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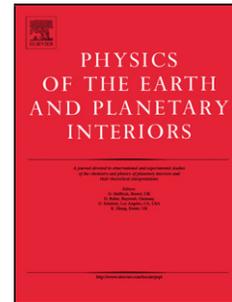
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1 Complex phase distribution and seismic velocity structure of the
2 transition zone: convection model predictions for a
3 magnesium-endmember olivine-pyroxene mantle

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Dedicated to Bernard de Jong on the occasion of his seventieth birthday

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Abstract

We have investigated the complex spatial distribution of mineral phases in the Earth's upper mantle, resulting from lateral variations of temperature in a convecting mantle, through numerical modelling of mantle convection. Our convection model includes a self-consistent thermodynamic description for an olivine-pyroxene composition in the SiO_2 , MgO system. The thermodynamic model is based on lattice vibrations and allows for the calculation of thermophysical properties as well as seismic wavespeeds.

Our modelling results show a complex structure in the behavior of physical properties, in particular the seismic shear wavespeed, in a depth range including the mantle transition zone, 400-700 km. We demonstrate that this behavior is related to the distribution of mineral phases in the olivine-pyroxene system. Especially near cold downwelling flows, representing subducting lithospheric plates, our model results show strong lateral variation of mineral phases and associated shear wavespeed. We show that, typically, pockets of contrasting mineral phases smaller than 100 km occur in subduction regions.

In line with current developments in seismic imaging of the mantle transition zone we have computed reflectivity profiles from the shear wavespeed distribution obtained from the convection results. We applied frequency filtering to the raw reflectivity data to investigate the requirements for resolving the heterogeneous structure of the transition zone. Our results show that heterogeneous structure from contrasting mineral phase regions is resolved in the reflectivity profiles, for periods below twenty seconds which may be feasible in seismic imaging applications. This opens a perspective for detailed mapping of mineral phase distribution in the mantle offering new constraints on the thermal conditions of the transition zone region, thus providing valuable constraints for geodynamic models of the upper mantle.

1 Introduction

The mantle transition zone in the depth range 400-700 km is characterized by a large number of mineral phases especially in regions with strong lateral temperature variation, related to subducting lithospheric slabs. Seismological mapping of the existing phase boundaries provides constraints on the geotherm in such regions from identification with phase diagram data for candidate mantle materials. This way Boehler (1996) estimated the temperature at the spinel to post-spinel '660 km' phase boundary at 1900 ± 100 K, based on a pressure of 23.9 GPa from the PREM model (Dziewonski and Anderson, 1981). A recent example of this procedure, extended to lateral variation, is an estimate of temperature distribution in the heterogeneous D" region in the bottom region of the mantle, from high resolution imaging of seismic reflectors, identified as the post perovskite phase boundary (Van der Hilst et al., 2007).

Lateral variation of the upper mantle transition zone has been investigated seismologically using underside reflections, observed as precursors of SS and PP phases (Shearer et al., 1999, Deuss and Woodhouse, 2001, Deuss et al., 2006), resulting in estimates of lateral variation of the depth of the '410' and '660 km' phase boundaries and regional variation in the visibility of the '520 km' phase boundary, associated with the wadsleyite (β) to ringwoodite (γ) transition in the (main) olivine component of the upper mantle. Recently Cao et al. (2010) applied seismic imaging methods, based on the Generalized Radon Transform (GRT) and related to the approach in (van der Hilst et al., 2007) and (Wang et al., 2008), to SS precursors originating from the transition zone for a tectonically undisturbed region of the Pacific. This study shows clear resolution of the topography of the '410' and '660 km' boundaries and laterally varying intermediate structure interpreted as the '520 km' discontinuity that is shown to resolve locally in two separate reflections in the shorter period ranges of the signal. This could be an indication for additional phase boundaries related to

53 mineral phases from the pyroxene system such as majorite and akimotoite that would be stable for
54 possible temperature conditions in the transition zone.

55 The above examples illustrate that seismic visibility of mineral phase boundaries in complex
56 configurations, as predicted for the mantle transition zone, is of great importance for constraining
57 local temperature, which in turn is of great value for dynamical reconstructions of the upper mantle.
58 In this paper we investigate this issue, of the seismic expression of the mineral distribution in the
59 transition zone, by means of numerical modelling of mantle convection, taking into account physically
60 self-consistent thermophysical parameters and mineral phase diagram of the olivine-pyroxene system.
61 To our knowledge no mantle convection studies have adressed the prediction of heterogeneous seismic
62 structure from the distribution of mineral phases in the transition zone, with the exception of (Jacobs
63 et al., 2006) restricted to an olivine mantle. Here our mantle convection model is based on the
64 magnesium endmember of the olivine-pyroxene mineralogy (Jacobs and de Jong, 2007). The same
65 model, further introduced in section 2.2 and the appendix, is also used to compute longitudinal
66 and shear wave speed. Other workers have computed seismic wave speed distributions from mantle
67 convection results without similar consistency between the mineral physics and the convection model
68 (Goes et al., 2004), (Schuberth et al., 2009a,b). We have chosen to apply the mineral physics model
69 of Jacobs and de Jong (2007), in spite of its restricted composition, because of its degree of internal
70 consistency and accuracy in representing available experimental data, that is superior to alternative
71 mineral physics models that include a wider range of compositions, as is further illustrated below
72 in section 2.2. The extension of our mineral physics model for a broader range of compositions, in
73 particular iron, aluminium and calcium, is work in progress (Jacobs and de Jong, 2009).

74 The magnesium endmember olivine-pyroxene model is a simplified model relative to a more re-
75 alistic, for instance pyrolitic, mantle composition (Ringwood, 1975), yet it contains the most signifi-
76 cant features of the mantle transition zone including the major phase transitions. The monovariant
77 phase transitions of the magnesium-endmember system produce corresponding sharp transitions in
78 physical properties including the seismic wave velocities. We use this endmember model for an
79 exploratory test (1) to investigate the applicability of a self-consistent thermodynamic model in
80 mantle convection computations, (2) to couple the self-consistently calculated sound wave velocities
81 with mineral phase partitioning in the mantle and (3) to investigate the expression of the different
82 mineral phases in seismic reflectivity traces.

