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1 **An inversion approach for analysing the physical properties of a**  
2 **seismic low-velocity layer in the upper mantle**

3

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15

16 **Abstract**

17 In this article, we propose a new inversion scheme to calculate the melt volume

18 fractions from observed seismic anomalies in a low-velocity layer (LVL) located atop

19 the mantle transition zone. Our method identifies the trade-offs in the seismic

20 signature caused by temperature, solid composition, melt volume fraction, and

21 dihedral angle at the solid-melt interface. Using the information derived from the

22 amplitude of *P*-to-*S* conversions beneath the western US, we show that the multiple

23 permissible solutions for melt volume fractions are correlated to each other. An  
24 existing solution can be directly transformed into a different solution whilst leaving the  
25 model output unaltered. Hence, the additional solutions can be rapidly derived given  
26 an initial solution. The calculation of multiple solutions reveals the universal properties  
27 to the whole range of solutions. A regional-averaged melt volume fraction of at least  
28 0.5% exists in every solution. In addition, the mantle potential temperature in the  
29 western US is broadly lower than 1550 K and the LVL in this region tends to be basaltic-  
30 rich. Using these insights, it is possible to give firm statements on the LVL and the solid  
31 mantle even though a unique interpretation does not exist.

32

33 **Keywords:** Shear wave, low-velocity layer, partial melting, inverse problem, non-  
34 uniqueness

35

## 36 **1 Introduction**

37 The mantle transition zone (MTZ), marked by a drastic change in the physical  
38 properties of the silicate mineral phases, plays a crucial role in the convective flow  
39 within the mantle. Owing to the sharp changes in density and volatile storage capacity  
40 across the boundaries of the MTZ, it can act as an impediment to mass transfer and  
41 sights of partial melting ([Bercovici and Karato, 2003](#); [Morra et al., 2010](#)). Indirect  
42 evidence of mass transfer between subducting slabs and surrounding mantle are  
43 obtained from the so-called 'superdeep diamonds' which bear geochemical signature  
44 of oxygen and carbon isotopic ratios that can be generated by mixing between mantle

45 and subducting slabs at these depths. Seismic observations also support the evidence  
46 of partial melting atop the MTZ. A low-velocity layer (LVL) located at ~350 km depth  
47 has been identified just above the mantle transition zone in numerous regions around  
48 the world, with lateral thickness from tens to over a few hundred kilometres (e.g. [Song  
49 et al., 2004](#); [Gao et al., 2006](#); [Courtier and Revenaugh, 2007](#); [Schaeffer and Bostock,  
50 2010](#); [Huckfeldt et al., 2013](#)). Characterized by 2 – 3% reductions in shear wave  
51 velocities, the LVL is characterized by a sharp interface with the overlying mantle,  
52 indicating the likely presence of a chemical anomaly, in particular partial melting.  
53 However, quantifying the fraction of melt has remained challenging as the  
54 environmental and chemical parameters, such as the mantle temperature, bulk solid  
55 composition and melt geometry, are not clearly understood.

56 The 350-km LVL has been frequently interpreted as a seismic signature of a small  
57 fraction of melt triggered by volatile elements released from subduction zones  
58 ([Revenaugh and Sipkin, 1994](#)) or mantle plumes ([Vinnik and Farra, 2007](#)). Since melts,  
59 characterized by zero shear modulus, disproportionately reduce shear wave velocities,  
60 seismic anomalies with low velocities are often qualitatively attributed to melting.  
61 Interpreting the origin of the seismic velocity anomalies in the LVL is complicated due  
62 to the competing influence of several parameters. While an increase in the  
63 temperature typically leads to seismic velocity reductions, the influence of bulk mantle  
64 composition on seismic velocities varies with depth ([Xu et al., 2008](#)). The multiple  
65 factors also likely affect each other. For instance, melting may leave a strong impact on  
66 the bulk solid composition, in particular the amount of basalt. The residual anomaly,

67 defined as the difference between the observed shear velocity and the reference  
68 velocity, can be attributed to the presence of melting, and used as a basis for  
69 calculating the volume fraction of melt in the LVL. Hence, calculation of the melt  
70 fraction requires accurate estimation of the reference seismic velocities, i.e. velocities  
71 in the absence of melting for given temperature and solid composition.

72 In addition, the non-uniqueness in the LVL interpretations arises from the fact  
73 that, in a partially molten layer, the seismic velocity reductions depend on both the  
74 melting extent and the microstructure of the melt-bearing aggregates ([Mavko, 1980](#);  
75 [von Bargaen and Waff, 1986](#); [Takei, 1998, 2002](#)). The dihedral angle (also known as  
76 wetting angle) at the solid-melt interface, controls the geometry of the load-bearing  
77 framework of partially molten rocks ([Hier-Majumder and Abbott, 2010](#)), trading off  
78 with inferred melt volume fraction . The chemical composition is also found to play a  
79 moderate role in reducing the seismic speeds ([Wimert and Hier-Majumder, 2012](#); [Hier-](#)  
80 [Majumder et al., 2014](#)), and may alter the dihedral angle ([Yoshino et al., 2005](#)). The  
81 numerical experiment of ([Hier-Majumder et al., 2014](#)) indicated the difficulties in  
82 distinguishing different types of melt from the seismic observations as the fraction of  
83 melt is very small. These therefore lead to extra non-uniqueness in the interpretation  
84 of seismic anomalies.

85 A number of previous studies mitigated the issue of competing influences by  
86 carrying out computationally expensive brute-force search to create lookup tables for  
87 inferred melt volume fractions corresponding to different controlling factors (e.g. [Hier-](#)  
88 [Majumder and Courtier, 2011](#); [Hier-Majumder et al., 2014](#); [Hier-Majumder and Tauzin,](#)

89 [2017](#)). While a brute-force search can produce a particular scenario of inversion,  
90 application of the approach is unable to ascertain if alternative solutions exist in the  
91 parameter space. Although, in principle, the entire range of solutions could be  
92 discovered through repetitive use of the algorithm given different combinations of the  
93 parameters, it fails to rigorously tackle the nature of variations in the inferred melt  
94 volume fractions caused by changes in the other factors. Therefore, a new inversion  
95 scheme is required to interpret these geophysical observations and to address the  
96 theoretical drawback of previous studies.

97       Here we present a mathematical formulation that uses the implicit symmetry of a  
98 petrologic model to understand the non-uniqueness in the melt fraction inference. The  
99 results from our work provide a more reliable evaluation of the long-standing problem  
100 in rock physics. The principle of symmetry has been successfully applied in a sequence  
101 stratigraphic problem ([Xiao and Waltham, 2019](#)), showing that the whole set of  
102 solutions are closely linked even when an inverse problem is non-linear. An existing  
103 solution can be directly transformed into another solution that leaves modelling  
104 products unchanged, in the same way that rotating a square by  $90^\circ$  can produce an  
105 identical geometry. In this way, the search for all possible solutions can begin with an  
106 initial solution generated through standard inversion techniques. The application of  
107 the symmetry method can then allow the additional solutions to be calculated from  
108 the initial solution.

109       Embedded with a predictive forward model of shear-velocities, our inversion  
110 scheme is used to revisit the nature of the 350-km LVL beneath the western US. The

111 seismically anomalous layer in this region has been reported underneath the Oregon-  
112 Washington border (e.g. [Song et al., 2004](#)), the Yellowstone (e.g. [Fee and Dueker,](#)  
113 [2004](#); [Jasbinsek and Dueker, 2007](#)), the Northern Rocky Mountains (e.g. [Jasbinsek and](#)  
114 [Dueker, 2007](#); [Zhang et al., 2018](#)), the Colorado Plateau/Rio Grande Rift (e.g. [Jasbinsek](#)  
115 [et al., 2010](#)), and California (e.g. [Vinnik et al., 2010](#)). Once the complete set of solutions  
116 has been derived, the lowest and highest possible fractions of melt within the LVL can  
117 be easily determined. As such, we can generate a robust statement on the partial  
118 melting effect in the LVL that does not rely on assumed values of the other  
119 parameters. The calculation can also offer more reliable information about the solid  
120 mantle, such as the plausible ranges of temperature and basalt fraction. For example,  
121 the estimates of melt content and associated parameters can be used to infer the  
122 budget of volatile elements in the mantle and the excess temperature of the mantle  
123 plumes beneath the region.

