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Original Citation:

Availability: This version is available at: 11577/3328375 since: 2020-11-27T17:11:57Z

Publisher: Blackwell Publishing Ltd

Published version: DOI: 10.1029/2019GC008462

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### On the origin of radial anisotropy near subducted slabs in the mid-mantle

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11	Key Points:
12	- Geodynamical modeling of anisotropy around slabs shows $V_{SV} > V_{SH}$ in the tran-
13	sition zone and $V_{SH} > V_{SV}$ in the topmost lower mantle.
14	• Shape-preferred orientation calculations do not fit seismic observations well, no-
15	tably for deeply penetrating slabs.
16	• Four possible easy slip systems of bridgmanite are found, agreeing with recent lab-
17	oratory experiments.

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#### 18 Abstract

Recent seismic studies indicate the presence of seismic anisotropy near subducted slabs 19 in the transition zone and uppermost lower mantle (mid-mantle). In this study we in-20 vestigate the origin of radial anisotropy in the mid-mantle using 3-D geodynamic sub-21 duction models combined with mantle fabric simulations. These calculations are com-22 pared with seismic tomography images to constrain the range of possible causes of the 23 observed anisotropy. We consider three subduction scenarios: (i) slab stagnation at the 24 bottom of the transition zone; (ii) slab trapped in the uppermost lower mantle; and, (iii) 25 slab penetration into the deep lower mantle. For each scenario we consider a range of 26 parameters, including several slip systems of bridgmanite and its grain boundary mo-27 bility. Modelling of lattice preferred orientation (LPO) shows that the upper transition 28 zone is characterised by fast-SV radial anisotropy anomalies up to -1.5%. For the stag-29 nating and trapped slab scenarios, the uppermost lower mantle is characterised by two 30 fast-SH radial anisotropy anomalies of  $\sim +2\%$  beneath the slab's tip and hinge. On the 31 other hand, the penetrating slab is associated with fast-SH radial anisotropy anomalies 32 of up to  $\sim +1.3\%$  down to a depth of 2,000 km. Four possible easy slip systems of bridg-33 manite lead to a good consistency between the mantle modelling and the seismic tomog-34 raphy images: [100](010), [010](100), [001](100) and  $<110>{\overline{1}10}$ . The anisotropy anoma-35 lies obtained from shape-preferred orientation calculations do not fit seismic tomogra-36 phy images in the mid-mantle as well as LPO calculations, especially for slabs penetrat-37 ing into the deep lower mantle. 38

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#### Plain Language Summary

Seismology studies reveal that subducting slabs show different characteristics across the Earth; some flatten in the upper mantle (at 660 km depth), others are trapped in the uppermost lower mantle (660-1,200 km depth) and a few penetrate into the deep lower mantle. Subducting slabs cause the surrounding mantle to deform, but the way in which the minerals deform in the mid-mantle (410-1,200 km depth) remains poorly understood.

Geodynamic modelling can help us to infer how the mantle flows and deforms around subduction zones. However, the pattern and evolution of mantle flow around the full range of subduction scenarios has yet to be studied in such detail. Therefore, in this study geodynamic modelling is used to explore a range of mid-mantle parameters that best fit observations around subduction zones from seismology studies. Deformation in the mid-

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mantle induced by subducting slabs, including deeply penetrating slabs, is found to be consistent with a mechanism known as dislocation creep, which involves the movement of defects in the crystal lattice of rocks in the deep Earth, and agrees with recent seismic, geodynamic and laboratory studies.

#### 54 1 Introduction

Subduction zones across the world provide a unique setting for studying mantle de-55 formation and its associated anisotropy. As tectonic plates plunge into the mantle, they 56 drive mantle flow around the subducted slabs. Some slabs penetrate to the lower man-57 tle, whereas others stagnate at the bottom of the transition zone, near the 660 km seis-58 mic discontinuity (e.g., Fukao & Obayashi, 2013; Goes et al., 2017). This leads to dis-59 tinct trajectories of mantle convection, which control the thermo-chemical evolution of 60 our planet (e.g., P. S. Hall et al., 2012). One of the most direct ways to constrain man-61 tle flow is by measuring seismic anisotropy, which can be caused by: (i) lattice-preferred 62 orientation (LPO) of intrinsically anisotropic mantle minerals due to mantle flow; or, (ii) 63 strain-induced shape preferred orientation (SPO) of isotropic materials with highly con-64 trasting seismic properties (for a review see e.g., Chang et al., 2014). 65

Seismic anisotropy is commonly found in layers of the Earth where deformation and 66 strain are highest (Montagner, 1998). There is abundant evidence of anisotropy in the 67 upper mantle (e.g., Silver, 1996; Fischer & Wiens, 1996) and in the D" region in the low-68 ermost mantle (e.g., Mitchell & Helmberger, 1973; Lay & Helmberger, 1983; Vinnik et 69 al., 1989; Ritsema, 2000; Nowacki et al., 2011). However, in the mid-mantle ( $\sim$ 410-1,200 70 km), which in this study is considered to be composed of the upper transition zone (UTZ, 71 410-520 km), lower transition zone (LTZ, 520-660 km) and uppermost lower mantle (ULM, 72  $\sim$ 660-1,200 km), the presence of anisotropy is debated (e.g., Beghein & Trampert, 2004; 73 Panning et al., 2010; Chang et al., 2014; De Wit & Trampert, 2015). Both experimen-74 tal and numerical modelling results suggest that certain mid-mantle minerals are intrin-75 sically anisotropic. In the UTZ, wadsleyite is anisotropic, with a single crystal  $V_S$  anisotropy 76 of 18% at ambient conditions, decreasing to  $\sim 9\%$  at pressures corresponding to a depth 77 of 410 km (J. S. Zhang et al., 2018). Tommasi et al. (2004) reported that wadsleyite is 78 able to generate LPO in response to a given flow process and Kawazoe et al. (2013) ex-79 perimentally found that [001](010) is the dominant slip system of wadsleyite for a wa-80 ter content of 50-230 wt. ppm H<sub>2</sub>O. However, Ohuchi et al. (2014) suggested that wad-81

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slevite has several slip systems of similar strength for different water content regimes, 82 and each regime will form an LPO. In the LTZ, ringwoodite has been reported to be nearly 83 perfectly isotropic at LTZ pressures (Mainprice et al., 2000). Bridgmanite, constituting 84 78% of the lower mantle, is anisotropic (e.g., Meade et al., 1995; Wenk et al., 2004; Main-85 price et al., 2008; Tsujino et al., 2016). It has been reported that bridgmanite has a single-86 crystal  $V_S$  anisotropy of 33% at ambient conditions (Yeganeh-Haeri, 1994), but that it 87 decreases to 8% at 1,000 km depth when using the extrapolated temperature and pres-88 sure derivatives of Wentzcovitch et al. (2004). Such estimates of bridgmanite single-crystal 89  $V_S$  anisotropy have been shown to be even larger when considering elastic properties cal-90 culated by Z. Zhang et al. (2013) (Ferreira et al., 2019). Ferropericlase, constituting 16% 91 of the lower mantle, remains nearly isotropic at 660 km depth, but its single-crystal  $V_S$ 92 anisotropy increases considerably with pressure, becoming up to 40% in the D" region 93 (Marquardt et al., 2009). It has been shown recently by Muir and Brodholt (2018) that, 94 in contrast to previous views, water does not have a significant effect on lower mantle 95 rheology. However, water may change the activity of the slip systems of bridgmanite, which 96 may in turn affect the resultant anisotropy (e.g., Jung et al., 2006). 97

Analysis of transmission electron microscopy on wadsleyite polycrystals deformed 98 in compression and simple shear in multi-anvil apparatus showed dislocations in glide 99 configuration as well as subgrains, indicating the presence of dynamic recrystallisation 100 and suggesting deformation by dislocation creep (Dupas et al., 1994; Sharp et al., 1994; 101 Dupas-Bruzek et al., 1998; Thurel & Cordier, 2003; Thurel et al., 2003). Regarding the 102 lower mantle, several seismic studies suggest that it is on average isotropic, apart from 103 the D" region (e.g., Chang et al., 2014). This led to the view that the dominant defor-104 mation mechanism in this region is diffusion creep (Karato et al., 1995). High temper-105 ature experiments on fabric developments by Karato et al. (1995) suggested that the ab-106 sence of anisotropy in the lower mantle is strong evidence for deformation by superplas-107 ticity, provided that grain size remains reasonably small (Edington et al., 1976). More 108 recently, numerical simulations of creep by Boioli et al. (2017) suggested that disloca-109 tion pure climb creep, which does not produce LPO, dominates in bridgmanite. On the 110 other hand, bridgmanite aggregates deformed during laboratory experiments display a 111 clear LPO at relatively small strains (Tsujino et al., 2016; Miyagi & Wenk, 2016). How-112 ever, the validity of the extrapolation of laboratory experiments to lower mantle condi-113 tions is questionable given the extremely different values of stress and strain rate. 114