83 In line with the above we have computed model predictions of the complex spatial distribution
84 of mineral phases and corresponding seismic wave velocities resulting from our convection model for
85 the whole mantle, in particular for the transition zone region. We convert the convection results
86 (spatial distribution of pressure and temperature) to shear velocity values for the upper 1000 km of
87 the mantle and correlate the resulting heterogeneous seismic velocity structures with corresponding
88 variations of both temperature and mineral phase distribution. To put the results in perspective
89 with recent developments in seismological reflectivity imaging of mantle structure, we compute 1-
90 D radial reflectivity profiles from our convection results and consider the effect of limited seismic
91 data bandwidth on the representation of the heterogenous structure by reflectivity time traces. This
92 modelling procedure can help in investigating the potential of seismological resolution of the detailed
93 structure of the transition zone. By focusing on the transition zone we avoid strong compositional
94 heterogeneity of other mantle regions such as the D'' zone at the bottom of the mantle, not accounted
95 for in our model (Xu et al., 2008).

96 Seismic expression of temperature variations in mantle convection models has been investigated
97 by Goes et al. (2004) who focus on large scale mantle plumes, and Schubert et al. (2009a,b), who
98 focus on lateral variation in 3-D global convection models in comparison with evidence from global

99 seismic tomography. In contrast we focus on modelling small scale heterogeneity in the transition
100 zone and its expression in high resolution seismic imaging methods.

101 In the next sections we first describe the convection model and underlying parameterization
102 of the mineral physics model. This is followed by a presentation of the results from convection
103 modelling and a discussion of the implications of the results and conclusions.

104 2 Description of the convection and thermodynamical model

105 2.1 Convection model

106 We apply a model of a compressible mantle, taking into account the effects of density increase with
107 pressure and solid state phase transitions. The model is defined for a two-dimensional cylindrical
108 domain geometry. The governing equations are,

$$109 \quad \partial_j(\rho u_j) = 0 \quad (1)$$

110 expressing mass conservation using a truncated anelastic liquid approximation (Jarvis and McKenzie,
111 1981, Steinbach et al., 1989, Steinbach, 1991, Ita and King, 1994). Conservation of momentum is
112 expressed in the Stokes equation for a highly viscous fluid of infinite Prandtl number,

$$113 \quad -\partial_i \Delta P + \partial_j \tau_{ij} + \Delta \rho g(r) e_i = 0, \quad i = 1, 2 \quad (2)$$

114 where $g(r)$ and e_i are, respectively, the amplitude and direction cosines of the local radial gravity
115 acceleration vector. The density perturbation $\Delta \rho$ in (2) is defined in terms of a reference profile ρ_r ,

$$116 \quad \rho(P, T) = \rho_r(P) + \Delta \rho(P, T) \quad (3)$$

117 where $\rho_r(P) = \rho(P, T_r(P))$ and $T_r(P) = \langle T(P) \rangle$ is a reference temperature profile computed from
118 a lateral average. The dynamic pressure gradient in (2) is defined by subtracting $\rho_r(P) g_i$ from the
119 gradient of pressure $\partial_i P$ in the Stokes equation.

120 Assuming that the effect of the rate of volume change, that scales with a bulk viscosity is
121 negligible on the convective time scale (Jarvis and McKenzie, 1980), the deviatoric shear stress
122 tensor for the compressible fluid is defined as,

$$123 \quad \tau_{ij} = \eta \left(\partial_i u_j + \partial_j u_i - \frac{2}{3} \partial_k u_k \delta_{ij} \right) \quad (4)$$

124 where the summation convention is implied for repeated indices and η is the temperature and
125 pressure dependent viscosity further specified in Table 1.

126 The energy transport equation used is,

$$127 \quad \rho c_p \frac{DT}{Dt} - \alpha \rho g w T = \partial_j (k \partial_j T) + \tau_{ij} \partial_j u_i + \rho H \quad (5)$$

128 D/Dt is the material time derivative and the second term describes the effect of adiabatic heating.
129 The terms on the right specify thermal conduction, heating by viscous dissipation and radiogenic
130 heating respectively. Further symbol definitions are given in Table 1.

Symbol	Definition	Value	Unit
h	Depth of the mantle model	$3 \cdot 10^6$	m
z	Depth coordinate aligned with gravity	-	-
P	Thermodynamic pressure	-	-
ΔP	Dynamic pressure	-	-
T	Temperature	-	-
$T_{surface}$	Surface temperature	373	K
ΔT	Temperature scale	3500	K
u_i	Velocity field component	-	-
w	Radial velocity aligned with gravity	-	-
$e_{ij} = \partial_j u_i + \partial_i u_j$	Strain rate tensor	-	-
$e'_{ij} = e_{ij} - \frac{1}{3} e_{kk} \delta_{ij}$	Strain rate deviator	-	-
$e' = (1/2 e'_{ij} e'_{ij})^{1/2}$	Second invariant of deviator	-	-
$\eta(T, z) = \eta_0 \exp(cz - bT)$	P,T dependent viscosity	-	-
	$b = \ln(\Delta\eta_T), c = \ln(\Delta\eta_P)$	-	-
	$\Delta\eta_T = 100, \Delta\eta_P = 10$	-	-
η_0	Viscosity scale value	10^{23}	Pa s
$\tau_{ij} = \eta e'_{ij}$	Viscous stress tensor	-	-
α_0	Thermal expansivity scale value	$3 \cdot 10^{-5}$	K^{-1}
ρ	Density	-	-
ρ_0	Density scale value	4500	kgm^{-3}
k	Uniform conductivity value	4.7	$Wm^{-1}K^{-1}$
$\kappa = \frac{k}{\rho c_p}$	Thermal diffusivity	-	-
c_p	Specific heat	-	-
c_{p0}	Specific heat scale value	1250	$Jkg^{-1}K^{-1}$
g	Gravitational acceleration	9.8	ms^{-2}
H	constant internal heating	$2 \cdot 10^{-12}$	Wkg^{-1}
$Ra = \frac{\rho_0 \alpha_0 g \Delta T h^3}{\kappa_0 \eta_0}$	Rayleigh number	10^6	-
$Di = \frac{\alpha_0 g h}{c_{p0}}$	dissipation number	0.47	-