124

## 125 **2 The 350-km LVL beneath the western US**

### 126 *2.1 Seismic observations*

127 The seismic data used here are teleseismic *P*-to-*S* conversions recorded on  
128 receiver functions from the Transportable Array of seismic stations in the western US  
129 (fig. 1). The portion of the seismic network consists in 820 seismic stations. Shear wave  
130 velocity contrasts at around 350 km have been derived for 583 sites over a 0.5° x 0.5°  
131 grid in latitude and longitude. The seismically anomalous layer covers an area of 1.8 ×  
132 10<sup>6</sup> km<sup>2</sup>, with lateral thickness from 25 to 90 km ([Hier-Majumder and Tauzin, 2017](#)).

133 2.2 Calculating shear wave velocities

134 To invert the shear wave speeds in the LVL from the seismic observations, we  
135 follow the computational approach outlined in [Hier-Majumder et al. \(2014\)](#). We use  
136 the results of conversion amplitudes at the top and the base of the LVL to estimate the  
137 velocity variations. To eliminate systematic variations in the amplitude of converted  
138 arrivals caused by the acquisition geometry (seismic wave incidence), we normalize the  
139 observed seismic amplitudes prior to computation. The normalized amplitude is  
140 calculated from the ratio of amplitudes of arrivals converted at the top of the LVL over  
141 arrivals converted at the olivine-wadsleyite mineralogical phase change at 410 km  
142 depth:

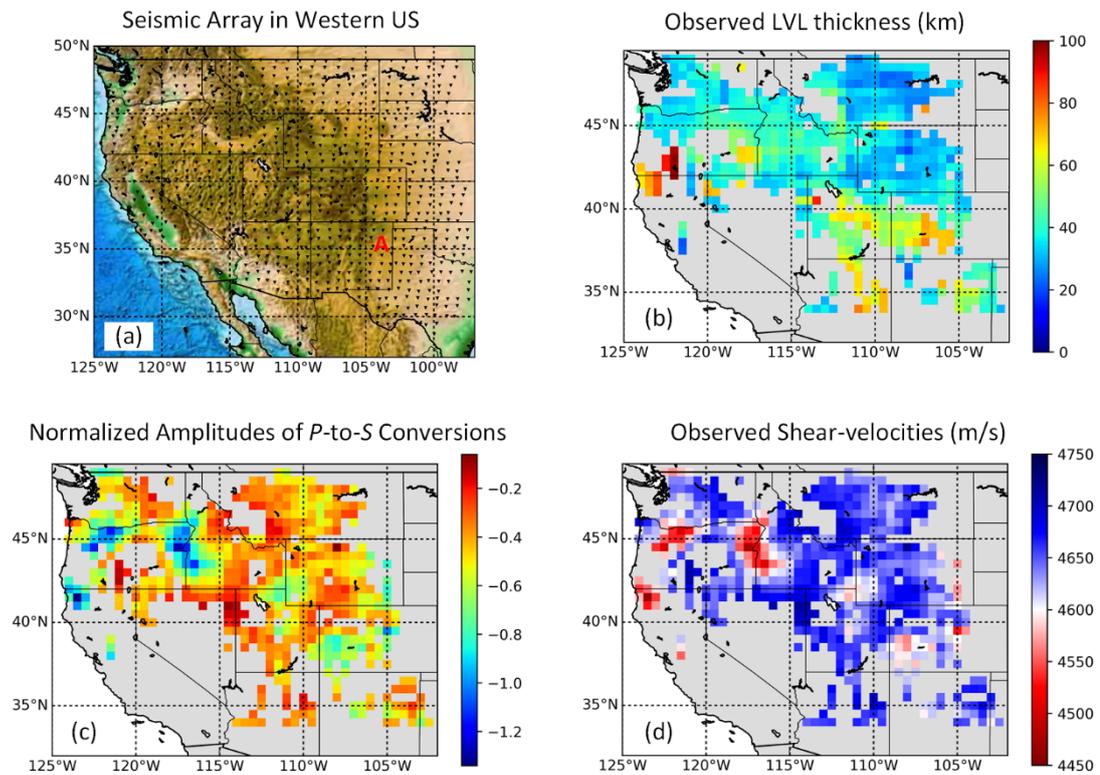
$$R_{\text{norm}} = \frac{A_{\text{LVL}}}{A_{410}} < 0 \quad (1)$$

143 , where  $A_{\text{LVL}}$  is the frequency-averaged amplitude at the top of the LVL recorded at  
144 each cell on the grid, and  $A_{410}$  is the frequency-averaged amplitude at the 410-km  
145 discontinuity in the same cell. Using the normalized  $R_{\text{norm}}$ , we then calculate the shear  
146 wave velocity ( $V_S^{\text{obs}}$ ) at each location from the normalized contrast between the shear-  
147 velocity immediately above the 350-km LVL ( $V_S^{350}$ ) and the velocity immediately below  
148 the 410-km discontinuity ( $V_S^{410}$ ):

$$V_S^{\text{obs}} = V_S^{350} \left( 1 + R_{\text{norm}} \frac{V_S^{410} - V_S^{350}}{V_S^{350}} \right) \quad (2)$$

149 We calculate  $V_S^{350}$  and  $V_S^{410}$  as the shear wave velocities at the depths of 350 km and  
150 410 km, respectively, from the Preliminary Reference Earth Model (PREM, Dziewonski

151 and Anderson, 1981). Compared to the global predictions from the PREM ( $\sim 4735\text{m/s}$  at  
 152 350 km depth), the estimated shear-velocities yield an average reduction of 1.6%.  
 153



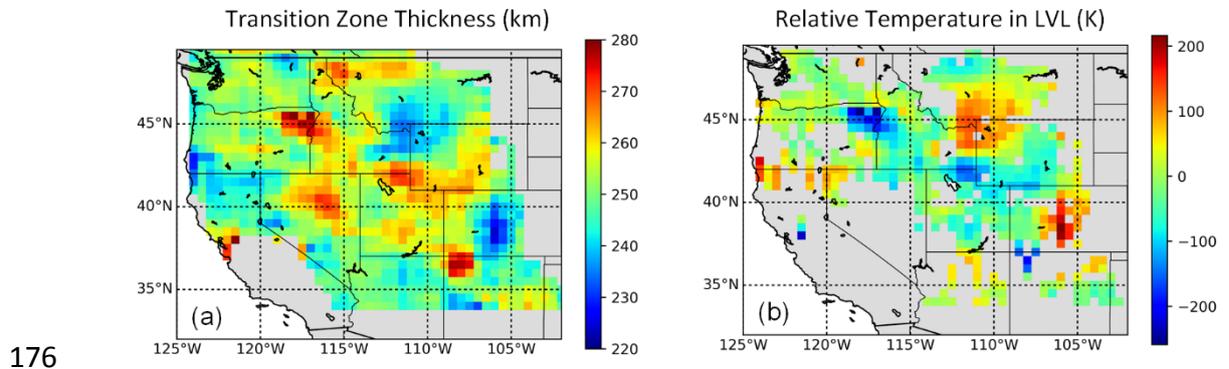
154  
 155 **Figure 1** Seismic observations of the 350-km LVL below the western US. (a) A map of the dense  
 156 seismic array of 820 sites ([black triangles, from Tauzin et al., 2013](#)). The seismic cell (106.5°W,  
 157 38°N) discussed later in this paper is labelled 'A'. (b) The 350-km LVL with lateral thickness is  
 158 identified beneath 583 sites ([from Hier-Majumder and Tauzin, 2017](#)). (c) Normalized amplitudes of  
 159 *P*-to-*S* converted arrivals. (d) Shear wave velocities in the LVL estimated from the seismic data