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Several shear-wave splitting studies have suggested anisotropy in the mid-mantle 115 (e.g., Vinnik et al., 1998), notably near subducting slabs down to the ULM (e.g., Wookey 116 et al., 2002; Chen & Brudzinski, 2003; Wookey & Kendall, 2004; Foley & Long, 2011; 117 Nowacki et al., 2015; Walpole et al., 2017). Several regional analyses focused e.g., on the 118 Tonga-Kermadec region, with Wookey and Kendall (2004) observing fast-SH shear waves 119 with a delay time of 0.7-2.2 s in the mid-mantle, and Foley and Long (2011) finding a 120  $\sim$ 1-3 s delay time attributed to the mid-mantle. However, such studies have difficulty 121 in isolating mid-mantle anisotropy from upper mantle effects and have limited depth res-122 olution and azimuthal coverage, which can restrict their interpretation. It has also been 123 possible to image anisotropy in the mid-mantle through global anisotropy tomography 124 studies since the 1980s (e.g., Nataf et al., 1984; Montagner & Tanimoto, 1991; Panning 125 & Romanowicz, 2004; Yuan & Beghein, 2013, 2014). One of the simplest forms of anisotropy, 126 radial anisotropy, corresponds to transverse isotropy with a vertical axis of symmetry, 127 and no azimuthal dependence (e.g., Bodin et al., 2015). Radial anisotropy describes the 128 difference between horizontally and vertically polarised shear waves, which can poten-129 tially distinguish between horizontal and vertical mantle flow. 130

Over the past decade or so, global radially anisotropic models have been developed 131 using different data sets and modelling schemes (for a review, see e.g., Chang et al., 2014). 132 The inclusion of body-wave travel time data allowed for anisotropy to be resolved in the 133 lower mantle (Panning & Romanowicz, 2006; Kustowski et al., 2008; Panning et al., 2010; 134 Auer et al., 2014; Moulik & Ekström, 2014), even if lowermost mantle anisotropy is dif-135 ficult to resolve globally (e.g., Kustowski et al., 2008; Chang et al., 2015). In addition, 136 to account for trade-offs between isotropic and anisotropic anomalies and discontinuities, 137 discontinuity perturbations have been included in inversions (e.g., Kustowski et al., 2008; 138 Visser et al., 2008; Moulik & Ekström, 2014). The use of huge data sets and, notably, 139 a large number of surface wave overtone dispersion measurements, has led to an improved 140 agreement between models. Chang et al. (2015) quantitatively compared recent mod-141 els and found: (i) an improved correlation between SGLOBE-rani (Chang et al., 2015) 142 and savani (Auer et al., 2014) of 0.5; this is an encouraging improvement compared to 143 previous studies, which do not show correlations larger than 0.3; (ii) fast-SV radial anisotropy 144 anomalies in the transition zone in SGLOBE-rani near subducted slabs, which also ap-145 pear in some other models (e.g., savani and SEMUCB-WM1 (French & Romanowicz, 146 2014)); and, (iii) fast-SH radial anisotropy anomalies in the ULM in SGLOBE-rani near 147

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subducted slabs (Ferreira et al., 2019), which also appear in *savani*, and seem consistent
with shear-wave splitting analyses. Given this increasing volume of observations, it is
timely to investigate the origin of anisotropy in the mid-mantle with geodynamic simulations and mantle fabrics calculations, which is the focus of this study.

The interpretation of radial seismic anisotropy is not straightforward and requires 152 a coordinated effort with other scientific disciplines, such as mineral physics and geody-153 namics (e.g., Chang et al., 2016; Chang & Ferreira, 2019; Ferreira et al., 2019). For ex-154 ample, LPO calculations depend on temperature, deviatoric stress, dominant creep mech-155 anism, the slip systems of anisotropic minerals, their elastic constants and water con-156 tent (see e.g., Karato et al., 2008; Mainprice, 2015). Yet, many of these properties are 157 imperfectly known, particularly in the deep mantle. Moreover, other mechanisms such 158 as extrinsic anisotropy through SPO also need to be considered (e.g., Faccenda et al., 159 2019). 160

Recent advances in computational modelling have provided new insights into the 161 elastic and rheological properties of the mantle. Anisotropy due to strain-induced LPO 162 has been modelled in the upper mantle (e.g., C. E. Hall et al., 2000; Becker et al., 2012; 163 Faccenda & Capitanio, 2013) and in the deeper mantle; in particular, a number of stud-164 ies have focused on the lowermost mantle (e.g., McNamara et al., 2002; Wenk et al., 2006; 165 Merkel et al., 2007; Walker et al., 2011). In contrast, few studies have focused on the mid-166 mantle. Nippress et al. (2004) used 2-D subduction models to show that finite strain pro-167 duced by the slab tip interaction with the 660 km discontinuity could be responsible for 168 anisotropy observed in the ULM. 3-D petrological-thermo-mechanical flow models of dy-169 namic subduction by Faccenda (2014) explored mid-mantle anisotropy produced by strain-170 induced LPO, indicating that high deviatoric stresses associated with subduction deform 171 transition zone and lower mantle aggregates by dislocation creep. This approach has been 172 subsequently used to interpret seismic observations of anisotropy in the uppermost lower 173 mantle (Ferreira et al., 2019) as well as anomalies associated with a deep plume-slab in-174 teraction (Chang et al., 2016). The investigation of mantle flow and seismic anisotropy 175 near subducted slabs in the mid-mantle is particularly difficult because complex 3-D pat-176 terns of mantle convection can develop (e.g., Faccenda & Capitanio, 2013; Faccenda, 2014). 177

<sup>178</sup> In this study we investigate the origin of mid-mantle (transition zone and ULM) <sup>179</sup> anisotropy using 3-D petrological-thermo-mechanical modelling of subduction dynam-

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ics combined with mantle fabrics calculations of mineral aggregates (Faccenda, 2014). 180 This work goes beyond that of Faccenda (2014) and Chang et al. (2016) by incorporat-181 ing a rheological model, and therefore an effective viscosity, that is consistent with 1-D 182 profiles of viscosity inverted from gravity data, including a mid-mantle viscosity hill in 183 the lower mantle (Rudolph et al., 2015; Mitrovica & Forte, 2004). We also incorporate 184 recent mineral physics results and first principle studies of lower mantle elastic constants. 185 We consider a variety of potential slip systems of bridgmanite, and take into account pos-186 sible contributions of mantle anisotropy from estimates of grain-scale SPO. Recently, Ferreira 187 et al. (2019) used a similar approach to interpret observations of radial anisotropy in the 188 uppermost lower mantle, but here we examine the whole mid-mantle. Moreover, we con-189 sider a greater range of subduction styles and modelling parameters, notably by intro-190 ducing a slab penetrating deeply into the lower mantle, and by using a variety of pos-191 sible slip systems. The resulting models are compared with tomographic images around 192 subducted slabs, in order to understand the mechanisms responsible for the observed ra-193 dial anisotropy. 194

#### <sup>195</sup> 2 Motivation from global radially anisotropic tomography

As explained in the previous section, despite discrepancies in studies of mid-mantle anisotropy, a number of recent seismic studies suggest the presence of radial anisotropy in the mid-mantle near subducted slabs. In this section we show illustrative examples of radial anisotropy in the global model SGLOBE-rani; for full details of the model and its robustness we refer the reader to the studies of Chang et al. (2015) and Ferreira et al. (2019). We focus on this model since we fully know all the details involved in its construction.

Figure 1 and Figure S1 in the Supporting Information show a selection of isotropic 203 and radially anisotropic cross-sections of seismic structure in SGLOBE-rani near sub-204 duction zones. A variety of subduction scenarios are shown: (i) slab stagnation at the 205 bottom of the transition zone (e.g., Honshu, Bonin, Northern Chile); (ii) slab trapped 206 in the ULM (e.g., Kurile, Kermadec, Eastern Java); and, (iii) slab penetration into the 207 deep lower mantle (e.g., Central America, Western Java, possibly Northern Peru). Pat-208 terns of radial anisotropy near subducted slabs in the mid-mantle show similar patterns 209 across the various subduction zones: the transition zone is characterised by fast-SV ra-210 dial anisotropy anomalies of up to  $\sim -3\%$ . In addition, a trend of two fast-SH anomalies 211

- of up to  $\sim +2\%$  are observed beneath the slab in the ULM, one beneath the steeply dipping portion of the slab and one beneath the slab's tip.
- In order to explain the presence of mid-mantle anisotropy around subduction zones, we can reduce the possible number of interpretations by comparing seismic tomography with predictions of geodynamic models. In this study we will compare SGLOBE-rani with calculations of radial anisotropy using 3-D geodynamic subduction models.