Table 1: Physical parameters

132 The thermal conductivity k is set to a uniform value. The physical properties ρ , c_p and α that appear
133 as coefficients in equation (5) are included in our model through a general interface based on pressure
134 temperature (P, T) domain tabulation of the material property values in the relevant pressure and
135 temperature range for the Earth's mantle, further discussed in sections 2.2 and A.3 (van den Berg et
136 al., 2002; Jacobs et al., 2006). The effect of heat exchange due to solid state phase transitions is not
137 included in the formulation of the energy equation (5). In the extended boussinesq approximation of
138 Christensen and Yuen (1985) this effect is included in terms of parameterizations of the Clapeyron
139 slope and the density contrast across the phase boundary, resulting in modified expressions for
140 effective heat capacity and thermal expansivity in the energy equation. Nakagawa et al., (2009)
141 have extended this approach to a compressible model using tabulated thermophysical properties for
142 a multicomponent model, where effective c_p and α are expressed in the temperature- and pressure
143 derivatives of the enthalpy. In our model calculations for the binary system MgO, SiO₂ we have

144 not included such extensions that would require differentiation of the enthalpy across discontinuities
145 at the monovariant phase transitions. We assume that this approximation will only have a minor
146 influence on the overall dynamics and temperature structure of our model. This is further discussed
147 in section 4.

148 The coupled model equations (1), (2) and (5) are solved using finite element methods. Domain
149 discretization, boundary and initial conditions and computational aspects of the coupling between
150 the model equations and the underlying mineral physics model are discussed in Appendix A.3.

151 2.2 Thermodynamical and mineralogical model

152 In our convection model the thermophysical properties density ρ , thermal expansivity α and specific
153 heat c_P , are derived from a thermodynamic formalism based on lattice dynamics. This formalism
154 by Jacobs and de Jong (2005, 2006, 2007), further denoted as ‘phonon-thermodynamic’ method,
155 incorporates the vibrational density of states, for the purely magnesian endmember model of the
156 MgO – SiO₂ system. The overall composition is specified by the mole fractions of the olivine and
157 pyroxene components, (Mg₂SiO₄)_{0.56}(MgSiO₃)_{0.44}.

158 The absence of at least iron in our model system, relative to a natural system, of pyrolitic
159 composition, prevailing in the mantle has three consequences. The first one is that density in our
160 model system is lower than for a pyrolitic mantle, affecting sound wave velocities and the pressure-
161 depth distribution. This is illustrated in Fig. 1 showing adiabatic profiles of seismic velocities,
162 derived from the phonon-thermodynamic model, for an Earth-like mineral composition within the
163 MgO – SiO₂ system. This figure shows that the main features of the mantle transition zone are
164 reproduced by our mineral physics model based on a restricted composition (not including Al, Ca
165 and Fe). The effect, of adding the major component Fe, on the seismic velocities of olivine, amounts
166 to an overall reduction of the velocity by about 1-2%. Secondly, addition of more elements to the
167 model system displaces phase boundaries. For instance the olivine-wadsleyite phase boundary will
168 shift to an approximately 1 GPa lower pressure when Fe content is increased from zero to 10%.
169 The wadsleyite-ringwoodite transition shifts in a similar way to lower pressure for increased iron
170 content. Thirdly, specific phase boundaries in the model system split up by the addition of other
171 elements, enclosing multi-phase regions. For instance the olivine-wadsleyite phase boundary splits
172 up in a field in which olivine and wadsleyite coexist when iron is added in our model. Although
173 the restricted model cannot be used to represent the ‘real Earth’ it is sufficiently realistic for our
174 present purpose of exploring the seismic expression of multiple phase regions in the transition zone
175 generated by the mantle convection proces.

176 Despite the issue of compositional completeness of our present thermodynamic model we empha-
177 size that the approach we follow here, is not restricted to a particular thermodynamic model. The
178 mantle convection computations are set up in a flexible way such that different thermodynamical
179 models, once available, can be applied, as illustrated further in section A.3 below. In future work
180 this will enable us to refine our present calculations with an extended thermodynamic model con-
181 taining more elements, and moreover to investigate effects of applying alternative thermodynamic
182 models.

183 A thermodynamic model incorporating iron, which is constrained by phonon data and applicable
184 in the range from zero Kelvin up to the melting point, is currently under development. Following
185 the work of Jacobs and de Jong (2009), we anticipate that this model is particularly important for
186 iron-bearing materials, which are characterized by antiferromagnetic-paramagnetic transitions at
187 low temperatures, e.g. 67 K for fayalite and 12 K for ringwoodite. This requires a thermodynamic

188 framework, which is adequate to reliably describe thermophysical properties from zero Kelvin up to
189 the melting temperature and to pinpoint inconsistencies in existing laboratory data.

190 A main advantage of the application of the phonon-thermodynamic method in numerical models
191 of mantle convection is that it enables one to compute the required thermo-physical parameters
192 as well as the phase diagram in a single self-consistent framework. This is important because for
193 many substances crucial experimental data, such as for thermal expansivity and bulk modulus,
194 have been measured at conditions far away from those prevailing in the mantle transition zone.
195 Therefore, to obtain values for thermodynamic properties at mantle conditions, any physical model
196 is forced to make large extrapolations of available thermodynamic data. For instance Jacobs and de
197 Jong (2005b) showed, by using a calphad-type parameterization technique, that thermal expansivity
198 and volume of gamma-Mg₂SiO₄ (ringwoodite) could not be constrained with sufficient accuracy to
199 enable a prediction of bulk sound velocity for gamma-(Mg_{0.91}Fe_{0.09})₂SiO₄ to within 0.8%, twice
200 the tomographic accuracy. Figure 12 of their work demonstrates that bulk sound velocity for this
201 substance modeled by Fabrichnaya (1998), Stixrude and Bukowinsky (1993) and their own work are
202 quite different, calling for a method which more tightly constrains thermodynamic data.

203
204 Such accuracy issues are also important because the representation of phase equilibrium boundaries
205 is quite sensitive to variations in the Gibbs energy in pressure-temperature space. For instance a
206 change in the Gibbs energy of akimotoite by about 500 J/mol (0.04 %) leads to a temperature shift
207 of about 300 K of the quadruple point where wadsleyite, ringwoodite, akimotoite and stishovite
208 are in equilibrium. Saxena (1996, 2010) gives a detailed analysis of how uncertainties in thermo
209 chemical properties affect the accuracy of the description of phase boundaries.