160

### 161 2.3 Evaluating relative temperature variations

162 We then evaluate the thermal variations in the LVL using the method outlined in  
 163 [Tauzin and Ricard \(2014\)](#). In this method, the relative temperature variations ( $\Delta T$ ) on  
 164 boundary topography are correlated with the relative thickness of the MTZ ( $\delta h$ ) and

165 the Clapeyron slopes (i.e. the change in temperature of phase transition with respect  
 166 to the change in pressure at which the phase transition occurs) for the olivine-  
 167 wadsleyite phase transitions at 410 km ( $\gamma_{410}$ ) and 660 km ( $\gamma_{660}$ ). We employ the data  
 168 of spatial variations in MTZ thickness beneath the western half of the US from [Tauzin](#)  
 169 [et al. \(2013\)](#). We also set the reference MTZ thickness at 250 km as [Tauzin and Ricard](#)  
 170 [\(2014\)](#) calculated from the IASP91 spherical model of [Kennett and Engdahl \(1991\)](#). We  
 171 follow the empirical scheme of [Tauzin and Ricard \(2014\)](#) and set  $\gamma_{410} = 3.0$  MPa/K and  
 172  $\gamma_{660} = 0.64 \gamma_{410} - 1.17$ . The uncertainties associated with the supplementary  
 173 parameters will be discussed in later sections. Using these methods, we calculate the  
 174 temperature variations in the LVL from the MTZ thickness beneath the seismic array.  
 175



176  
 177 **Figure 2** Thickness of MTZ (a) and relative temperature variations in the LVL (b) estimated from the  
 178 MTZ thickness ([after Tauzin and Ricard, 2014](#))

179

180 **3 Forward modelling**

181 The forward model of shear-velocities presented here incorporates four primary  
 182 controls, including the mantle potential temperature, bulk solid composition, melt  
 183 volume fraction and dihedral angle at the solid-melt interface. The simulation of shear

184 wave speeds in the LVL consists of two independent phases. Firstly, we estimate the  
185 reference velocities from the properties of the solid mantle. Secondly, we calculate the  
186 changes in velocities as waves travelling through a melt-bearing aggregate using a  
187 micromechanical model that involves both the fraction and geometry of the melt.

188

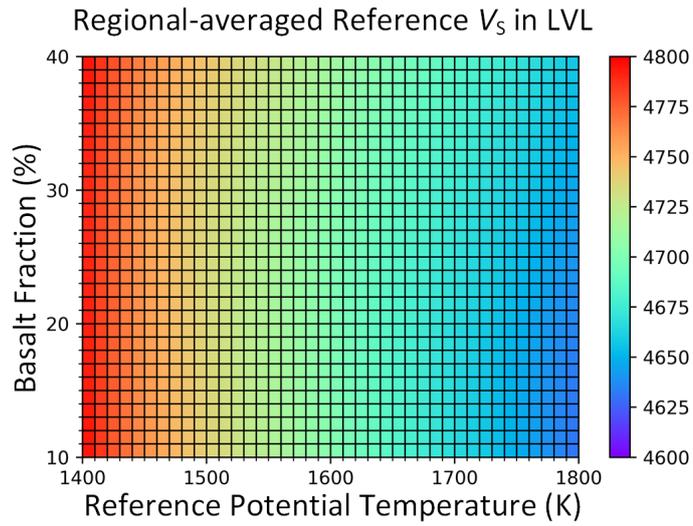
### 189 *3.1 Estimating reference velocities*

190 We estimate the reference shear wave speeds in the solid mantle accounting for  
191 the thermal and compositional properties of the mineral. The mantle temperature  
192 below each site can be expressed as

$$T = T_0 + \frac{dT}{dz} z_{LVL} + \Delta T \quad (3)$$

193 , where  $T_0$  is the potential temperature of the reference mantle,  $dT/dz$  is the  
194 adiabatic temperature gradient which is suggested as 0.4 – 0.5 K/km in the upper  
195 mantle ([Katsura et al., 2010](#)),  $z_{LVL}$  is the depth of LVL and  $\Delta T$  is the relative  
196 temperature variation at a given location. We set  $z_{LVL}$  at the average depth of 352 km  
197 as observed from the seismic profiles. To quantify the mantle composition, we follow  
198 the definition from [Xu et al. \(2008\)](#) which parameterizes the solid bulk as a mechanical  
199 mixture of mid-ocean ridge basalt and harzburgite. The composition of the solid  
200 mantle can therefore be expressed as the volume fraction of basaltic component. We  
201 can then formulate the reference shear wave velocities as  $V_S^{\text{ref}} = V_S^{\text{ref}}(T_0, C)$ , where  
202  $T_0$  and  $C$  are the potential temperature and basalt fraction of the mantle, respectively.

203 Reference shear wave speeds applied here are derived from the mineral physics  
204 database of [Xu et al. \(2008\)](#), in which seismic velocities are tabulated with associated  
205 combinations of potential temperatures and basalt fractions. In the database,  
206 potential temperatures range from 1000 to 2000 K with increments of 100 K whereas  
207 basalt fractions range from 0 to 100% with increments of 5%. While we can select a  
208 given value of  $C$  for the calculation, the temperature at any point on the seismic grid is  
209 determined from the MTZ thickness as discussed above. As a result, we interpolate the  
210 value of seismic velocity for the temperature evaluated at each location using a  
211 second-order polynomial interpolation between two tabulated values. Using this  
212 interpolation, we are able to calculate the value of reference shear wave speed at each  
213 point for a given bulk basalt volume fraction and a given reference potential  
214 temperature. Figure 3 presents the predictions of regional-average shear wave speeds  
215 for a range of potential temperatures and basalt fractions at a constant pressure of  
216 11.7 GPa. The thermal and compositional effects can trade off with each other and  
217 thus different combinations of the two variables may lead to the same velocities.  
218



219

220 **Figure 3** A heatmap showing the predicted regional-averaged reference shear wave velocities at

221 11.7 GPa in response to different combinations of reference potential temperature and basalt

222 fraction in the LVL beneath the western US

223

### 224 3.2 Partial melting and velocity reductions

225 To simulate the influence of partial melting on seismic velocities, we employ the

226 modelling scheme of [Takei \(2002\)](#), where the shear wave speed variation  $\xi$  is governed

227 by the effective elastic moduli of the aggregate:

$$\xi = \sqrt{\frac{N/\mu}{\bar{\rho}/\rho_s}} \quad (4)$$

228 , where  $N$  is the elastic modulus of the intergranular skeletal framework that indicates

229 the strength of contact between the neighbouring grains;  $\mu$  is the shear modulus;  $\rho_s$  is

230 the density of the solid bulk; and  $\bar{\rho}$  is the volume-averaged density of the entire

231 aggregate which is calculated as:

$$\bar{\rho} = \rho_m \varphi + \rho_s (1 - \varphi) \quad (5)$$

232 , where  $\rho_m$  is the density of the melt;  $\varphi$  is the volume fraction of melt within the  
233 aggregate.

