppm (sub 200 ppm) water tends to partition to the PpV phases, while at higher amounts, water should move to the CaPv phase. Also, the use of pure end-member phases neglects the effects of phenomena such as electronic spin transitions observed in (Mg,Fe)O at lower mantle conditions (e.g. Antonangeli et al. 2011; Yang et al. 2015;
Figure 15. Volumetric mapping of radial anisotropic parameter ($\xi = (V_{SH}/V_{SV})^2$) within the slab for Model 001 (a–d) and Model 010 (e–f) showing (a), an oblique view of slab volume showing $\xi > 1$ indicated by iso-contour of constant $\xi = 1.02$ (2% $V_{SH}$ fast) and (b) area of slab with $\xi < 1$ indicated by iso-contour of $\xi = 0.98$ (2% $V_{SV}$ fast). (c–d) viewed from above with the pPv–Pv reverse phase transition demarcated by yellow line. Figure bound values indicated by the color. Cartoon slabs on the right guide the reader about slab flow direction with 3-D velocity projection of $S$-wave anisotropy shown for each flow section for both models. Vertical axis shows depth in km while the colatitude ($y$) and longitude ($x$) were converted to Cartesian coordinates during the meshing process.

Texture simulations with VPSC assume that plastic deformation occurs purely by dislocation glide. Without constraints on the amount of contribution from non-rotational deformation mechanisms in the lower mantle, we assume that only 50% of the strain causes crystal rotations. But other mechanisms are ignored such as diffusion resulting in grain growth which is particularly significant in polyphase materials as was explored experimentally (e.g. Marquardt & Miyagi 2015; Chandler et al. 2021) and with finite element models (Kasemer et al. 2020). For example, in Pv–MgO aggregates softer MgO appears to develop minimal CPO. This leads us to the mechanism of dynamic recrystallization—nucleation of new grains and grain growth—which likely plays a significant role at lower mantle conditions. It was introduced into the VPSC model (e.g. Wenk et al. 1997; Wenk & Tomé 1999) and applied to upper mantle convection (Blackman et al. 2002), but so far never used for lower mantle models, largely because of lack of experimental data.

Furthermore, although we incorporated phase-transformations into the deformation model, the associated energetic effects (Oganov & Ono 2004) as well as the choice of Clapeyron slope of this transition could have significant effects on the local temperature and viscosity and therefore strain rates and active deformation mechanisms within the slab. Further studies are needed to address these technically challenging questions, coupled with more detailed measurements of seismic anisotropy at the edges of and within mantle upwellings.
Our incorporation of melting remains a first approximation and includes two large assumptions (1) We do not account for any increased density effect due to Fe that may occur in the melt and which may increase any velocity reductions we suggest in our model and (2) when testing various amounts of melt in our model we do not adjust the density of the aggregate. We feel this assumption is valid for less than 5% of melt as it is anticipated that the density of a pure end-member melt at these conditions would have a similar density to that of the surrounding aggregate and fluctuations of a few % or less would have little effect on the density contribution to the calculated anisotropy. Future geodynamic models which include the addition of partial melting would however have the effect of lowering the viscosity where melt is located which could act to increase the strain rate locally imparting accelerated effects on texture development as well as the calculated anisotropy of the aggregate.

5 CONCLUSIONS

We have modelled the effect of both forward and reverse Pv–pPv phase transitions and partial melting on seismic anisotropy in a subducting slab being deformed along the CMB as well as areas of upwelling. Our study provides insights on how phase transformations in the Pv–pPv system and temperature variations related to dynamic flow patterns contribute to explaining the observed seismic anisotropy patterns in the deep mantle. We find that incorporating a texture inheritance for the forward and reverse Pv–pPv phase transitions is significant for interpreting observations of seismic anisotropy in D″. We argue that Pv alone cannot produce the combination of isotropic shear velocities and anisotopic signatures seen in D″ and therefore another phase or factor must contribute. We find that only a model with (001) dominant slip for pPv provides results consistent with a strong but complicated anisotropy, with $V_{SH} > V_{SV}$ in regions of faster than average isotropic $V_s$ (e.g. graveyards of slabs), a tilted fast axis of anisotropy near the borders of the LLSVPs and flow-aligned or absent anisotropy as observed in hotter than average regions of upwelling.

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Author Contribution: All authors contributed to the vision and design of the project and to the resulting analysis. BC developed the codes for visualization and performed the mineral physics and seismological calculations with the assistance of LC. ML conducted the geodynamic modelling experiments. All authors contributed to writing the paper.

COMPETING INTERESTS

The authors declare no competing interests.

DATA AVAILABILITY STATEMENT

The data underlying this paper will be shared on reasonable request to the corresponding author.

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Seismic anisotropy in the lowermost mantle