210 For all mineral phases present in the model phase diagram of Fig. 5, even for the phases stable
211 at high pressure, experimental data, such as heat capacity, thermal expansivity and bulk modulus,
212 are available at 1 bar pressure. These 1-bar data do not suffer from uncertainties associated with
213 equations of state of pressure reference materials, as is the case for data obtained at high pressure.
214 It is therefore of great importance to constrain thermodynamic analyses of these phases with 1 bar
215 experimental data. Such data are very well fitted by methods based on polynomial expressions for
216 these properties, (Fabrichnaya et al., 2004), (Saxena, 1996), (Holland and Powell, 1998).

217 However it has been demonstrated by Jacobs and Oonk (2000) that the methods based on
218 polynomial approximations are difficult to use when thermodynamic properties are extrapolated to
219 conditions prevailing in the lower mantle because of physical anomalies that occur in the computed
220 thermal expansivity. Therefore the methods based on polynomials do not perform well, compared
221 to alternative methods, for instance methods based on Mie-Grüneisen-Debye theory, when applied
222 for the full pressure and temperature range of the Earth's mantle.

223 Significant progress in representing experimental data at lower mantle pressures has been made
224 by Stixrude and Lithgow-Bertelloni (2005). They used the Mie-Grüneisen-Debye method (MGD)
225 to construct a thermodynamic database for the CFMAS system. However due to the simplified
226 construction of the Vibrational Density of State (VDoS) inherent to the Debye model and the use of
227 the quasi-harmonic approximation, experimental data at 1-bar conditions are less well represented
228 by the MGD method compared to the polynomial approach. This is illustrated for forsterite in Fig.
229 2, where computed values of the specific heat at constant pressure are compared with experimental
230 data.

231 Jacobs and de Jong (2005, 2007) introduced a method, based on Kieffers (1979) more elaborate
232 model for the VDoS that also includes the effect of anharmonicity. This method, here labeled MGK-
233 a, combines an accurate representation of both 1-bar and high pressure (lower mantle) experimental

234 data. As a consequence the MGK-a method is better constrained by, both 1-bar and high pressure,
235 experimental data.

236 Figure 2 shows for forsterite, that including anharmonicity combined with a realistic VDoS
237 improves the representation of 1-bar heat capacity significantly. The effect of anharmonicity on
238 vibrational frequencies has been measured for forsterite by Gillet (1991, 1997). Its effect on the
239 heat capacity of forsterite is about 2.5% at 2000 K and 1 bar pressure and it propagates for about
240 0.4% in the Gibbs energy. Although this effect seems small at first sight, Jacobs and de Jong (2005)
241 showed that it has a significant effect on location and slope of the phase boundary between forsterite
242 and wadsleyite. Neglecting anharmonicity shifts this phase boundary by 2 GPa to lower pressures,
243 whereas the slope decreases with almost a factor two. Not only forsterite, but also other mineral
244 phases such as perovskite and akimotoite are affected by anharmonicity, impacting the position and
245 slopes of phase boundaries as has been demonstrated by Jacobs and de Jong (2007).

246 In view of the demonstrated impact on the phase diagram, of both a detailed VDoS representation
247 and of anharmonicity, in the lattice dynamics model, a unique characteristic of the MGK-a method,
248 we consider this the most reliable method available to date for the computation of both the phase
249 diagram and the thermo physical properties of the mantle convection model specified in (2)-(5), for
250 an olivine-pyroxene system.

251 The thermodynamic formalism (MGK-a) by Jacobs et al. (2007) is based on microscopic proper-
252 ties such as vibrational frequencies and microscopic Grüneisen parameters. Relative to polynomial
253 representations of thermodynamic data, this method is additionally constrained by Raman and
254 Infrared spectroscopic data, resulting in more tight constraints of thermodynamic data. Jacobs
255 et al. (2006) applied this to Mg_2SiO_4 to obtain better constrained thermodynamic properties for
256 ringwoodite. In contrast to many thermodynamic parameterizations available in the literature their
257 vibrational model is tightly constrained by experimental data below room temperature, such as
258 low temperature heat capacity data, resulting in a better partitioning of physical effects at high
259 temperature, such as intrinsic anharmonicity in forsterite and akimotoite and cation disorder in
260 majorite. This also implies better constrained descriptions of entropy and enthalpy, necessary for
261 the determination of Clapeyron slopes. This high degree of physical self-consistency and agreement
262 with experimental data is considered particularly important in modeling complex, heterogeneous,
263 configurations in the mantle transition zone.

264 Thus the properties ρ , c_P and α , required in model calculations based on equations (2), (5),
265 together with both seismic velocities v_p , v_s , can be computed for the complete (P, T) range of the
266 Earth's mantle, in a single physically self-consistent framework, without relying on separate param-
267 eterizations for individual mineral phases, as is common practice in models based on an (extended)
268 Boussinesq approximation (EBA), (Christensen and Yuen, 1985, Steinbach et al., 1989, Zhao et
269 al., 1992). In this respect our method is similar to the methods applied by Ita and King (1994),
270 Piazonni et al. (2009) and Nakagawa et al. (2009), that are based on thermodynamical models, with
271 varying degree of self-consistency in the representation of thermophysical parameters and seismic
272 wave velocities. The phonon-thermodynamic method is further outlined in the appendix.

273 3 Results of numerical modelling

274 We have modelled thermal convection in a 2-D cylindrical domain with an opening angle of ninety
275 degrees. The ratio of the core radius and the outer radius R_c/R is 0.54, similar to the value for
276 Earth. The depth of the mantle is set to 3000 km. The model is both bottom and internally heated.
277 Uniform and constant radiogenic heating is applied, set to a value $H = 2 \cdot 10^{-12}$ W/kg, slightly

278 lower than the chondritic value, in agreement with the smaller surface/volume ratio of the 2-D
 279 cylindrical domain, compared to the 3-D spherical case. Temperature is prescribed constant at the
 280 outer surface and the core mantle boundary with a temperature contrast $\Delta T = 3500$ K across the
 281 mantle. Zero heatflux symmetry conditions are imposed on the radial boundaries.

282 Computations were started from an initial adiabatic temperature field, with a potential tempera-
 283 ture $T_p = 1600$ K, truncated at the top- and bottom thermal boundary layers. The model equations
 284 were integrated in time for about 1 Gyr.

285 A newtonian, temperature and pressure dependent viscosity model is used with an exponential
 286 parameterization defined in Table 1.