234 In eq. 4, the elastic modulus  $N$  is determined by both the melt volume fraction  $\varphi$   
235 and the contiguity ( $\psi$ , i.e. the area fraction of the intergranular contact) of the melt:

$$N = \mu(1 - \varphi)[1 - (1 - \psi)^n] \quad (6)$$

236 The contiguity  $\psi$  depends on the melt volume fraction  $\varphi$  and the dihedral angle  $\theta$   
237 between the solid grains and the melt; and  $n$  is an exponent also depending on  $\psi$   
238 ([Takei, 2002](#)). The simulations of contiguity applied here are based on the micro-  
239 structural model of [von Bargaen and Waff \(1986\)](#) which formulates the contiguity  $\psi$  as  
240 the proportion that the contact area of grains occupy among the total contact area in a  
241 partial molten aggregate:

$$\psi = \frac{2A_{gg}}{2A_{gg} + A_{gm}} \quad (7)$$

242 , where  $A_{gg}$  and  $A_{gm}$  are the grain-grain contact area and grain-melt contact area per  
243 unit volume, respectively. The values of  $A_{gg}$  and  $A_{gm}$  are calculated from the given  
244 melt volume fraction and dihedral angle using polynomial functions:

$$\begin{cases} A_{gg} = \pi - b_{gg}\text{power}(\varphi, p_{gg}) \\ A_{gm} = b_{gm}\text{power}(\varphi, p_{gm}) \end{cases} \quad (8)$$

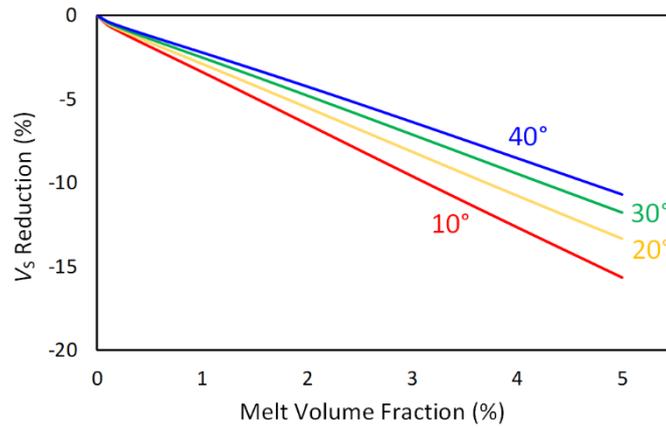
245 The required constants  $b_{gg}$ ,  $b_{gm}$ ,  $p_{gg}$  and  $p_{gm}$  are approximated from quadratic  
246 polynomials of the dihedral angle (in degree), of which the values are outlined in [von](#)  
247 [Bargaen and Waff \(1986\)](#). Wimert and Hier-Majumder (2012) indicated this

248 approximation of contiguities can produce satisfactory fits with experimental  
249 measurements from partially molten aggregates with melt volume fractions below 5%.

250 Combining equations 3—7 enables the contiguity to be expressed as a function of  
251 the melt volume fraction  $\varphi$  and dihedral angle  $\theta$ , i.e.  $\psi = \psi(\varphi, \theta)$ . Moreover, shear  
252 wave speed anomalies  $\xi$  caused by partial melting can be formulated as a function  
253 with respect to melt volume fraction and dihedral angle:

$$\xi(\varphi, \theta) = \sqrt{\frac{(1 - \varphi)[1 - (1 - \psi(\varphi, \theta))^n]}{1 - \varphi(1 - \rho_m/\rho_s)}} \quad (9)$$

254 We estimate the densities of solid bulk  $\rho_s$  and melt  $\rho_m$  using the third-order Birch-  
255 Murnaghan equation of state (EOS), as [Ghosh et al. \(2007\)](#) suggested for carbonated  
256 peridotite melt. We implement the mathematic approximations using a Python  
257 computational toolkit for microscale geodynamic study, named as Multiphase Material  
258 Properties forward model ([MuMaP, Hier-Majumder, 2017](#)). The modelled shear wave  
259 velocity reductions (in percentage) in response to a variety of melt volume fractions  
260 and dihedral angles are illustrated in fig. 4. Each of the curves in the cross-plot  
261 represents the shear wave velocity reductions caused by the melt with volume  
262 fractions from 0 to 5% at a fixed dihedral angle, showing that the velocity in the  
263 partially molten aggregates decreases rapidly as the fraction of melt increases. The  
264 upward shifting of the curves indicates that, for the same melt volume fraction, a  
265 smaller dihedral angle can result in greater reductions in the shear wave speed.  
266 However, different combinations of dihedral angles and melt volume fractions may  
267 produce the same extent of shear-velocity reduction.



268

269 **Figure 4** Predicted shear wave velocity reductions for different melt volume fractions and dihedral

270 angles. The corresponding dihedral angles to the curves are annotated on the plot. Each curve

271 shows the velocity reductions caused by changes in melt volume fraction at a fixed dihedral angle

272

#### 273 **4 Model inversion**

274 The forward modelling approach described in the preceding section predicts the

275 shear wave velocity reductions in response to associated parameters. Alternatively, if

276 seismic data of the LVL are available, it is possible to calculate the velocity reductions

277 as a ratio of the observed velocity over the reference velocities:

$$\xi = \frac{V_S^{\text{obs}}}{V_S^{\text{ref}}(T_0, C)} \quad (10)$$

278 When embedded with an inversion scheme, the numerical model can be used to

279 deduce the multiple controls on seismic velocities. The inversion procedure can begin

280 with an initial solution that is built upon petrologic and seismological constraints. We

281 then investigate how to exploit and utilize the symmetry of the model, which can allow

282 us to alter the initial solution directly into another solution whilst giving the same

283 observations. In this way, the additional solutions to the inverse problem can be  
284 rapidly derived by repetitively use of the transformation.

285

#### 286 4.1 An initial solution based on a priori knowledge

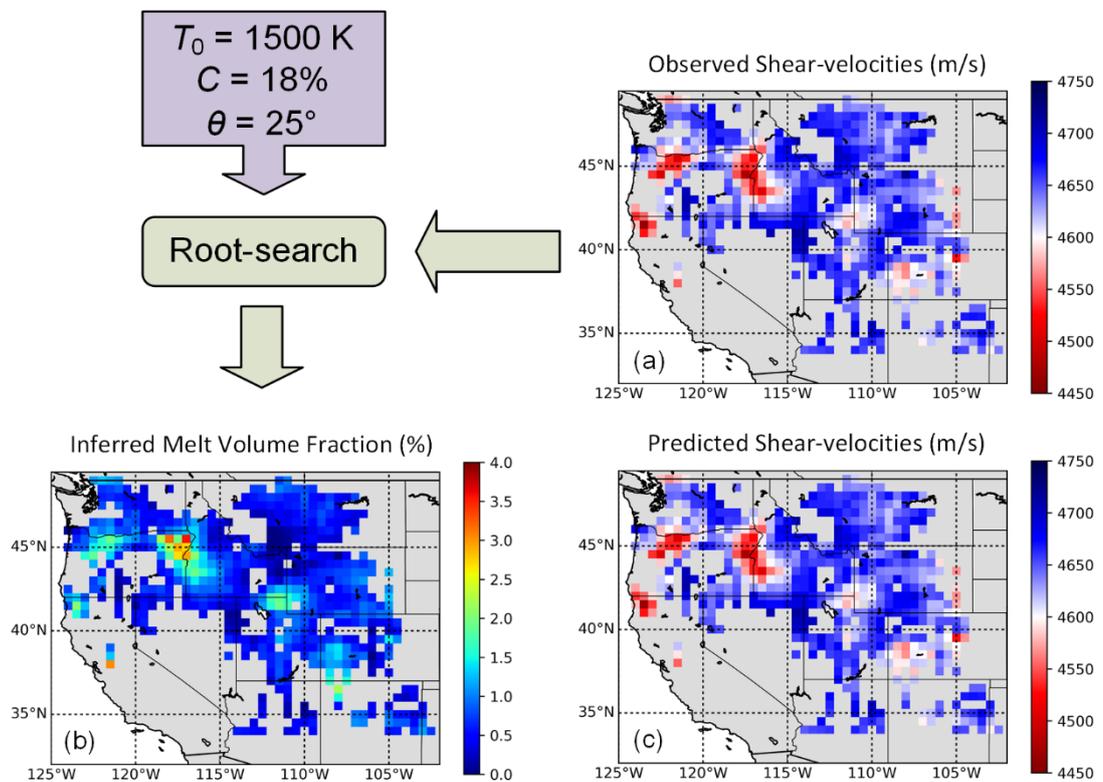
287 To incorporate the forward model and the observed data in a single framework,  
288 we firstly combine eq. 9 and 10:

$$\sqrt{\frac{(1 - \varphi) \cdot [1 - (1 - \psi(\varphi, \theta))^n]}{1 - \varphi(1 - \rho_m/\rho_s)}} = \frac{V_S^{\text{obs}}}{V_S^{\text{ref}}(T_0, C)} \quad (11)$$