#### <sup>218</sup> 3 Methodology

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#### 3.1 Geodynamical simulations

We use a series of 3-D petrological-thermo-mechanical models in order to simulate subduction, built upon the methodology from Faccenda (2014) and Ferreira et al. (2019). These models use a 3-D geodynamic framework, I3MG, based upon a mixed Eulerian-Lagrangian finite difference scheme (Gerya, 2009). The model domain is defined by 6,000  $\times$  3,000  $\times$  3,000 km, using 293  $\times$  293  $\times$  69 Eulerian nodes (x, y, z coordinates, respectively; where y is the vertical coordinate).

The initial model set-up (Figure S2) includes a 30 km thick crust overlying a 1 Myr 226 old background mantle and a 80 Myr old oceanic plate. The plate, which is 3260 km long, 227 90 km thick, 1000 km wide, subducts self-consistently aided by a gently dipping 335 km 228 long slab. A strain-dependent low coefficient of friction of  $\mu$ =0.02-0.005 at zero defor-229 mation and at maximum strain, respectively, is set for the crust; this lubricating layer 230 allows self-consistent subduction of the plate. This is then increased at a depth of 100 231 km to  $\mu=0.1$  to simulate crust eclogitisation, ensuring the crust remains strong down to 232 the transition zone. 233

We define the thermal structure of the model using a half-space cooling model above 90 km depth, and an adiabatic geotherm of  $0.5 \text{ K} \cdot \text{km}^{-1}$  below. Mantle phase transitions are obtained from density and enthalpy maps taken from PERPLE\_X (Connolly, 2005) as a function of pressure and temperature for pyrolite. The Clapeyron slope of the mantle discontinuities can be derived from the density map in Figure S2b.

All the model parameters used in our study are shown in Table S1. In order to limit the number of parameters studied, we focus largely on varying the mantle's viscosity to achieve different subduction simulations. We calculate the effective viscosity for a visco-

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plastic material by combining a Druger-Prager yielding criterion and low-T Peierls, highT dislocation and diffusion creep mechanisms (see Table S2 for the equations used). We
simulate three subduction scenarios of: (i) slab stagnation at the bottom of the transition zone; (ii) slab trapped in the ULM; and, (iii) slab penetration into the deep lower
mantle.

For our subduction scenarios of a slab stagnation at the bottom of the transition 247 zone and trapped in the ULM, we employ a relatively low viscosity (weak) asthenosphere, 248 a viscosity jump at 660 km depth, and a viscosity hill at around 1,500 km depth, pro-249 ducing a strong mid-mantle (Morra et al., 2010; Marquardt & Miyagi, 2015; Rudolph 250 et al., 2015). Deformation in the upper mantle is accommodated mostly by dislocation 251 creep, whereas it is only active at deviatoric stresses above 10-20 MPa in the lower man-252 tle (Figure S2c). Whilst such values are taken from olivine flow laws, it is generally ac-253 cepted that this amount of stress is sufficient to activate dislocation creep (e.g., McNa-254 mara et al., 2002). 255

The pre-exponential factors for diffusion and dislocation creep in the upper and lower mantle are the only varying rheological parameters in each of our subduction models. This simulates regional variations in the composition of the mantle (e.g., Ballmer et al., 2017). For the deeply penetrating subduction model, the employed pre-exponential factors for diffusion and dislocation creep result in the absence of the mid-mantle viscosity hill, which would otherwise prevent deep slab penetration.

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#### 3.2 Mantle fabric modelling

Following Faccenda (2014) and Ferreira et al. (2019), we calculate the strain-induced lattice-preferred orientation (LPO) of Lagrangian aggregates which are passively advected by means of the Eulerian velocity field obtained by the macro-flow modelling. Throughout the model evolution, the fabric development of each aggregate is calculated using a modified version of the kinematic model D-Rex (Kaminski et al., 2004), which accounts for deformation history, non-steady-state deformation and strain-induced LPO of midmantle aggregates (e.g., Faccenda & Capitanio, 2012, 2013; Faccenda, 2014).

We use a harzburgitic upper mantle composition (Ol:Ens=70:30, 0-410 km depth) and a pyrolitic mantle composition in the transition zone (Wd:Grt=60:40, 410-520 km; Rw:Grt=60:40, 520-660 km) and lower mantle (Brd:Fp=80:20, 660-3,000 km) (Mainprice,

2015). Whole crystal aggregates undergo phase transitions at arbitrary density crossovers 273 that represent the boundary between two different rock types (Ol:Ens $\rightarrow$ Wd:Grt=3,650 274  $kg \cdot m^{-3}$ ; Wd:Grt  $\rightarrow$  Rw:Grt = 3,870 kg  $\cdot m^{-3}$ ; Rw:Grt  $\rightarrow$  Brd:Fp=4,150 kg  $\cdot m^{-3}$ ) (Figure S2). 275 During subduction, upper mantle and transition zone mantle aggregates are entrained 276 around the slab down into the lower mantle, except near the slab's tip (Figure S3). Given 277 that little is known about the topotactical growth of crystal aggregates undergoing phase 278 transitions given a pre-existing fabric, we adopt the approach of resetting the LPO af-279 ter each phase transition by randomising the crystal orientation. 280

We only compute the fabric development for phases that display significant single-281 crystal visco-elastic anisotropy, such as olivine, enstatite, wadsleyite and bridgmanite, 282 and only for the fraction of viscous deformation accommodated by dislocation creep. There-283 fore crystal aggregates of cubic phases, including ringwoodite, garnet and ferropericlase, 284 are orientated randomly throughout the model evolution, as they are mostly isotropic 285 in the mid-mantle (e.g., Carrez et al., 2007). In this study, we only display anisotropy 286 generated by significantly deformed aggregates due to the subducting slab (whereby  $\ln\left(\frac{FSE_{max}}{FSE_{min}}\right) >$ 287 (0.5). This is consistent with our interpretation of anisotropy anomalies near the slabs 288 in the seismic tomography, which have been shown to be statistically distinct groups of 289 anomalies by a cluster analysis (Chang & Ferreira, 2019). 290

In our models, the ratio of dislocation to diffusion creep is stress-dependent, which is accounted for in the large-scale flow model. A low transition stress value favouring dislocation creep is used for the upper mantle and transition zone (Turcotte & Schubert, 2014), whereas in the lower mantle the dislocation creep mechanism is only active above deviatoric stresses of 10-20 MPa (Figure S2c and Figure 2a-f) (e.g., McNamara et al., 2002).

In order to calculate the strain-induced LPO of anisotropic minerals, we use the 297 normalised Critical Resolved Shear Stress (CRSS) for slip systems of olivine, enstatite 298 and wadsleyite from available experimental data as compiled in Faccenda (2014). For 299 bridgmanite, we test several potential slip systems proposed from experimental studies 300 and from ab-initio simulations (e.g., Cordier et al., 2004; Wenk et al., 2004; Mainprice 301 et al., 2008). At ULM pressures and temperatures we consider: [100](010), [100](001), 302  $[010](100), [001](100), [001](010), [001]{\overline{1}10}, <\overline{1}10>(001), <110>{\overline{1}10}.$  In turn, each 303 slip system was tested by imposing a CRSS five times lower than all other slip systems 304

(e.g., Tommasi et al., 2004). Whilst this method considers only the softest slip system 305 at a time, it remains a reasonable simplification when dynamic crystallisation is efficient 306 enough. We use bridgmanite elastic tensors and their P-T derivatives derived from Z. Zhang 307 et al. (2013) at ULM conditions (Table S3). We can then obtain the full elastic tensor 308 of each aggregate by Voigt-averaging the crystal elastic properties (scaled at local P-T 309 conditions) according to their volume and orientation. For further comparison, we ob-310 tain another fabric from static (0 K) ab-initio atomic scale modelling run at ULM pres-311 sures (e.g., Carrez et al., 2007; Mainprice et al., 2008). 312