287 Fig. 3 shows results for a representative snapshot of the temperature distribution resulting from
 288 the convection model, at a model time of 837 Myr. The snapshot shown is characteristic for the
 289 model results with narrow cold downwellings, descending all the way to the core mantle boundary.
 290 These downwellings migrate along the outer boundary, similar to subducting lithospheric plates
 291 subject to trench migration and slab roll-back. The temperature field is shown in the top row of
 292 frames. The bottom row displays corresponding plots of the lateral variation of the seismic shear
 293 wavespeed. The temperature field is characterized by two colliding cold downwellings and a region
 294 of hot upwelling, in the area indicated by 1500 km wide zoom-in windows, outlined in black in
 295 frame (a), that correspond to frames (b) and (c). The cold downwellings show only limited dynamic
 296 interaction with the endothermic phase boundaries near 700 km depth, with a slight deflection
 297 of the right hand downwelling. This is related to the small value of the Clapeyron slope, -1.9
 298 MPa/K, of the post-spinel phase transition at the bottom of the transition zone in our model. The
 299 temperature distribution of the zoom-in windows is smooth and without significant features related
 300 to the transition zone.

301 Lateral variation of the seismic shear velocity δv_s is shown in frames (d,e,f) that correspond
 302 to the temperature frames (a,b,c) respectively. The lateral variation is defined with respect to a
 303 smooth background profile, to bring out more clearly the discontinuities in the velocity, related to
 304 the different phase boundaries, $\delta v_s(\mathbf{x}) = (v_s(\mathbf{x}) - \langle v_s(r) \rangle) / \langle v_s(r) \rangle$. The smooth background
 305 profile $\langle v_s(r) \rangle$ is computed from the horizontally averaged values by applying a boxcar moving
 306 average filter with a 200 km halfwidth.

307 The velocity and temperature variations shown in Fig.3 are closely correlated in the lower mantle
 308 region away from the D'' region, where several lens-like structures of post-perovskite show up in the
 309 seismic velocity (Hernlund et al., 2005, van der Hilst et al., 2007).

310 This indicates that seismic velocity is related in a simple way to temperature and pressure,
 311 in this region without phase transitions. This situation is quite different for the transition zone
 312 region between about 400 and 700 km depth as illustrated particularly in Fig. 3e,f. The large scale
 313 structure of the smooth temperature field associated with the vertical downwellings is dominant in
 314 the lateral variation but much of the small scale structure of the velocity anomalies is not reflected
 315 in the smooth variation of the temperature field.

316 A smooth relation between temperature and seismic wavespeed is underlying interpretations of
 317 seismic travel time tomography (Goes et al., 2004), (Schuberth et al., 2010b). The poor correlation
 318 between small scale lateral variation of shear wave speed and temperature illustrated in Fig. 3
 319 shows that assumption of such relation is not applicable for small scale variation in the depth range
 320 of the transition zone. A clear difference in correlation of seismic velocity and temperature, between
 321 regions inside and outside the transition zone is illustrated more directly in Fig. 4, showing discrete
 322 samples of wavespeed data obtained from several isobaric cross-sections at different sample depths,
 323 taken from the convection results.

324 Only the data samples taken at 797 km depth (27.5 GPa), in the shallow lower mantle occupied
325 by post-spinel, show a continuous relation between shear velocity and temperature.

326 The velocity-temperature plots of Fig. 4 can be interpreted with the phase-diagram for the
327 magnesium endmember model applied in the convection model shown in Fig. 5. Horizontal dashed
328 lines in Fig. 5 indicate the pressure values of the isobaric velocity-temperature plots in Fig. 4.

329 The intersection of the 9.4 GPa isobar, at 300 km depth, with the phase boundary curve of the
330 ortho- and clino enstatite transition at about 1750 K corresponds to the transition shown in the
331 bottom velocity-temperature curve in Fig. 4. The loop in the sampling curves for 300 and 636 km
332 depth of Fig. 4 is a result of the spread in pressure in the sample points that are located in a 20 km
333 depth range around the indicated depth.

334 In a similar way the intersection of the 21 GPa isobar, at 636 km depth, with the wadsleyite-
335 ringwoodite ($\beta \rightarrow \gamma$) phase boundary near 1800 K corresponds to the velocity transition of the
336 middle curve in Fig. 4. The latter phase transition corresponds to the ‘520 km’ discontinuity that
337 has been the target of a growing number of seismological investigations (Shearer et al., Deus et al.,
338 2001,2006, Cao et al., 2010). In our modelling results this transition occurs around 650 km depth
339 as will be shown below. The fact that this transition occurs at depths greater than 520 km in our
340 model is a consequence of the absence of iron in the magnesium endmember composition model used
341 here. This composition related pressure shift of the $\beta \rightarrow \gamma$ transition has been calculated from the
342 thermodynamic database of Saxena (1996) as 1.25 GPa. This effect is amplified in a shift to smaller
343 depth, due to the increased pressure gradient associated with the density increase resulting from
344 adding 10 % iron. Fig. 4 clearly illustrates that interpreting lateral variation in seismic velocity in
345 terms of temperature variation only, will not produce correct results in a multi-phase environment
346 like the mantle transition zone.

347 That strong lateral variation of physical properties, related to variation in mineral phase, can
348 occur in the mantle transition zone, especially in regions of large lateral variation in temperature, is
349 illustrated in Figure 5, by three radial temperature profiles. The profiles are labeled by their angular
350 coordinate, positioned in the zoom-in window around the cold downwellings of Fig. 3b,e. Adiabats
351 with a range of potential surface temperatures of 1400-1800 K are drawn for reference in Figure 5.
352 This temperature range also includes the red profile, positioned between the two cold downwellings,
353 that corresponds to a background reference profile, more representative for the mantle outside the
354 cold disturbance of the downwelling flows. From the temperature excursion across several phase
355 boundaries of the two low temperature geotherms, associated with the downwelling flows, it is clear
356 that several mineral phases can exist at a given depth/pressure depending on the laterally varying
357 temperature field. This is more directly illustrated in Fig. 6 showing the mineral phase distribution,
358 frames (a,b) and corresponding lateral variation of the shear velocity δv_s (c,d) for the two zoom-in
359 windows indicated by black boxes in Fig. 3(a,d). Dashed lines in Fig. 6a correspond to the radial
360 temperature profiles shown in the phase diagram of Fig. 5. Individual pockets of different mineral
361 associations intersected by the radial profiles can be identified with the help of the phase diagram
362 of Fig. 5. Fig. 6a shows a complex configuration of regional domains occupied by contrasting
363 mineral phases, indicated by the same phase labels as in Fig. 5. The large negative temperature
364 perturbations, of up to 1000 K, of the two cold downwellings, shift the local geotherms across several
365 stability fields in the phase diagram in Fig. 5. This causes the strong lateral variation in the phase
366 distribution shown in Fig. 6a.