289 , which gives four unknowns (i.e.  $T_0$ ,  $C$ ,  $\theta$  and  $\varphi$ ) in one equation. To solve melt volume  
290 fraction  $\varphi$  from the eq. 11, the reference potential temperature  $T_0$ , basalt fraction  $C$   
291 and dihedral angle  $\theta$  need to be specified. We initially assume the reference potential  
292 temperature to be 1500 K in the region. We set the basalt fraction at 18%, as  
293 suggested in [Xu et al. \(2008\)](#) for common peridotite. The dihedral angle at the grain-  
294 melt interface varies with the chemical composition of the melt. For example, [Minarik  
295 and Watson \(1995\)](#) proposed dihedral angles varying from 25 to 30° at the interface  
296 between carbonate melt and molten aggregates; [Mei et al. \(2002\)](#) suggested a dihedral  
297 angle of 28° for molten aggregates with hydrous basalt melt. Here we initially assume a  
298 dihedral angle of  $\theta = 25^\circ$ . Given these *a priori* assumptions,  $T_0$ ,  $C$  and  $\theta$  are specified,  
299 and hence the melt volume fraction can be solved from eq. 11.

300 We then calculate the corresponding melt volume fraction  $\varphi$  using a modified  
301 Newton-Raphson root-search algorithm ([Press et al., 2007, chap. 9.1](#)), same as the  
302 calculation in [Hier-Majumder and Tauzin \(2017\)](#). The algorithm begins with a bracket

303 for the melt volume fraction between  $1 \times 10^{-4}\%$  and 10% and iterates the searching  
 304 process until a convergence of  $10^{-4}\%$  is achieved in the inferred fraction. Figure 5  
 305 shows the initial solution derived from the inversion using the seismic observations  
 306 and the constraints on  $T_0$ ,  $C$  and  $\theta$ . The melt fractions in the region vary spatially and  
 307 yields an average of 0.72%. The synthetic velocities reproduced from the forward  
 308 model (fig. 5c) proves a good match to the real observations (fig. 1d).  
 309



310

311 **Figure 5** An initial solution found from the inverse problem. The observed shear wave velocities (a)  
 312 and reference values of  $T_0$ ,  $C$  and  $\theta$  are used to provide constraints on the inversion. A particular  
 313 inference of the melt vol. % within the LVL (b) is then generated using a root-search approach. The  
 314 regionally averaged fraction is calculated as 0.72% given  $T_0 = 1500 \text{ K}$ ,  $C = 18\%$  and  $\theta = 25^\circ$ . Using  
 315 the inferred melt vol. % and the reference values, shear wave velocities (c) can be reproduced from  
 316 the forward model

317 4.2 Symmetric transformation

318 The above calculation generates a single solution to the inverse problem. Since the  
319 inverse problem is non-unique with respect to the input parameters  $T_0$ ,  $C$  and  $\theta$ , there  
320 are, in principle, an infinite number of alternative solutions that can reproduce  
321 identical seismic observations. Here we develop a quantitative approach to prove the  
322 non-uniqueness and, more crucially, the transformation from an existing solution to an  
323 alternative solution. The symmetry of the numerical model is found by properly  
324 modifying the input parameters to obtain an unchanged output model. To start with,  
325 we formulate the forward model of shear wave speed as:

$$\mathbf{V}_S = F(T_0, C, \theta, \boldsymbol{\varphi}) \quad (12)$$

326 , where  $\mathbf{V}_S$  is the shear wave speeds in the LVL beneath the seismic sites;  $F$  denotes a  
327 general, non-linear function (in this work,  $F$  is the forward model from the code  
328 MuMaP\_fwd) and  $\boldsymbol{\varphi}$  is a vector of melt volume fractions in the LVL. Note that 583  
329 seismic sites are analysed in this study, and hence the vector lengths are 583 for both  
330  $\mathbf{V}_S$  and  $\boldsymbol{\varphi}$ . We then generate three perturbations  $\delta T_0$ ,  $\delta C$  and  $\delta \theta$  respectively into the  
331 three variables  $T_0$ ,  $C$  and  $\theta$ . These small changes in the model inputs thus give rise to  
332 residuals in the modelled velocities, i.e.  $\Delta \mathbf{V}_S$ . This can be written as:

$$\Delta \mathbf{V}_S = F(T_0 + \delta T_0, C + \delta C, \theta + \delta \theta, \boldsymbol{\varphi}) - F(T_0, C, \theta, \boldsymbol{\varphi}) \quad (13)$$

333 , which may be approximated in a linear form using the first-order Taylor's series:

$$\frac{\partial F}{\partial T_0} \delta T_0 + \frac{\partial F}{\partial C} \delta C + \frac{\partial F}{\partial \theta} \delta \theta = \Delta \mathbf{V}_S \quad (14)$$

334 , where  $\partial F/\partial T_0$ ,  $\partial F/\partial C$  and  $\partial F/\partial \theta$  are finite derivatives of the function  $F$  with  
 335 respect to  $T_0$ ,  $C$  and  $\theta$ . We then calculate changes required in the melt volume  
 336 fractions (i.e.  $\delta\boldsymbol{\varphi}$ ) to compensate the changes in velocities resulting from the  
 337 perturbations. This can be expressed as:

$$F(T_0 + \delta T_0, C + \delta C, \theta + \delta\theta, \boldsymbol{\varphi} + \delta\boldsymbol{\varphi}) - F(T_0, C, \theta, \boldsymbol{\varphi}) = \mathbf{0} \quad (15)$$

338 Approximation based on the Taylor's series gives:

$$\frac{\partial F}{\partial T_0} \delta T_0 + \frac{\partial F}{\partial C} \delta C + \frac{\partial F}{\partial \theta} \delta\theta + \frac{\partial F}{\partial \boldsymbol{\varphi}} \delta\boldsymbol{\varphi} = \mathbf{0} \quad (16)$$

339 , where  $\partial F/\partial \boldsymbol{\varphi}$  is the finite derivative of the function  $F$  with respect to  $\boldsymbol{\varphi}$ . We then  
 340 solve  $\delta\boldsymbol{\varphi}$  by combining eq. 14 and 16:

$$\delta\boldsymbol{\varphi} = -\frac{\Delta V_s}{\partial F/\partial \boldsymbol{\varphi}} \quad (17)$$

341 In this equation,  $\partial F/\partial \boldsymbol{\varphi}$  can be calculated from the forward model. We make small  
 342 changes in  $\boldsymbol{\varphi}$  and then run the model to predict the corresponding velocities. The  
 343 values of  $\partial F/\partial \boldsymbol{\varphi}$  are given by the difference in the modelling outputs divided by the  
 344 small changes in  $\boldsymbol{\varphi}$ . Note that  $\delta\boldsymbol{\varphi}$ ,  $\partial F/\partial \boldsymbol{\varphi}$  and  $\Delta V_s$  are all vectors with a length of 583  
 345 as there are 583 locations in total. Given the perturbations  $\delta T_0$ ,  $\delta C$  and  $\delta\theta$  and the  
 346 required adjustments in melt volume fractions  $\delta\boldsymbol{\varphi}$ , the model  $F(T_0 + \delta T_0, C + \delta C, \theta +$   
 347  $\delta\theta, \boldsymbol{\varphi} + \delta\boldsymbol{\varphi})$  can produce the same shear wave speeds as given by the initial solution.  
 348 The new solution can then be used as a basis for another transformation. Iterative  
 349 transformation can therefore derive all the additional solutions to the inverse problem.  
 350