- We test the effect of the grain boundary mobility  $(M^*)$  on the strength and loca-313 tion of the computed anisotropy (Figure 3a-c). In D-Rex,  $M^*$  is a dimensionless param-314 eter that controls the efficiency of grain-boundary migration (GBM), a process in which 315 grains with low internal energy grow at the expense of grains with high internal energy 316 (Kaminski & Ribe, 2001). In deformed polycrystalline aggregates, newly formed grains, 317 having undergone recrystallisation, have low internal energy and are well orientated with 318 the easy slip system to accommodate flow. Therefore, they grow more than other grains 319 and dominate the LPO. The higher the  $M^*$ , the faster the LPO forms. 320
- There are also other parameters that affect the computed anisotropy, such as the 321 nucleation rate  $(\lambda^*)$  and grain boundary sliding, which can be modelled by the thresh-322 old volume fraction below which grains do not deform anymore by dislocation creep ( $\chi$ ) 323 (i.e. do not rotate and have zero internal energy) and the relative CRSS of different slip 324 systems. We use  $\lambda^*=5$  and confirmed that using  $\lambda^*>5$  does not lead to a significant vari-325 ation of LPO strength (Kaminski & Ribe, 2001; Faccenda, 2014). For  $\lambda^* < 2$ , although 326 the anisotropy is stronger and more dominated by hard grains, the LPO does not agree 327 with that found by (Mainprice et al., 2008) nor with experiments in which there is a clear 328 alignment of one of the crystallographic orientations with the shear direction at very low 329 strain (e.g., Tsujino et al. (2016); see Figures S4 and S5 in the Supporting Information). 330 Regarding grain boundary sliding, we use  $\chi=0.3$  (Kaminski et al., 2004). If we increase 331 it, then only the very large grains will deform by dislocation creep, and thus the LPO 332 will be weaker. On the other hand, if we decrease  $\chi$  even further, we would only slightly 333 strengthen the LPO as the LPO is dominated by the very large grains.  $\chi = 0$  makes no 334 sense because the dynamic recrystallisation and grain size reduction/growth are intrin-335 sic processes of dislocation creep. Furthermore, reducing the contrast in the CRSS among 336 the different slip systems, decreases the strength of the LPO as more slip systems are 337

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competing to accommodate the strain. Hence, for the sake of simplicity, in this study 338 we choose to test  $M^*$  since it has been shown to have the most direct effect on the mag-339 nitude of the anisotropy (Kaminski & Ribe, 2001; Boneh et al., 2015). In the upper man-340 tle, olivine has a  $M^*$  value of  $125\pm75$  taken from model predictions by Kaminski and 341 Ribe (2001) and calibrated against the experimental results from S. Zhang and Karato 342 (1995). In the transition zone,  $M^*$  of wadslevite is set to 125 following the results of Faccenda 343 (2014). For bridgmanite, we vary this constant between 10 (Boneh et al., 2015) and 200 344 as there is currently little available data to calibrate it. Figure 3a-c shows that increas-345 ing  $M^*$  in the lower mantle increases the strength of the computed radial anisotropy be-346 neath the slab. As explained in the caption of Figure 3, we only display anisotropy that 347 has been induced by the subducting slab. This is supported by a clustering analysis by 348 Chang and Ferreira (2019), which showed that the anisotropy anomalies around subducted 349 slabs in SGLOBE-rani are a statistically distinct class of anomalies. 350

In all mantle fabric models used in this study, the  $M^*$  value for bridgmanite is set to 125 because it provides a radial anisotropy of  $\sim +2\%$  beneath the slab. This is consistent with the seismic tomography images in Figure 1 (and Figure S1), and with shearwave splitting measurements (e.g., Walpole et al., 2017). In addition, bridgmanite's  $M^*$ value needs to be high to justify the LPO with the very low amount of deformation induced by the stagnating slab. Lower values of  $M^*$  would lead to a poor fit to the observations (Figure 3a-c).

While it is generally accepted that dislocation creep is the dominant deformation 358 mechanism in the upper mantle and transition zone (e.g., Karato & Wu, 1993; Weert-359 man & Weertman, 1975; Kohlstedt & Goetze, 1974; Trampert & van Heijst, 2002; Shi-360 mojuku et al., 2009), we explore the effect of the level of deformation absorbed by dis-361 location creep in bridgmanite on the LPO calculations. In light of recent experiments 362 by Girard et al. (2015), it was reported that bridgmanite crystals are likely to absorb 363 less deformation than the bulk deformation in the lower mantle because they are stiffer 364 than ferropericlase. Thus, we compare the results obtained when bridgmanite absorbs 365 only 30% of the bulk deformation with those obtained when bridgmanite absorbs all de-366 formation. The results, shown in Figure 3, show that when bridgmanite absorbs 30% of 367 the deformation (Figure 3d,e,f), the resultant ULM anisotropy is very weak ( $\sim +0.5\%$ ). 368 On the other hand, when bridgmanite absorbs all the deformation (Figure 3a,b,c) the 369 resultant ULM anisotropy is more consistent with that found in the seismic tomogra-370

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phy images. However, it is worth noting that, even when bridgmanite absorbs only 30%of the deformation, significant ULM anisotropy could be generated with a substantially larger value of  $M^*$  or, with a higher amount of subduction-induced deformation than considered in this study or, as mentioned above, with a lower nucleation rate or grain boundary sliding.

In addition to LPO, extrinsic radial anisotropy is also estimated by modelling grainscale shape-preffered orientation (SPO) using the effective medium theory, following the approach of Backus (1962), Faccenda et al. (2019) and Ferreira et al. (2019) A short summary of the approach used can be found in the Supporting Information (Text S1).

#### 380 4 Results

In this section we present the results obtained from our 3-D modelling approach 381 for the three subduction scenarios considered. We recall that these different scenarios 382 were achieved mainly by varying the viscosity contrast between the upper and lower man-383 tle, for the simulation parameters presented in the Table S1. The subduction models are 384 compared with tomography images. To aid in their comparison, we interpolate our man-385 the fabrics calculations into a grid with spacing  $200 \times 100 \times 200$  km (x, y, z co-ordinates, 386 respectively), which is more comparable with the resolution of the tomography models 387 than the higher resolution used in the geodynamical simulations ( $\sim 20 \times 20 \times 40$  km). In 388 the future we plan to filter the geodynamical models using the resolution matrix of the 389 tomography models. However, given the global parameterisation used in the tomogra-390 phy models, that is an effort that goes beyond the scope of this study. 391

392

#### 4.1 Slab stagnating at the bottom of the transition zone

Figure 4 and Movie S1 show the results obtained for a slab stagnating at the bottom of the transition zone. The slab arrives at the 660 km discontinuity after ~8 Ma, at a shallow dip angle, owing to a fast trench retreat. The viscosity jump at 660 km depth, together with the negative Clapeyron slope of the 660 km discontinuity and the shallow dip angle, generate relatively low stresses at this depth (Christensen, 1996), ultimately leading to slab stagnation.

Viscosity-depth profiles for each of our subduction models are shown in Figure S6.
For the stagnating case (Figure S6b), the effective viscosity of the surrounding mantle

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is reduced by the subducting slab compared to the background mantle (with the exception of the sharp peak caused by the high viscosity of the slab itself). This is shown in
the upper mantle but is most evident below 660 km depth. Figure 2g shows how the strain
rate is high below the hinge of the retreating slab, which decreases the effective viscosity of the lower mantle and reduces the viscosity contrast with the overlying transition
zone. In turn, this facilitates the entrainment of mantle transition zone material below
660 km depth.

Sub-horizontal green velocity vectors near the stagnant part of the slab in Figure 408 2g show that the slab's tip advances slowly over the 660 km discontinuity. This explains 409 the low strain rate below the slab's tip. Strain rate is higher above the stagnating plate 410 because of the return flow opposite to the direction of plate motion. Subduction induces 411 a lower mantle upwelling beyond the slab's tip and up to the right boundary of the model 412 (6,000 km in the x-coordinate, at a relatively low velocity). The induced mantle flow is 413 fastest above the stagnant part of the slab, where the trench retreats. It is worth not-414 ing that this leads to some lower mantle regions in Figure S6a with lower viscosity than 415 the upper mantle. This is possible given what we know of the real Earth, based on the 416 history of slab subduction. In particular, a number of slab avalanche events have been 417 documented by van der Meer et al. (2018); these slabs would have greatly loaded the 660 418 km discontinuity, increasing the stress on the lower mantle and thus reducing its viscos-419 ity. 420

LPO generation can be explained by studying the strain the slab induces on the 421 surrounding mantle. Figure 5 and Movie S2 show the maximum finite strain ellipsoid 422 (FSE) axis on the mantle surrounding the slab. Horizontal sliding of the slab over the 423 660 km discontinuity generates simple shear deformation in the mid-mantle near the stag-424 nant part of the slab. The maximum FSE axis in the ULM is oriented parallel to the stag-425 nant part of the slab and strain is highest beneath the slab where there is contact with 426 the 660 km discontinuity, and also surrounding the slab's tip. High strain beneath the 427 slab's tip is generated upon contact with the 660 km discontinuity; this produces an area 428 of fast-SH radial anisotropy of  $\sim +2\%$ . Subsequent trench retreat encourages stagnation 429 and the loading of the slab on the 660 km discontinuity generates further strain accom-430 modated by dislocation creep (Figure 2a). Hence, the anisotropy builds away from the 431 slab's tip, forming a second fast-SH radial anisotropy anomaly beneath the steeply dip-432 ping portion of the slab, again of  $\sim +2\%$ . The fast-SH anisotropy anomalies are confined 433

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within the 660-1,000 km depth range and show some separation. The UTZ is characterised
by ~-1.5% fast-SV radial anisotropy due to anisotropic wadsleyite. Part of the UTZ above
the stagnant part of the slab remains isotropic, due to upwelling and downwelling of the
mantle, producing constant phase changes of olivine to wadsleyite and LPO resetting.
Fast-SV radial anisotropy anomalies of <-1% are present beyond the slab's tip due to</li>
induced poloidal flow rotating the lower mantle aggregates.