367 Frame 6b shows similar lateral variation in the mineral phase distribution for a zoom-in window
368 with a smaller, hot, mantle anomaly. The lateral variation of temperature is mainly reflected here
369 in the variation of the thickness of the various mineral phase layers. The forementioned phase

370 boundary between wadsleyite and ringwoodite, associated with the ‘520 km’ discontinuity, occurs
 371 in two different settings here. First as the transition $\beta + ak \rightarrow \gamma + ak$ that is more prominent in
 372 the core of the cold downwellings. The local thickening of the $\beta + ak$ layer is a consequence of
 373 the diamond shaped stability field of this mineral assemblage shown in Fig.5. Second, in warmer
 374 areas, as the transition $\beta + pv \rightarrow \gamma + pv$. This results in an intermittent behavior of the $\beta \rightarrow \gamma$
 375 boundary illustrated in 6a,b, which could be related to lateral variations in seismic observations of
 376 the ‘520 km’ boundary reported by (Deuss, 2009) and (Cao et al., 2010). If such detail of the $\beta \rightarrow \gamma$
 377 transition would indeed be observable in the seismic data this would provide strong constraints on
 378 lateral variation of the temperature field in the transition zone.

379 In the modelling results the bottom of the transition zone that represents the boundary between
 380 the upper and lower mantle consists of a layer of ringwoodite and perovskite, that transforms into a
 381 post-spinel assemblage of periclase and perovskite for pressures higher than the endothermic post-
 382 spinel transition. The pyroxene component has transformed to perovskite at shallower level at the
 383 nearby strongly endothermic transition of akimotoite to perovskite (Chudinovskikh and Boehler,
 384 2004, Jacobs and de Jong, 2007). The magnitude of the Clapeyron slope in (Jacobs and de Jong,
 385 2007) of 4.1 MPa/K is smaller than the value of 6 MPa/K reported in (Chudinovskikh and Boehler,
 386 2004). The Clapeyron slope of the ringwoodite to postspinel transition of (Jacobs and de Jong,
 387 2007) is -1.9 MPa/K. The relatively small magnitude of the latter transition and the splitting of the
 388 phase transition to perovskite of the olivine and pyroxene reduce the dynamic effect of the composite
 389 endothermic phase boundary between the upper and lower mantle, in line with the weak interaction
 390 of the cold downwellings with these phase boundaries as shown in Fig. 3.

391 The radial profile at 37° , halfway between the cold downwellings, is representative for the global
 392 horizontally averaged mantle. The corresponding geotherm in Fig. 5 is close to an adiabat of
 393 1700K. The transition zone has a five layer configuration here with, from top to bottom 1) $\beta +$
 394 clino-enstatite, 2) $\beta +$ majorite, 3) $\beta +$ akimotoite, 4) $\beta +$ pv 5) $\gamma +$ perovskite. The transition
 395 zone is followed by the lower mantle consisting of a post spinel assemblage of perovskite $MgSiO_3 +$
 396 periclase MgO .

397 Fig. 6c,d show the lateral variation of the shear velocity for the corresponding zoom-in windows
 398 of frames (a) and (b). There is a strong correlation between the velocity anomalies and the mineral
 399 phase distribution, to the degree that individual pockets of contrasting mineral content can be
 400 identified in the anomaly pattern of the shear velocity. This is in contrast with the corresponding
 401 smooth temperature field distributions shown in Fig. 3(b,c).

402 The ‘410 km’ seismic discontinuity is clearly visible in the velocity frames as the boundary
 403 between second and third phase layer from the surface. This phase boundary shows the well-known
 404 uplift near the core of the two cold downwellings, in agreement with the positive Clapeyron slope of
 405 the $\alpha \rightarrow \beta$ phase transition (Turcotte and Schubert, 2002). The phase boundary between layer 1 and
 406 2, related to the transition from ortho-enstatite to clino-enstatite shows an even greater topography
 407 related to the high value of the Clapeyron slope, that increases for lower temperatures, as shown in
 408 Fig. 5.

409 Fig. 7 shows a compilation of radial distributions of temperature (a,c) and seismic shear velocity
 410 (b,d). The different curves in each frame correspond to the profiles indicated by dotted lines in Fig.
 411 6a,b. The black curves in frames (a) and (c) correspond to the horizontally averaged geotherm that
 412 is close to the 1700K adiabat in the transition zone.

413

414 The curves in frames (c),(d) correspond to profiles near 70° in a less disturbed and warmer upper
 415 mantle region. The geotherms in Fig. 7a show temperature contrasts over 1000 K, illustrating the

416 wide range of temperatures found in the mantle transition zone, in areas of subducting lithosphere.

417 Corresponding profiles of the shear wavespeed are shown in Fig. 7b,d. The smoothed global
418 background profile, $\langle v_s(r) \rangle$, used in the calculation of lateral variations of shear velocity, is
419 plotted as a dashed curve. Seismic discontinuities corresponding to the phase boundary crossings of
420 the different temperature profiles can be clearly recognized, showing substantial differences between
421 the different profiles, in particular in Fig.7b, representing the region with stronger lateral variation
422 in temperature.

423 The direct correlation between mineralogy and lateral variation of seismic velocity shown in
424 these results clearly demonstrates that the temperature dependence of the seismic wave velocities
425 is strongly non-linear because of the mineralogy involved. This is in contrast with assumptions
426 underlying methods of temperature and density estimation from seismic tomographic data.