### 351 4.3 Calculating multiple solutions

352 Using the forward model and symmetric transformation, we then examine the  
353 entire parameter space and calculate alternative solutions. The parameter space can  
354 be considered as a 3-D volume of which the three dimensions are potential  
355 temperature ( $T_0$ ), basalt fraction ( $C$ ) and dihedral angle ( $\theta$ ). We define the ranges of  
356 the parameters as 1400 to 1800 K in potential temperature, 10 to 40% in basalt  
357 fraction and  $10^\circ$  to  $40^\circ$  in dihedral angle. We also set the increments at 10 K in  
358 potential temperature, 1% in basalt fraction and  $1^\circ$  in dihedral angle. Therefore, the  
359 parameter space is finely sampled and thus the transformation approach can apply.  
360 Each position in the parameter space can be described using the coordinates in the  
361 three dimensions. If a solution exists in position  $(T_0, C, \theta)$ , then the corresponding melt  
362 volume fraction vector can be written as  $\varphi(T_0, C, \theta)$ . Once a solution is found, the  
363 solutions in neighbouring positions can also be determined. Because the  
364 transformation can be applied both forward and backward, six neighbouring solutions  
365 should be examined, including  $\varphi(T_0 + \delta T_0, C, \theta)$ ,  $\varphi(T_0 - \delta T_0, C, \theta)$ ,  $\varphi(T_0, C + \delta C, \theta)$ ,  
366  $\varphi(T_0, C - \delta C, \theta)$ ,  $\varphi(T_0, C, \theta + \delta\theta)$  and  $\varphi(T_0, C, \theta - \delta\theta)$ . We calculate the additional  
367 solutions through the following procedure:

- 368 (1) Create an empty list. Add the coordinate of the initial solution into the list.
- 369 (2) For each solution in the list, calculate the solutions in the neighbouring  
370 positions that are inside of the parameter space but not existing in the list.
- 371 (3) Add the solutions found in step (2) into the list.
- 372 (4) Return to step (2) and repeat the workflow until no new solution can be

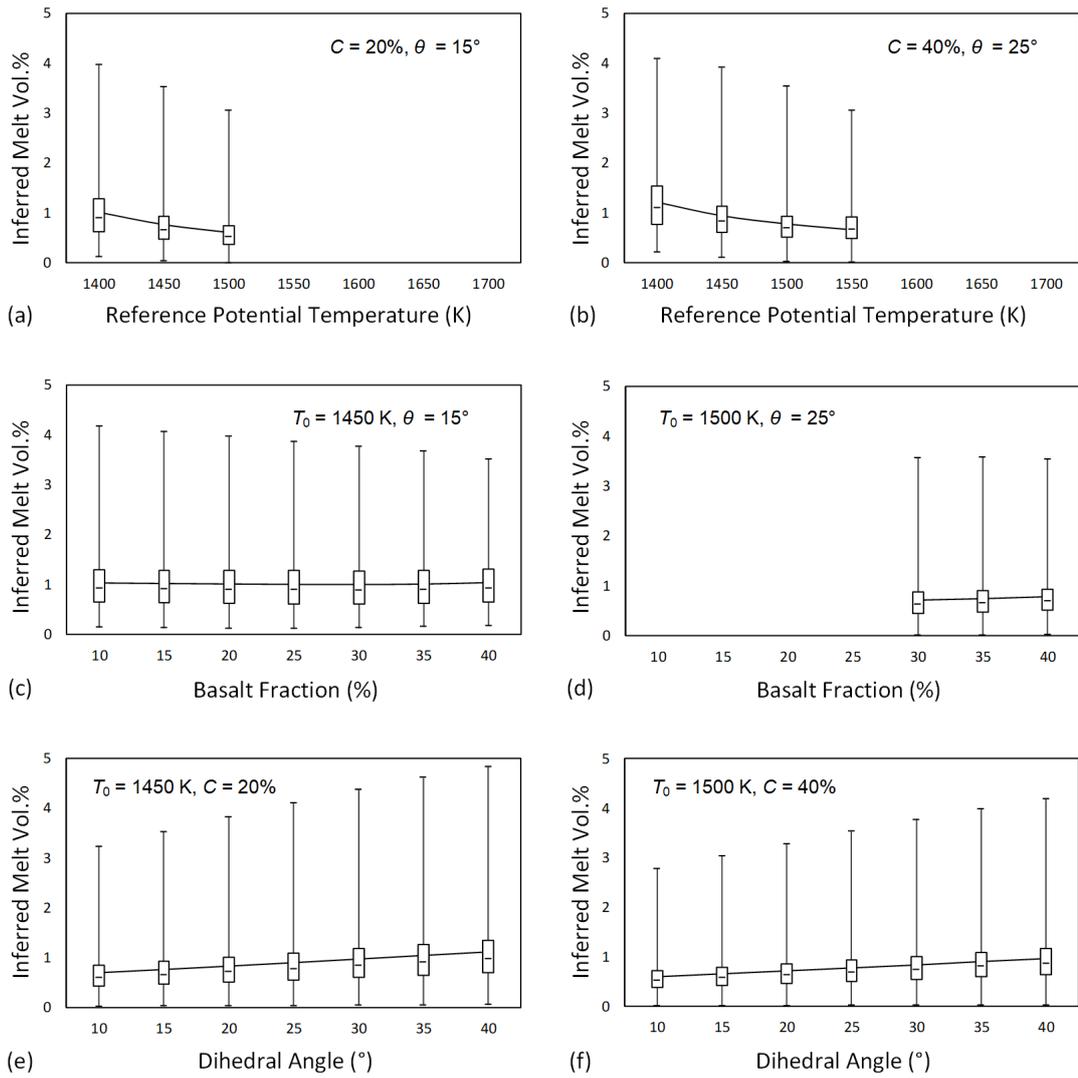
373 added into the list.

374 Note that this is different from a brute-force search which involves a root-  
375 searching approach for calculating the melt volume fraction beneath every location  
376 given different combinations of  $T_0$ ,  $C$  and  $\theta$ . In contrast, the symmetric transformation  
377 is straightforward as it can simultaneously derive the melt volume fraction beneath the  
378 whole area. Since this method works directly on the behaviour of the solution with  
379 respect to perturbations, it also allows us to predict regions where solution does not  
380 exist and the solution containing the lowest possible average melt fractions, which was  
381 intractable with the method described by [Hier-Majumder et al. \(2014\)](#).

382

#### 383 *4.4 Complete solutions to the inverse problem*

384 Using the above computational procedure, we derive all the solutions in the  
385 parameter space. All the possible solutions can reproduce the same synthetic shear  
386 wave velocities from the forward model. Significant spatial variations in the inverted  
387 melt volume are found in every solution. Because the melt volume fraction should  
388 always be non-negative, the calculated vectors of  $\varphi$  where one or more negative  
389 values exist should be removed. Given this requirement, limits can be placed to bound  
390 the symmetric transformation, i.e. not every combination of potential temperatures,  
391 basalt fractions and dihedral angles in the parameter space is compatible with the  
392 seismic observations, though not a unique solution to the inverse problem can be  
393 found. Example of the variations in calculated melt volume fractions and the  
394 transformation limits in the multiple controlling factors are demonstrated in fig. 6.