In order to further understand the nature of the observed anisotropy anomalies, 440 we ran the fabrics calculations keeping track of the initial rock type for each aggregate 441 (Figure S3). We find an interesting upwelling of transition zone material in the upper 442 mantle wedge. Moreover, Figure S3 shows that except near the slab tip, the region with 443 positive radial anisotropy is made mostly of upper mantle and transition zone aggregates 444 that have been dragged down into the lower mantle (and have transformed into lower 445 mantle aggregates) by the subducting plate. Figure 4a shows good agreement between 446 the radial anisotropy in the seismic tomography images and our LPO fabric calculations 447 for a slab stagnating at the 660 km discontinuity. At least qualitatively, the modelled 448 LPO replicates well the observed anisotropy in the mid-mantle. In the uppermost man-449 tle, the seismic tomography images show negative  $\xi$  perturbations which do not appear 450 in the geodynamics models. This is possibly due to (i) the fossil slab anisotropy yield-451 ing negative  $\xi$  perturbations when the slab is dipping above a certain angle (e.g., Song 452 & Kawakatsu, 2012), while the slab in our modelling is isotropic, and (ii) upwellings trig-453 gered by the slab, which are not considered in the geodynamical modelling. The com-454 puted ULM anisotropy shows two separate anomalies, with one anomaly beneath the slab's 455 tip and the other beneath the steeply dipping portion of the slab. Nevertheless, these 456 anomalies are less separated than in the seismic tomography images. As explained in the 457 methods section, we tested nine possible slip systems of bridgmanite in the LPO calcu-458 lations (Figure 4b). Upon comparison with the tomography images, it is clear that four 459 slip systems are compatible with the observed fast-SH radial anisotropy anomalies in the 460 ULM: [100](010), [010](100), [001](100) and  $<110>\{\bar{1}10\}$ . 461

As previously reported by Ferreira et al. (2019), modelled grain-scale SPO also replicates well the fast-SH radial anisotropy anomalies observed in the subslab, of up to  $\sim+2.5\%$ due to the large contrast in mineral isotropic elastic properties in the region between the post-spinel and the post-garnet reactions. However, there is less separation between the two anisotropic anomalies than in the LPO calculations, and they are present down to

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greater depths (~1,100 km) than when considering a LPO mechanism. On the other hand,
 the SPO modelling is not compatible with the fast-SV radial anisotropy anomalies ob served in the transition above the stagnant part of the slab.

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#### 4.2 Slab trapped in the uppermost lower mantle

Slab penetration through the 660 km discontinuity is achieved by reducing the viscosity contrast between the upper and lower mantle, as can be seen in Figure S6c-d. In this case, the subduction rate is slower than that of the slab stagnating at the bottom of the transition zone. The slab's tip reaches the 660 km discontinuity after  $\sim$ 14 Ma, and with a steeper dip angle than in the stagnating case (Movie S3). This generates a large stress on the discontinuity, facilitating penetration over  $\sim$ 40 Ma.

The creation of radial anisotropy in the ULM is similar to that seen in the stag-477 nating case, as can be seen in Figure 6 and Movie S3. When the slab's tip hits the 660 478 km discontinuity and consequently begins to stagnate, the large generated stress leads 479 to the first fast-SH radial anisotropy anomaly in the ULM. The slab's tip then remains 480 relatively stationary whilst trench retreat causes the slab to unload across the 660 km 481 discontinuity. This generates further stress at the discontinuity, which leads to the sec-482 ond fast-SH anisotropy anomaly in the ULM. Eventually, the stagnant part of the slab 483 penetrates through the 660 km discontinuity into the ULM. Strain-induced LPO calcu-484 lations lead to fast-SV anomalies up to  $\sim -1.5\%$  in the UTZ and to fast-SH anomalies of 485  $\sim +1.7\%$  in the ULM. 486

During penetration through the 660 km discontinuity, the entrained material be-487 neath the slab, which causes the fast-SH radial anisotropy observed, is pushed downwards 488 to a depth extent of  $\sim 1,300$  km. The velocity vectors shown in Figure 2h show a down-489 ward motion at a relatively fast velocity (red arrows around the slab), resulting in the 490 forcing down of the subslab material. The consequent penetration, after a stable period 491 of stagnation, takes place in  $\sim$ 7 Ma. During this period, the velocity of the mantle in 492 the whole model domain is also larger than in the stagnating case due to a faster sub-493 duction rate, and there is a noticeably larger return flow. The mantle moves fastest in 494 the upper mantle above the slab, but unlike the stagnating case, mantle flow is also fast 495 beneath the slab due to slab penetration. 496

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497 Strain beneath the penetrating part of the slab is higher than strain beneath the 498 stagnant slab in the previous scenario, but also acts over a larger depth range, as seen 499 in Figure 5b, and in Movie S4. This is due to the lower viscosity of the lower mantle than 500 in the stagnating scenario, and to the slab arriving at the 660 km discontinuity at a steeper 501 angle, generating a larger stress on the discontinuity.

Figure 6b shows the radial anisotropy produced when considering the nine possi-502 ble bridgmanite slip systems previously stated. We find that four slip systems lead to 503 radial anisotropy compatible with the anisotropy observed in the seismic tomography: 504 [100](010), [010](100), [001](100) and  $<110>\{\overline{1}10\}$ . This agrees with those found in the 505 stagnating slab scenario. SPO modelling again shows fast-SH anisotropy below the slab. 506 However, the anisotropy anomalies around the slab in the lower mantle are only up to 507 +1% (peaking at +1.4% beneath the slab's tip) due to the majorite-bridgmanite phase 508 transformation, which is weaker than in the seismic tomography images. Similar to the 509 previous section, SPO modelling also yields fast-SH radial anisotropy in the transition 510 zone, which disagrees with fast-SV radial anisotropy observed in both the seismic tomog-511 raphy and LPO images. 512

513

#### 4.3 Slab penetrating deep into the lower mantle

By further decreasing the effective viscosity of the lower mantle compared to the 514 two previous subduction scenarios (see Table S1), the slab penetrates below 1,000 km 515 depth as seen in Figure S6e, Figure 7a, and Movie S5. Slab penetration is helped by a 516 steeper dip angle than in the previous two cases when the slab reaches the 660 km dis-517 continuity, by slow trench retreat and by a weaker resistance imposed by the 660 km dis-518 continuity. Indeed, the slab bends slightly at the 660 km discontinuity due to the vis-519 cosity increase, and consequently a large stress is induced around the slab's tip (see Movies 520 S5 and S6). However, the viscosity contrast between the upper and lower mantle is not 521 strong enough to prevent slab penetration and thus, the slab is able to continue pene-522 trating deep into the lower mantle. 523

Figure 7a shows that fast-SV radial anisotropy anomalies are present in the ULM, whilst fast-SH radial anisotropy anomalies, of up to  $\sim +1.3\%$  are present beneath the slab's tip. Movie S5 shows how the fast-SH radial anisotropy is created upon slab tip interaction with the 660 km discontinuity and how its strength increases with further subduc-

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tion. Strain generated beneath the slab's tip is distributed over a larger area (see Fig-528 ure 5c,f and Movie S6) than in the two previous sections, thus generating a larger area 529 of induced anisotropy but of weaker strength than in the two previous subduction sce-530 narios. Figure 2i shows that the strain rate is much larger in the entire model domain 531 compared to the previous two subduction scenarios. This is due to a faster rate of sub-532 duction, hence a faster and larger poloidal flow is induced in the mantle. Similarly to 533 the trapped slab scenario, flow is vertical all around the end of the slab, producing a fast-534 SV anisotropy anomaly of  $\sim$ -1%. The UTZ yields some fast-SV radial anisotropy anoma-535 lies, although the majority of the transition zone remains isotropic due to the large poloidal 536 flow resetting anisotropy at phase change boundaries. 537

Figure 7b shows that the same four slip systems, as in the two previous sections, lead to seismic anisotropy comparable to the seismic tomography cross-sections. Grainscale SPO modelling yields a pattern of anisotropy similar to the LPO modelling. The ULM remains largely isotropic, but fast-SH radial anisotropy anomalies appear above and below the slab's tip at depths of ~1,200-1,800 km. However, the strength of the fast-SH radial anisotropy is significantly weaker than that seen in the LPO model, at ~+0.3%. This does not match the seismic tomography image shown in Figure 7a.