427 Detailed seismic velocity structure of the mantle transition zone, including lateral variation,
428 is an important target of seismological investigation, (Shearer et al.,1999, Deus and Woodhouse,
429 2001, Deuss et al, 2006, Lebedev et al., 2002, Cao et al., 2010). Studies like those by Deuss and
430 co-workers and Cao et al., 2010, using SS precursors originating from underside reflections of the
431 transition zone layering, produce reflectivity-time traces as a measure of radial distribution of ve-
432 locity contrasts. Here we have computed a similar approximation of the radial distribution of the
433 shear wave reflectivity from the radial derivative of the logarithmic seismic impedance. The com-
434 puted reflectivity-depth profiles were then converted to time traces by a conversion from depth to
435 two-way traveltime, using the spatially variable shear wave speed, followed by equidistant interpo-
436 lation of the time traces with a sample frequency $f_s = 2.56$ Hz. Fig. 8 shows a spectral analysis
437 of a representative reflectivity time trace that samples the transition zone in the region of complex
438 phase distribution corresponding to Fig. 6a, near the radial profile labeled 35° . The signal power
439 is concentrated near a frequency of 0.1 Hz that corresponds to wavelength's between about 50 and
440 60 km in the transition zone. Structures of such wavelength are reasonably well resolved by our
441 finite element mesh with a nodal point spacing of 6 km in the transition zone. We tested the effect
442 of the finite element resolution on our results by comparison with a model computation with half
443 the number of nodal points with respect to the model results shown. This comparison produced
444 practically identical results in particular also in the powerspectrum shown in Fig. 8. The mesh
445 resolution is further specified in section A.3.

446 The raw reflectivity data traces obtained by the forementioned procedure are shown in Fig. 9a,
447 for the region corresponding to Fig. 6a. To investigate the seismic signal bandwidth required to
448 resolve the underlying velocity structure we applied low-pass frequency filtering to the raw reflectivity
449 traces. The result of second order Butterworth filtering of the raw data traces with corner periods
450 of 20 and 40 seconds are shown in frames b) and c) of Fig. 9 respectively.

451 The corresponding shear velocity distribution for the region is shown in Fig. 10, for interpretation
452 of the reflectivity traces. This figure shows clearly contrasting velocity values that coincide with the
453 different phase regions shown in Fig. 6. The discontinuities outlining the different phase regions in
454 Fig. 10 are closely correlated with the pattern of reflectivity maxima in Fig. 9. Pockets of anomalous
455 'low temperature' phases like the ringwoodite regions in the cold downwellings are clearly visible in
456 the reflectivity traces.

457 Table 2 lists reflectivity maxima corresponding to several phase boundaries, mostly related to
458 the pyroxene component, that can be identified in locations, away from the irregular structures
459 related to the two cold downwellings in the mantle region shown.

Time in seconds	Phase transition
200	α -olivine + clino-enstatite \rightarrow β -olivine + clino-enstatite
225	β -olivine + clino-enstatite \rightarrow β -olivine + majorite
240	β -olivine + majorite \rightarrow β -olivine + akimotoite
not-resolved	β -olivine + akimotoite \rightarrow γ -olivine + akimotoite
270	γ -olivine + akimotoite \rightarrow γ -olivine + perovskite
280	γ -olivine + perovskite \rightarrow periclase + perovskite

Table 2: Approximate two-way travel times and phase transitions related to the reflectivity maxima for the background mantle parts of Fig. 9.

The ‘520 km’ seismic discontinuity, associated with the $\beta \rightarrow \gamma$ transition of the olivine component, is represented in our modelling results by the contrast between the $\beta + ak$ (green in Fig.6ab) and $\gamma + pv$ (pink in Fig.6ab) layers near the boundary between the upper and lower mantle. In the reflectivity traces of Fig.9 this transition is visible as the second peak from the bottom near 270 seconds. The thin layer of $\gamma + ak$, replaced laterally by $pv + \beta$, as shown in Fig.6ab is not resolved in the reflectivity traces.

The ‘520 km’ discontinuity is observed in a peridotite mantle, of pyrolitic composition, roughly halfway between the $\alpha \rightarrow \beta$ (‘410 km’) and $\gamma \rightarrow MgO + pv$ (‘660 km’) phase boundaries (Deus and Woodhouse, 2001, Cao et al., 2010). Another reason for the relative proximity of the ‘520’ and ‘660 km’ boundaries, besides the forementioned absence of iron in our magnesian endmember model, is the rather high background temperature of the mantle model where the geotherm intersects the spinel to post-spinel boundary ($\gamma + pv \rightarrow MgO + pv$) in Fig. 5 at a temperature of about 2050 K, higher than the experimental value 1900 ± 100 K in (Boehler, 2000). This explanation by a temperature effect is in agreement with the occurrence of two thicker pockets of ringwoodite and akimotoite ($\gamma + ak$), in the phase distribution shown in Fig. 6a, intersected by dashed profile lines, corresponding to the two colder geotherms labeled 35° and 39° in the phase diagram of Fig. 5. From Fig. 9 it can be concluded that the main mineral phase distribution of the transition zone, in the present magnesian endmember model, are clearly expressed in the reflectivity structure, at least for the period range below 20 seconds, well accessible in broadband seismological data, as illustrated in 9b.

4 Discussion and conclusions

Recent progress in mapping sharp contrasts in seismic shear wavespeed in the transition zone (Deuss et al., 2006, Cao et al., 2010) calls for an assessment of phase related heterogeneity generated in mantle dynamical models. In order to investigate such heterogeneous structure of the mantle transition zone, resulting from lateral variation in temperature, we have modelled thermal convection in the Earth’s mantle, applying a mineral physics model from which the complex phase diagram for the olivine-pyroxene system can be derived in a self-consistent manner.

Our mantle convection model includes thermophysical properties such as density, thermal expansivity and specific heat, for the magnesium endmembers of a olivine-pyroxene mantle. We have computed lateral variations in seismic shear wave velocities applying the same lattice vibrational model as used in the computation of thermophysical properties (Jacobs and de Jong, 2007).

Our computations are based on a restricted chemical composition of the model material, in particular without the approximately 10% iron content of a pyrolitic mantle composition (Ringwood,

494 1975). We applied this model in our calculations because of the available corresponding thermo-
495 physical database (Jacobs and de Jong, 2007) that is unique in accurate prediction of both the
496 phase diagram and material properties specific heat, thermal expansion and density, as discussed in
497 section 2.2. The absence of iron in our model results in a shift to higher pressure of major phase
498 transitions of the model olivine component, olivine-wadsleyite and wadsleyite-ringwoodite, associ-
499 ated with the ‘410 km’ and ‘520 km’ seismic discontinuity respectively (Bina and Helffrich, 1994,
500 Jacobs and de Jong, 2005b). In contrast the spinel-postspinel boundary corresponding to the ‘660
501 km’ discontinuity is less affected by the model iron content. The restricted composition also implies
502 a lower model density and associated pressure gradient, which also results in a depth increase of
503 the phase boundaries. The monovariant phase transitions of our mineral physics model do not have
504 multi-phase regions characteristic for models containing solid solutions. This implies that phase
505 transitions in our model are associated with discontinuities in physical properties, in contrast to a
506 model containing 10% iron in solid solution that shows smoother transitions between phase domains
507 (Bina and Helffrich, 1994, Stixrude, 1997). In this sense our model results represents an endmember
508 case for the computation of the seismic expression of phase boundaries in the transition zone.