395

396 **Figure 6** Series of box-plots showing the estimated melt vol.% beneath all locations with median

397 indicated by the horizontal line within each box, upper/lower quartiles indicated by the

398 upper/lower edges of the box and maximum/minimum indicated by whiskers of the boxes. (a) & (b)

399 Inferred melt vol.% as a function of reference potential temperature with fixed basalt fraction and

400 dihedral angles. (c) & (d) Inferred melt vol.% as a function of basalt fractions with fixed reference

401 potential temperature and dihedral angle. (e) & (f) Inferred melt vol.% as a function of dihedral

402 angle with fixed reference potential temperature and basalt fractions. Note that no solution can be

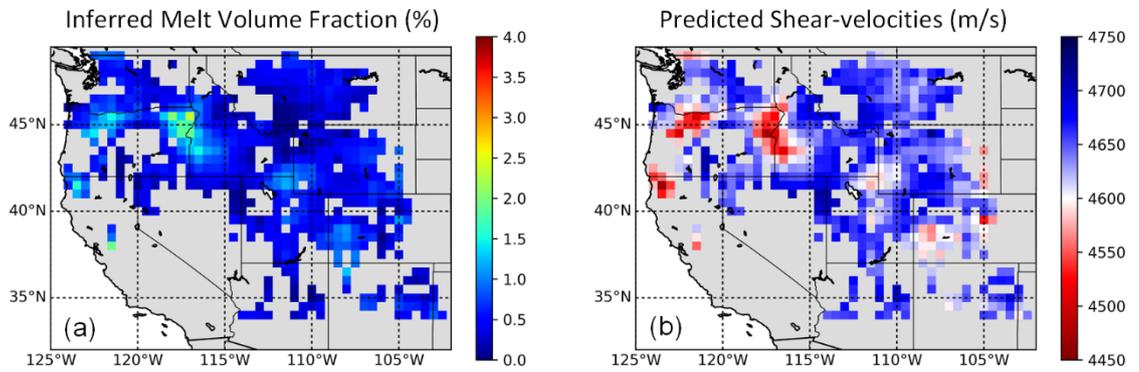
403 found given  $T_0 \geq 1500$  in (a),  $T_0 \geq 1550$  K in (b) and  $C \leq 30\%$  in (d)

404

405       The model output illustrated in fig. 7 is an end-member solution showing that the  
406 lowest possible averaged melt volume fraction is 0.51%, associated with  $T_0 = 1550$  K,  $C$   
407 = 40% and  $\theta = 10^\circ$ . In this solution, the melting is not predicted beneath some regions,  
408 for instance at the triple border between Idaho, Montana and Wyoming. Considering  
409 the sharp boundary atop the LVL, this may just be an artefact because the variations in  
410 solid bulk are unlikely to produce the rapid velocity reductions. However, this solution  
411 is still meaningful since it places a lower-bound below the regional-averaged melt  
412 volume fraction within the observed LVL. In contrast, the highest possible averaged  
413 melt volume fraction that exists in the parameter space yields 1.47%, associated with  
414  $T_0 = 1400$  K, basalt fraction  $C = 10\%$  and dihedral angle  $\theta = 10^\circ$ , as shown in fig. 8.  
415 Examples of the trade-offs between the estimated melt volume fraction below a given  
416 location and the multiple controls are displayed in fig. 9 by cross-plotting the estimates  
417 and the corresponding controlling factors. Whilst the forward model used here is non-  
418 linear, application of the proposed method has indicated the trajectories that link  
419 together the multiple solutions in the parameter space.

420

$T_0 = 1550 \text{ K}$   
 $C = 40\%$   
 $\theta = 10^\circ$



421

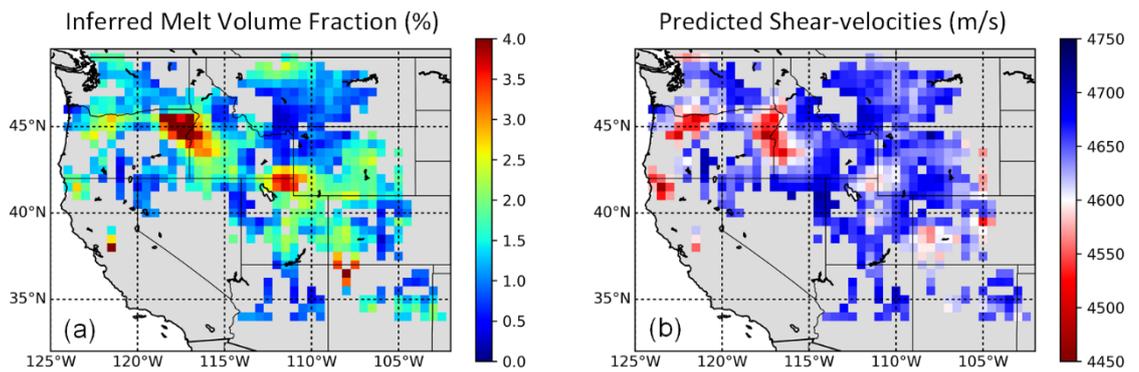
422 **Figure 7** The end-member solution with the minimum melt vol. % within the LVL beneath the w.

423 The regional averaged melt vol. % is 0.51% given  $T_0 = 1550 \text{ K}$ ,  $C = 40\%$  and  $\theta = 10^\circ$ . Note that this

424 solution is directly derived from the initial solution, rather than from a brute-force search

425

$T_0 = 1400 \text{ K}$   
 $C = 10\%$   
 $\theta = 40^\circ$

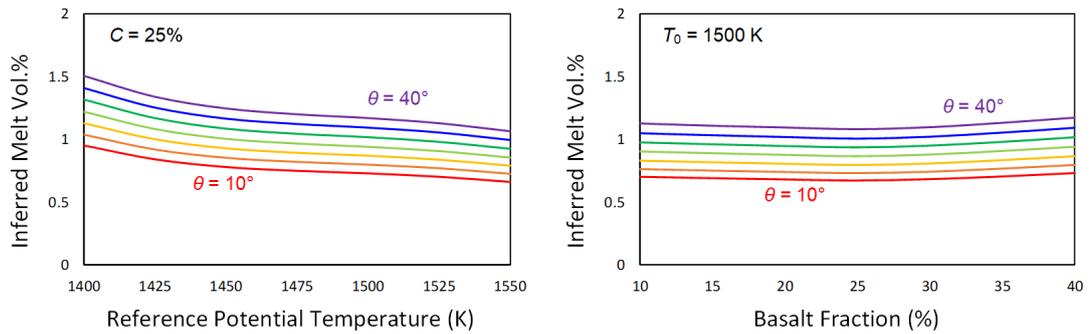


426

427 **Figure 8** The end-member solution with the maximum melt vol. % within the LVL beneath the

428 region. The regional averaged melt vol. % is 1.47% given  $T_0 = 1400 \text{ K}$ ,  $C = 10\%$  and  $\theta = 40^\circ$ . Note

429 that this solution is directly derived from the initial solution, rather than from a brute-force search



430

431 **Figure 9** Cross-plots of inferred melt volume fraction beneath 106°W, 35°N (label A in fig. 1a)

432 versus (a) the reference potential temperature for different dihedral angles ranging from 10° to 40°

433 (annotated on the plot) with constant intervals of 5° given a fixed basalt composition and (b) the

434 basalt fraction in the bulk composition for a range of different dihedral angles given a fixed

435 potential temperature

436

## 437 **5 Discussion**

438 Using a numerical inversion approach, we have examined the LVL at 350 km

439 underneath the western US. The shear-velocity anomalies and impedance contrasts in

440 this zone have been thought to indicate a small fraction of volatile-rich melt ([Hier-](#)

441 [Majumder and Tauzin, 2017](#)) released either by the decarbonation during the Farallon

442 slab subduction ([Thomson et al., 2016](#)) or by the dehydration from the upwelling of

443 the Yellowstone mantle plume or small-scale convection within the MTZ ([Bercovici and](#)

444 [Karato, 2003](#); [Richard and Bercovici, 2009](#); [Zhang et al., 2018](#)). Despite the presence of

445 petrological and geochemical evidences of melting near the MTZ, determination of the

446 quantity of melting from seismic signatures remains hard work owing to the trade-offs

447 that exist between various controlling factors. Due to the lack of geophysical and

448 geochemical constraints, it is difficult, if not impossible, to distinguish the individual

449 effects of temperature, composition and partial melting. A recent study has further  
450 suggested that these multiple controls are strongly correlated, leading to a  
451 disagreement between the experimental measurements and theoretical estimates  
452 ([Freitas et al., 2019](#)).