#### 545 5 Discussion

Our study presents calculations of radial anisotropy in the mid-mantle for three subduction scenarios. LPO and SPO anisotropy mechanisms have been considered, with LPO leading to anisotropic features more consistent with observations than a SPO mechanism, especially around penetrating slabs. This is highlighted in Figure S7, where radial anisotropy due to SPO is significantly weaker in the deeply penetrating case compared to the LPO. Specifically, no radial anisotropy greater than +1% develops due to SPO in the deeply penetrating slab scenario.

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#### 5.1 Transition zone

Figure 8 compares 1-D profiles of depth-dependent radial anisotropy between the three models of subduction and seismic tomography. It is important to note that these profiles are averages of the geodynamic models and of the tomographic images of subduction regions, and therefore radial anisotropy values are smaller than the maximum

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values previously stated. The geodynamic models (Figure 8a, b and c) coherently show that the transition zone is characterised by fast-SV radial anisotropy anomalies ( $\xi < 1\%$ ) of on average ~0.5% when considering LPO modelling, but SPO modelling implies the transition zone is isotropic, or has fast-SH radial anisotropy ( $\xi > 1\%$ ). Given that the seismic tomography 1-D profiles at subduction regions (Figure 8d) show ~-0.5% fast-SV anisotropy, LPO can explain this observation but SPO cannot.

Many shear-wave splitting studies struggle to separate contributions of mid-mantle 564 anisotropy from the transition zone and the ULM. However, Nowacki et al. (2015) found 565 shear-wave splitting of  $\leq 2.4$  s in the transition zone, attributing this to the presence of 566 hydrous phases in the region but not to the development of LPO, disagreeing with our 567 results. Chen and Brudzinski (2003) found SH waves arriving up to 3 s earlier than SV 568 waves in the transition zone in the Fiji-Tonga region. Whilst this finding is not consis-569 tent with the results presented in this study, it does agree with the presence of a plume 570 interacting with the Tonga-Kermadec slab (Chang et al., 2016). 571

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#### 5.2 Uppermost lower mantle

For the uppermost lower mantle, Figures 8a, b and c show that four slip systems 573 of bridgmanite ([100](010), [010](100), [001](100) and  $\langle 110 \rangle \{\bar{1}10\}$ ) yield fast-SH radial 574 anisotropy anomalies. The tomography images for the subduction zone regions plotted 575 in Figure 8d are comparable to the results for the slip systems in Figures 8a, b and c, 576 agreeing with an average maximum fast-SH radial anisotropy value of +0.5% in the ULM, 577 but not below 1,200 km depth. Whilst the seismic tomography suggests that subduc-578 tion regions have radial anisotropy anomalies of  $\xi < 1\%$  in the lower mantle beneath 1,200 579 km depth, all three geodynamic models show anomalies that remain  $\xi > 1\%$ . This could 580 be explained by the fact that the resolution of the tomography images is limited beneath 581  $\sim$ 1,400 km depth (Chang et al., 2015). On the other hand, this could also suggest that 582 our results are affected by errors in the model parameters, such as grain boundary mo-583 bility and relative slip system activities. 584

When a slab reaches the 660 km seismic discontinuity, it is expected to produce large stresses in the ULM, which in turn can induce mineral alignment, producing anisotropy (e.g., Nippress et al., 2004). Our results confirm this. Indeed, our calculations of LPO lead to a pattern of anisotropy in the ULM similar to that observed in the SGLOBE-

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rani and savani tomographic models (i.e., two separated fast-SH anomalies of up to +2%589 beneath stagnant slabs and next to penetrating slabs). The comparison of our LPO mod-590 elling to the seismic tomography, to first order, fits the assumption that LPO is randomly 591 re-set at phase changes. The support of this hypothesis, as opposed to inheritance of LPO 592 across phase changes, provides an interesting insight into this relatively unknown area 593 of interest. The inheritance of LPO at phase changes is important to consider in future 594 studies and requires further constraints from laboratory experiments. For slabs stagnat-595 ing at the bottom of the upper mantle, SPO calculations around the 660 km seismic dis-596 continuity are also compatible with the seismic images. 597

Several shear-wave splitting studies have reported observations of seismic anisotropy 598 in the ULM broadly compatible with fast-SH radial anisotropy anomalies (e.g., Wookey 599 et al., 2002; Wookey & Kendall, 2004; Mohiuddin et al., 2015). In addition, studies in 600 the Tonga-Kermadec region show that SH waves lead SV by a few seconds (Wookey & 601 Kendall, 2004), which was interpreted as due to either strain-induced LPO or to SPO 602 of subducted material into the ULM. Mohiuddin et al. (2015) observed significant split-603 ting (delay times >1 s) of S phases at the base of the transition zone in subduction re-604 gions. They hypothesised a layer of  $\sim 5\%$  anisotropy with a thickness of  $\sim 200$  km in the 605 mid-mantle around stagnating slabs. However, they also found that the strength of anisotropy 606 and the thickness of the layer trade off directly; thus, their results are comparable to the 607 values found in this study, since we find weaker anisotropy  $(\sim +2\%)$  in a thicker region 608  $(\sim 540 \text{ km})$ . A subsequent shear-wave splitting study by Walpole et al. (2017) reported 609 tilted transverse isotropy in the ULM with a fast symmetry axis orientated sub-parallel 610 to the subduction direction, agreeing with our results. Splitting times of  $\sim 1$  s in the ULM, 611 would require a layer of 2% anisotropy  $\sim 180$  km thick. Given that the thickness of the 612 anisotropic anomalies in tomographic images is likely affected by limitations in resolu-613 tion (Chang et al., 2015), this is broadly compatible with our results. 614

Faccenda (2014) conducted the first calculations of seismic anisotropy around subduction zones and obtained  $\sim +2\%$  fast-SH radial anisotropy anomalies down to  $\sim 1,000$ km depth. However, that study did not test potential slip systems of bridgmanite or take into account possible anisotropy contributions from SPO. Also, although the rheology of the lower mantle is still largely unknown, the mantle viscosity values used in this study are likely more realistic than when using the olivine flow law used in Faccenda (2014).

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#### 5.3 Bridgmanite slip systems

The four potential easy slip systems of bridgmanite identified in this study agree 622 with recent uni-axial deformation experiments in a Kawai-type deformation-DIA appa-623 ratus (Tsujino et al., 2016) who found a bridgmanite fabric dominated by the slip sys-624 tem [001](100), at ULM conditions of 25 GPa and 1,873 K. Miyagi and Wenk (2016) used 625 a diamond anvil cell apparatus to report bridgmanite's dominant slip system as [100], 626 [010] and <110> on the (001) planes, at pressures <55 GPa, agreeing with our slip di-627 rections but not with our slip plane. An earlier study by Cordier et al. (2004) suggested 628 [100](001) and [010](001) dislocations based on X-ray line-broadening analysis of sam-629 ples recovered from a deformation experiment at 25 GPa and 1,673 K, but both slip sys-630 tems disagree with our findings. 631

Slip systems of bridgmanite have also been investigated numerically using the Peierls-632 Nabarro model and calculation of generalised stacking faults and the Peierls-Nabarro-633 Galerkin model to evaluate Peierls stresses (Ferré et al., 2007; Gouriet et al., 2014). These 634 studies find that [010](100) and [100](010) should be the easiest slip systems, agreeing 635 with our results. A study of the interaction between the Samoan plume and Tonga-Kermadec 636 slab (Chang et al., 2016) highlighted [100](010), [100](001),  $\langle \bar{1}10 \rangle (001)$  and  $\langle 110 \rangle \{ \bar{1}10 \}$ 637 as potential bridgmanite easy slip systems. Our study agrees with two of these slip sys-638 tems, suggesting that the results of Chang et al. (2016) may require higher mid-mantle 639 temperature due to the interaction between the slabs and the plume. 640

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#### 5.4 Geodynamic modelling

Our geodynamic modelling of slab subduction relies on a rheological model where 642 the high-temperature effective viscosity strongly depends on the pre-exponential factor 643 and a depth-dependent activation enthalpy for both diffusion and dislocation creep mech-644 anisms. Previous models, such as those in Faccenda (2014), utilised only the olivine flow 645 law with pressure-dependent activation enthalpy, which produces a very high effective 646 viscosity already at 1,000 km depth. In contrast, the present rheological model is more 647 consistent with existing constraints on the 1-D viscosity profile of the Earth, including 648 a viscosity hill in the mid-lower mantle (e.g., Rudolph et al., 2015), and the relative con-649 tribution of dislocation creep mechanism in the lower mantle that is significant only at 650 high stresses (e.g. McNamara et al., 2002; Cordier et al., 2004; Mainprice et al., 2008). 651

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The latter effect is needed to prevent lower mantle fabrics and seismic anisotropy to de-652 velop everywhere in the lower mantle around subduction zones, which is not observed 653 in the SGLOBE-rani and savani tomographic models. For the stagnating scenario, the 654 negative Clapeyron slope and fast trench migration are essential for slab stagnation across 655 the 660 km discontinuity. A layer of reduced viscosity has been suggested to aid in the 656 stagnation of slabs at the 660 km discontinuity (Mao & Zhong, 2018); we performed this 657 test to find that the low viscosity layer had the effect of absorbing more deformation, 658 resulting in a wider area of diffused anisotropy in the ULM. This hindered the separa-659 tion of two fast-SH anomalies in the ULM, which are observed in the tomography im-660 661 ages.