453 Our numerical scheme based on a symmetry is able to cover all solutions. Using a  
454 forward model, we firstly generate an arbitrary solution assuming  $T_0 = 1500$  K,  $C = 18\%$   
455 and  $\theta = 25^\circ$ . This is a successful solution as the shear wave velocities it predicts are  
456 consistent with the observations. The inverse problem is then linearized to find  
457 neighbouring solutions to the initial solution. As the controlling parameters have only a  
458 limited range of plausible values (in this work  $1400 \leq T_0 \leq 1800$  K,  $10\% \leq C \leq 40\%$  and  
459  $10^\circ \leq \theta \leq 40^\circ$ ), the symmetry gives a quasi-complete set of solutions subject to the  
460 necessary constraint that the melt volume fraction in the upper mantle must always be  
461 non-negative. This constraint can be justified as the effects of temperature and  
462 composition are already taken into account. Given the above treatment, it is then a  
463 simple matter to find the combinations of parameters that reveals the end-member  
464 possibilities (e.g. maximum and minimum degrees of partial melting).

465 The modelling results show that a regional-averaged melt volume fraction of  
466 approximately 0.51% is necessary to explain the sharp shear-velocity reductions at 350  
467 km beneath the western US. This is the minimum extent of melting required to  
468 produce the observed LVL, whatever the solid mantle conditions and the geometry of  
469 the melt are. As [Hier-Majumder and Courtier \(2011\)](#) suggested, at such a small level of  
470 melting, a near neutrally buoyant melt can migrate over the LVL due to surface

471 tension, whereas the drainage efficiency of both buoyant and dense melts is likely  
472 insignificant.

473 As no solution has been found to be associated with a reference potential  
474 temperature higher than 1550 K, we can place an upper-bound on the variations in the  
475 reference potential temperature. The modelling output also shows that the range of  
476 variations in basalt fraction depends on the assumed reference potential temperature.  
477 At a low reference potential temperature (e.g. 1400 K), the basalt fraction may vary  
478 from 10% to 40%. In contrast, at a higher reference potential temperature, solutions  
479 can only be in the basaltic-rich zone (e.g. fig. 6d). For instance, [Hier-Majumder and](#)  
480 [Tauzin \(2017\)](#) estimated the reference potential temperature as approximately 1550 K.  
481 If this is the case, then we can make a statement that the basalt fraction in the LVL  
482 beneath the western US is no less than 40%. Hence, whilst the thermal and  
483 compositional conditions are still under-constrained, our model work offers more  
484 reliable information about the mantle physical properties.

485 In addition, our inverse method unravels trade-offs between parameters. As the  
486 forward model is non-linear, there is no simple analytical tool for determining these  
487 competing effects. The numerical approach proposed here allows estimating the rates  
488 of change in the inferred melt volume fraction caused by changes in other parameters.  
489 According to the modelling outputs, the significance of the trade-offs between inferred  
490 melt volume fractions and other parameters can be summarized as:

491 (1) For a given dihedral angle and a given basalt fraction, the inferred melt  
492 volume fractions present a strong negative correlation with the assumed

493 reference potential temperatures (fig. 6a & b).

494 (2) For a given reference potential temperature and a given dihedral angle, the  
495 inferred melt volume fractions are insensitive to the assumed basalt fractions  
496 (fig. 6c & d).

497 (3) For a given reference potential temperature and a given basalt fraction, the  
498 inferred melt volume fractions present a modest positive correlation with the  
499 assumed dihedral angles (fig. 6e & f).

500 In this analysis, a number of assumptions are made about the mantle: it is in a  
501 state of chemical disequilibrium (described as a mechanical mixture of basalt and  
502 harzburgite), melt films are not playing a role in velocity reduction, the transition zone  
503 thickness reflects temperature variations, the Clapyron slope is known, and receiver  
504 function estimates of MTZ thickness are accurate.

505 This study calculates the temperature variations from the thickness of the MTZ  
506 using the empirical correlation proposed by [Tauzin and Ricard \(2014\)](#). The empirical  
507 model relies on several assumptions, for example that only temperature varies MTZ  
508 thickness and that no vertical variation occurs in temperature from the MTZ to the LVL.  
509 As observed from tomographic models (with low vertical resolution), the MTZ has  
510 consistent structures over the whole range of depth, in particular the stalled Juan de  
511 Fuca/Farallon slab ([Burdick et al., 2008](#); [Schmandt et al., 2011](#); [Hier-Majumder and  
512 Tauzin, 2017](#)). Although an entirely consistent MTZ should not be expected, dealing  
513 with the absolute topography of discontinuities to infer the temperatures would likely  
514 introduce more uncertainties, as would require a precise correction of the effect of

515 shallow velocity heterogeneities from 3-D tomographic models, which have their own  
516 limitations.

517 Another assumption involved here is that one can extract reliable MTZ thickness  
518 from receiver functions, while interference effects from seismic phases that do not  
519 interact with MTZ boundaries can be neglected. It has indeed been shown through  
520 modeling that the effect of interfering phases is small (Tauzin et al., 2013). The move-  
521 out of these phases is different from the one from direct conversions ([Guan and Niu,](#)  
522 [2017](#)) and stacking along move-out curves for direct conversions is efficient in  
523 removing their effect. Besides, slant-stack diagrams and slowness weighted stacking  
524 (e.g. [Guan and Niu, 2017](#); [Hier-Majumder and Tauzin, 2017](#)) show no evidence for  
525 interference effects in several locations of the western US.

526 Apart from the primary controls on the seismic velocities we have investigated,  
527 there are other factors that can influence the seismic wave speeds. In this work, the  
528 Clapeyron slopes  $\gamma$  are set to values from a compilation of experimentally obtained  
529 values ([Tauzin and Ricard, 2014](#)). The values of matrix density  $\rho_s$  and melt density  $\rho_m$   
530 are set to constants as suggested in previous studies. The thickness of MTZ applied  
531 here are also from supplementary dataset whereas alternative empirical models (e.g.  
532 [Keifer and Dueker, 2019](#)) would produce different scenarios. These additional  
533 complications can lead to substantial uncertainties in estimated melt volume fractions.  
534 However, the inversion technique presented here is independent from the forward  
535 model and can easily be adapted to include these factors. While in this paper the  
536 application of the inversion has been demonstrated using 1-D column simulation, the

537 technique could be applied to more sophisticated models that are spatially 2-D or 3-D.  
538 For future work, we intend to apply our modelling approach to investigating the LVL  
539 identified in other regions that differ in tectonic settings, for example, the Hawaii  
540 Islands (Huckfeldt et al., 2013) which are dominated by mantle plumes. An effort will  
541 be done for accounting for uncertainties from seismic data and propagate it into  
542 mantle melting estimates.

543

## 544 **6 Conclusions**

545 The interpretation of the observed seismic structures in the upper mantle, like  
546 many other geophysical inverse problems, is hampered by the fundamental challenge  
547 of non-uniqueness. In this work, we investigate the influence of thermal,  
548 compositional and melting effects on the pervasive LVL at 350 km beneath the western  
549 US. We develop an inversion scheme, based on the principle of symmetry, for  
550 generating the full range of solutions in the parameter space. Although a unique  
551 solution is not available, the calculation of an ensemble of solutions allows extracting  
552 the properties that are common to all solutions. A key result of our inversion is that a  
553 minimum fraction of  $\sim 0.5\%$  melt by volume is necessary to explain the seismically  
554 anomalous layer in the region. The scheme also encapsulates the ranges of variations  
555 in the thermal and compositional factors. Consequently, the application of the  
556 proposed inversion technique can provide more robust interpretation of seismic  
557 velocity reductions within the mantle.

558

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567

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