On the other hand, the steeper dip angle of the slab associated with the relative 662 slower trench migration rates in the trapped and penetrating scenarios, respectively, aid 663 slab penetration through the 660 km discontinuity. This agrees with the results of geo-664 dynamical modelling by Agrusta et al. (2017), whereby a viscosity increase in the lower 665 mantle is not by itself enough to control subduction dynamics; trench migration and the 666 Clapeyron slope also play an important role. Nippress et al. (2004) used instantaneous 667 2-D flow calculations in an early subduction setting to investigate lower mantle anisotropy. 668 Despite the differences between their modelling scheme and ours, it is interesting that 669 when comparing an early stage of our FSE modelling for the penetrating slab scenario 670 (as seen in Movie S6) to theirs, we see that in both models the longest FSE axis align 671 in the same direction. 672

Our rheological model accounts for a combined dislocation-diffusion creep mech-673 anism, similar to that of Hedjazian et al. (2017). We have varied the criteria used to ac-674 tivate dislocation creep by varying the pre-exponential factors of the diffusion and dis-675 location creep flow laws. This has allowed us to (1) obtain different subduction scenar-676 ios, which is not possible with kinematic models such as those of Hedjazian et al. (2017), 677 and, at the same time, (2) vary the contribution of one creep mechanism relative to the 678 other. Unlike this study, Hedjazian et al. (2017) identified areas deformed by diffusion 679 creep in the upper mantle. In our model, dislocation creep is predominant over diffusion 680 creep in most P-T-stress conditions in the upper mantle and transition zone. As a re-681 sult, the anisotropy at these depths represents an upper bound estimate. Nevertheless, 682 this assumption is realistic for the anisotropy estimated near the slab where stresses are 683 generally high (about 1 MPa), agreeing with the conclusion of McNamara et al. (2002). 684

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#### 5.5 Limitations

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As previously mentioned, a study of Girard et al. (2015) found that bridgmanite 686 is substantially stronger than ferropericlase and largely accommodates strain in the lower 687 mantle. Whilst Girard et al. (2015) suggested that bridgmanite only absorbs 30% of de-688 formation in the lower mantle, when taking such results into account in our modelling, 689 we obtained weak fast-SH radial anisotropy anomalies of <+1% in the ULM which are 690 not compatible with the seismic tomography images. In addition, our results disagree 691 with those found in a recent study by Boioli et al. (2017) that suggests a pure climb de-692 formation mechanism whereby seismic anisotropy due to LPO is not present in the lower 693 mantle. It is worth to note, however, that the experimental crystal aggregates deformed 694 by Girard et al. (2015) contain 30% of ferropericlase. If this is the case, it is unclear which 695 other mechanism could explain the observed radial anisotropy anomalies, as grain-scale 696 SPO, for example, does not produce significant anisotropy for penetrating subducting 697 slabs. This is substantially higher than the 17% volume fraction found in pyrolite, with 698 the consequence that bridgmanite could accommodate more deformation at the expense 699 of the less abundant ferropericlase. Our LPO and SPO modelling have only been com-700 pared to one tomography model. Ferreira et al. (2019) showed a good level of agreement 701 between the radial anisotropy patterns in SGLOBE-rani and in its contemporaneous sa-702 vani model near slabs in the mid-mantle. Future comparisons with new anisotropy to-703 mography models will be important to further test the geodynamical models. 704

On the other hand, our micro- and macro-geodynamic modelling also have their 705 own limitations, which are mainly related to the rheological properties of mantle's min-706 erals. In particular, relative slip system activities and the flow law parameters for man-707 tle aggregates are still uncertain, especially in the lower mantle. For mid-mantle aggre-708 gates, we only consider the slip system with the lowest CRSS, however, the conclusions 709 of this study may be different if two or more slip systems have the same CRSS. Given 710 the existing large uncertainties of the CRSS of the different slip systems of bridgman-711 ite, investigating the contributions of two or more slip systems remains an area for fu-712 ture work. Nevertheless, this is a common assumption used when the uncertainties of 713 the CRSS of the different slip systems are significantly high (Tommasi et al., 2004), which 714 is the case e.g. for bridgmanite. The contribution to lower mantle anisotropy from fer-715 ropericlase is also not taken into account in this study, which has been reported to be 716 the dominant cause of anisotropy across and below the pressure-induced iron spin tran-717

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sition (below about 1,200 km depth) (Marquardt et al., 2009). There are also trade-offs
involved in the modelling, for example between the grain boundary mobility and the amount
of deformation absorbed by a mineral, such as bridgmanite. Future mineral physics efforts in these directions will help us better constrain our geodynamic and mantle fabric calculations.

It is worth noting other potential causes of anisotropy in the mid-mantle. At middle-723 transition zone conditions, representative dense hydrous magnesium silicate (DHMS) phases 724 B and D remain stable. Superhydrous phase B remains less anisotropic than wadsleyite, 725 but in contrast phase D can be more anisotropic than wadsleyite (Mookherjee & Tsuchiya, 726 2015). However, these minor phases have a limited thermal stability field, being mostly 727 stable within the slab (e.g., Frost, 1999; Pamato et al., 2015). Thus, they are are unlikely 728 to be responsible for large scale anisotropy. Further calculations of extrinsic anisotropy 729 associated with compositional heterogeneity by Faccenda et al. (2019) suggested mod-730 est SPO throughout the mantle, apart from around the 660-km discontinuity, where anisotropy 731 could be possibly related to grain-scale shape-preferred orientation. An alternative mech-732 anism to explain the observations is the alignment of fluid-pockets in the uppermost lower 733 mantle. (e.g., Holtzman & Kendall, 2010). These structures could be generated as a con-734 sequence of the entrainment of hydrous TZ material at lower mantle depths by the slab. 735 As lower mantle minerals have very low hydrogen solubility, partial melting of the meta-736 somatized mantle rocks could occur. A small fraction of subhorizontally aligned melt pock-737 ets would be then sufficient to explain the positive radial anisotropy below stagnating 738 slabs. 739

#### 740 6 Conclusion

Using 3-D petrological-thermo-mechanical modelling, three subduction models were 741 investigated: (i) slab stagnation at the bottom of the transition zone; (ii) slab trapped 742 in the ULM; and, (iii) slab penetration into the deep lower mantle. Mantle fabric cal-743 culations were conducted to investigate possible contributions to radial anisotropy in the 744 mid-mantle from LPO and SPO mechanisms. The UTZ develops a disjointed mantle fab-745 ric of fast-SV radial anisotropy when considering LPO, where induced poloidal flow re-746 sets some anisotropy at phase transitions. The LTZ remains isotropic due to the cubic 747 symmetry and low single crystal anisotropy of ringwoodite and garnet aggregates. SPO 748 modelling shows fast-SH radial anisotropy anomalies in the majority of the transition 749

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zone, which does not match the seismic tomography images. Fast-SH radial anisotropy 750 anomalies of  $\sim +2\%$  appear in the ULM when considering the LPO mechanism, and grain-751 scale SPO could also contribute to radial anisotropy at ULM depths, but not below deeply 752 penetrating slabs due to the small contrast in isotropic elastic moduli. These observa-753 tions agree with seismic tomography images and with results from shear-wave splitting 754 analysis (Wookey & Kendall, 2004; Walpole et al., 2017). We tested nine potential slip 755 systems for bridgmanite, of which four lead to a good consistency between the mantle 756 fabric modelling and the seismic tomographic images: [100](010), [010](100), [001](100)757 and <110>{ $\overline{110}$ }. Recent deformation experiments at ULM conditions imply the dom-758 inant slip system of bridgmanite is [001](100) (Tsujino et al., 2016), which was also high-759 lighted by this study. 760

With global radially anisotropic tomographic models starting to show improved cor-761 relation, comparing them with geodynamic modelling is proving a powerful tool to in-762 terpret seismic anisotropy. Whilst there are still limitations in the geodynamic modelling, 763 in particular the fact that the rheology of the mantle is still largely unknown, this study 764 gives support to LPO being the preferred mechanism for the observed radial anisotropy 765 in the mid-mantle. Given that subducting slabs likely exert high stress in the surround-766 ing mantle, the observed radial anisotropy anomalies suggest that dislocation creep is 767 active in the mid-mantle. 768

#### 769 Acknowledgments

This research was initially supported by the Leverhulme Trust (project F/00~204/AS), 770 followed by support by NERC project NE/K005669/1 and the Korea Meteorological Ad-771 ministration Research and Development Program under grant KMI 2018-09312. W.S. 772 was supported by the Natural Environment Research Council [grant number NE/L002485/1]. 773 A.M.G.F. also thanks discussions supported by COST Action ES1401-TIDES. M.F. was 774 supported by the ERC StG #758299 NEWTON and the Progetto di Ateneo FACCP-775 TRAT12 granted by the Universita' di Padova. Geodynamic simulations were performed 776 on Galileo Computing Cluster, CINECA, Italy, thanks to the computational time assigned 777 to M.F. under the NUMACOP, NUMACOP2 and NUMACOP3 projects. We thank our 778 colleagues John Brodholt, David Dobson and Alex song for fruitful discussions. We are 779 grateful to the editor Maureen Long and two anonymous reviewers for their valuable com-780 ments, which helped improve this manuscript. We are also grateful to Carolina Lithgow-781

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Bertelloni and Lars Stixrude for providing HeFESTo's results and to Zhigang Zhang for 782 providing bridgmanite's full elastic constants from ab-initio calculations. The code for 783 the large scale subduction models (I3MG) was kindly provided by Taras Gerya, and the 784 mantle fabric calculations used a modified version of the code D-REX available at http:// 785 www.ipgp.fr/~kaminski/web\_doudoud/DRex.tar.gz. Once published, the results of the 786 geodynamical simulations will be freely available in NERC's data repository. SGLOBE-787 rani can be downloaded from the IRIS website at http://ds.iris.edu/ds/products/ 788 emc-sglobe-rani/. 789

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Figure 1. Cross-sections of perturbations in Voigt average and radially anisotropic structure of subduction zones in the Western Pacific. Cross-sections of the global tomography model SGLOBE-rani beneath Northern Kurile, Southern Kurile, Honshu, Northern Bonin, Southern Bonin, Northern Mariana, Western Java, Eastern Java and Kermadec.  $V_S$  denotes perturbations in the Voigt average model  $\left(V_{Voigt}^2 = \frac{2V_{SV}^2 + V_{SH}^2}{3}\right)$  with respect to PREM (Dziewonski & Anderson, 1981) down to the core-mantle boundary and  $\xi$  denotes perturbations in radial anisotropy  $\left(\xi = \frac{V_{SH}^2}{V_{SV}^2}\right)$  down to 1,400 km depth (below this depth the resolution is more limited, see Chang et al., 2015). Focal depths from EHB data (Engdahl et al., 1998) with an upper bound of 60 km are superimposed on the cross-sections as grey circles. The depths of 410 km, 660 km and 1,000 km are represented by solid black lines. For reference, we use the same geographical locations and codes (Cross-sections Northern Kurile J, Southern Kurile E, Honshu E, Northern Bonin G, Southern Bonin E, Northern Mariana J, Western Java J, Eastern Java E and Kermadec H) as in -37-



Figure 2. Fraction of deformation accommodated by dislocation creep  $(\frac{\eta_{eff}}{\eta_{disl}}; \text{ top row})$ , second invariant of the stress tensor  $(\sigma'_{II}; \text{ middle row})$  and mantle velocity vectors overlain upon the second invariant of the strain tensor  $(\varepsilon'_{II}; \text{ bottom row})$  for stagnant (first column), trapped (second column) and penetrating (third column) slab models.



Figure 3. The effects of mantle fabric parameters on radial anisotropy. From left to right: the effect of increasing the grain boundary mobility (M\*) to 10 (a, d), 125 (b, e) and 200 (c, f) respectively, where dislocation creep accommodates 100% of the bulk deformation in the lower mantle. From top to bottom: the effect of changing the amount of the bulk deformation accommodated by dislocation creep in the lower mantle from 100% to 30%. All images show radial anisotropy produced by significantly deformed aggregates  $\left(\ln\left(\frac{FSE_{max}}{FSE_{min}}\right)>0.5\right)$  and interpolated to a grid with spacings 200 × 100 × 200 km (x, y, z coordinates, respectively). The slab is coloured in grey.



Comparison of seismic tomography with geodynamic modelling for a slab stag-Figure 4. nating at the bottom of the transition zone. (a) Comparison between cross-sections of radially anisotropic structure from SGLOBE-rani beneath Honshu and results from geodynamic simulations for a slab stagnating at the bottom of the transition zone. The top image shows a cross-section of perturbations in radial anisotropy  $\left(\xi = \frac{V_{SH}^2}{V_{SV}^2}\right)$  from SGLOBE-rani at Honshu (crosssection Honshu C from Fukao & Obayashi, 2013). The green contours correspond to an outline of the Voigt average fast anomalies from SGLOBE-rani, in the range of 1.25-1.5%. This contour is based on observations and therefore aids in the understanding of the relationship between the slab and anisotropy anomalies. Below this is the computed LPO due to dislocation creep for the [001](100) bridgmanite slip system. We show in the bottom right hand corner the corresponding  $dV_S$  (km/s) calculated at lower mantle P-T conditions for a 80:20=Brd:Fp mixture deformed in horizontal simple shear ( $\xi$ =1.0); red is minimum; blue is maximum. Cubic MgO crystals are random. The bars in the  $dV_S$  maps indicate the polarisation of the fast shear wave component for different propagation directions. Below this is a geodynamic image showing grain-scale SPO assuming a perfectly layered medium for a pyrolitic medium. (b) LPO due to dislocation creep for the nine slip systems of bridgmanite where each slip system is set five times weaker than the rest, ab-initio calculations are from Mainprice et al. (2008). All geodynamic images have a resolution -40of  $200 \times 100 \times 200$  km (x, y, z coordinates, respectively) and show radial anisotropy produced when the minimum  $\ln\left(\frac{FSE_{max}}{FSE_{min}}\right) > 0.5.$ 



Figure 5. 3-D representations of the finite strain ellipsoid (FSE) for the three subduction scenarios considered in this study. The orientations of the maximum  $(a_1)$  FSE axis for the mantle aggregates where  $\ln\left(\frac{a_1}{a_3}\right) > 0.5$  are shown, providing a clear LPO. The bar length is proportional to  $\ln\left(\frac{a_1}{a_3}\right)$ , as well as the colour scale. The slab is coloured in grey.



Figure 6. Comparison of the seismic tomography model SGLOBE-rani (Chang et al., 2015) with geodynamic modelling results for a slab trapped in the uppermost lower mantle. Figure details are the same as in Figure 4, but for trapped slab. The seismic tomography image is from Northern Kurile (cross-section Northern Kurile J from Fukao & Obayashi, 2013).



Figure 7. Comparison of the seismic tomography model SGLOBE-rani (Chang et al., 2015) with geodynamic modelling results for slab penetration deep into the lower mantle. Figure details are the same as in Figures 4 and 6, but for a deeply penetrating slab. The seismic tomography image is from Western Java (cross-section Western Java I from Fukao & Obayashi, 2013).



Figure 8. Comparisons of 1-D average radial anisotropy  $\left(\xi = \frac{V_{SH}^2}{V_{SV}^2}\right)$  depth profiles from the mantle fabrics simulations (a-c) and from the tomographic model SGLOBE-rani (d) (Chang et al., 2015). The mantle fabric 1-D profiles represent mean values of anisotropy present in the whole model domain as shown in Figures 4, 6 and 7. For LPO, the nine possible bridgmanite slip systems and ab-initio calculations from Mainprice et al. (2008) are plotted, along with SPO calculations. The results are shown for the subduction scenarios of slab stagnation at the bottom of the transition zone (a), slab trapped in the uppermost lower mantle (b) and slab penetration deep into the lower mantle (c). Panel (d) shows depth-dependent 1-D average profiles of radial anisotropy in the model SGLOBE-rani for eleven subduction zones considered: Northern Kurile, Southern Kurile, Honshu, Northern Bonin, Southern Bonin, Northern Mariana, Eastern Java, Western Java, Kermadec, Northern Central America, Northern Peru; their averages are calculated by considering all points in a  $2^{\circ} \times 2^{\circ}$  grid of the tomographic model SGLOBE-rani that align with all five profiles of each subduction region as defined in Fukao and Obayashi (2013) in grey, their average (red) and the global 1-D average (black). Horizontal dashed lines at 660 km and 1,200 km are used to represent the depth bounds of the uppermost lower mantle. We choose not to interpret anisotropy beneath  $\sim 1,400$  km in (d) due to the poor balance between SV- and SH-sensitive travel-time data in the body-wave datasets used in current tomography models to constrain lower mantle structure (e.g., Chang et al., 2014, 2015).