509 Our model calculations were done with the simplifying assumption that the effect of latent heat
510 exchange due to phase transitions can be neglected to first order in the large scale dynamics and
511 global temperature distribution. The dynamical effect of the phase boundary on the mantle flow
512 operates mainly through the phase related density contrast in the righthand side of the Stokes
513 equation (2). The localized temperature effect from the latent heat exchange produces a shift in the
514 transition pressure that is estimated to be smaller than about 0.4 GPa. We note that this value is
515 similar to the uncertainty in the experimental determination of phase boundaries (Frost, 2003). In
516 view of the forementioned shift of the transition-depth of phase boundaries, resulting from absence
517 of iron in our model, estimated at about 1 to 2 GPa for $\alpha \rightarrow \beta$ and $\beta \rightarrow$ ringwoodite respectively,
518 the effect of latent heat is acceptable.

519 In spite of these differences with a more realistic mantle composition, our model reproduces
520 thermophysical properties, including seismic wavespeeds, as well as mineral phase boundaries to
521 within experimental uncertainty, for the magnesium endmember of the olivine-pyroxene system. Self-
522 consistency of the underlying mineral physics model and high accuracy in representing experimental
523 data, as discussed in section 2.2, is an important characteristic of our convection model, especially
524 when applied to mantle regions with a large number of mineral phases with contrasting physical
525 properties such as the upper mantle transition zone.

526 We have analysed the distribution of mineral phase and corresponding shear wavespeed, com-
527 puted from the pressure-temperature fields obtained in the mantle convection calculations. In rel-
528 atively undisturbed regions, away from cold downwellings and hot mantle plumes, the modelling
529 results show heterogeneity mainly in the variation of layer thicknesses of the different phase associa-
530 tions. Here we observe interesting similarities with seismological results from SS and precursors from
531 underside reflections of the transition zone (Deuss et al., 2006, Cao et al, 2010). The seismological
532 results show lateral variations in amplitude and depth of seismic reflectors interpreted as topography
533 of the ‘410’ and ‘660 km’ phase boundaries. The ‘520 km’ boundary has a more regional character
534 (Deuss, 2009) and frequency dependent signature that could be related to phase transitions in the
535 pyroxene component (Cao et al., 2010). In our model results ringwoodite occurs in association with
536 stishovite and with akimotoite in the core of a cold downwelling. Away from cold downwellings a
537 thin layer of ringwoodite and akimotoite exists intermittantly replaced by an equally thin layer of
538 wadsleyite and perovskite. This layering can be identified in the reflectivity traces computed from
539 the wavespeed distributions. This configuration is related to the vicinity of the stability fields for

540 these phase associations, along an isobar of 22 GPa, in the phase domain of Fig. 5. The lateral
541 boundaries between these associations pinpoint the temperature of the ‘quadruple point’ at 22 GPa
542 in Fig. 5 and the middle (black) data set shown in Fig. 4. This example illustrates the possibility
543 of lateral variation in the signature of seismic reflectors due to phase transitions of the pyroxene
544 component.

545 Other transitions in the pyroxene component that are clearly visible in the reflectivity traces
546 of Fig. 9 are clinoenstatite to majorite, close to the ‘410 km’ discontinuity, and the majorite to
547 akimotoite transition about halfway in the transition zone.

548 The strongest heterogeneity in our model results is found in regions with cold downwelling flows,
549 simulating lithospheric subduction, where the geotherm deviates by up to 1000 K from the horizon-
550 tally averaged background value. This heterogeneity shows up as distinct pockets of mineral phase
551 with corresponding, contrasting seismic velocity distribution, where the outlines are clearly visible
552 in the reflectivity traces. It should be noted here that our modelling results have been obtained as-
553 suming equilibrium thermodynamics, thereby neglecting possible effects of phase transition kinetics
554 that may become significant in the coldest cores of old subducting lithospheric slabs (Daessler et al.,
555 1996; Vacher et al., 1999).

556

557 Our main objective in this paper has been to investigate the heterogeneity due to the complex phase
558 diagram of a magnesium endmember olivine-pyroxene system, for the mantle depth range including
559 the transition zone, and relate the results to recent developments in seismological reflectivity imaging
560 of the mantle.

561 We have shown that lateral variations of temperature result in a laterally heterogeneous phase
562 distribution, especially near subduction regions. The results show that the distribution of seismic
563 shear wavespeed is clearly dominated by the phase distribution rather than by the temperature field.

564 The major phase transitions of both the olivine and pyroxene subsystems show up clearly in the
565 reflectivity traces computed from the shear velocity distribution in the signal bandwidth with periods
566 below 20 s, indicating that these phase boundaries can, in principle, be imaged by seismological
567 methods. Geodynamical models that can generate the detailed structure of the transition zone
568 region can therefore be helpful in the interpretation of such seismological data.

569 Further progress requires that multi-phase regions, in particular related to a finite iron composi-
570 tion will be modelled. This requires the extension of our thermodynamic data base with iron, which
571 is currently in progress (Jacobs and de Jong, 2009).

572

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726 **A Thermodynamic formalism and computation of thermophysical** 727 **parameters and seismic wave velocities**

728 **A.1 Background of the thermodynamical model**

729 In our modelling experiments thermophysical properties ρ, α, c_P and the seismic wave velocities
730 were derived from a formalism based on thermodynamics and lattice dynamics. This phonon-
731 thermodynamic formalism was developed in (Jacobs and de Jong, 2005, 2007). There are several
732 important differences between this formalism and recently published alternative formulations and
733 corresponding databases by Stixrude and Lithgow-Bertelloni (2005), Connoly (2005) and Piazzoni et
734 al., (2007). The latter databases employ the Debye model to obtain thermal pressure, but polynomial
735 expressions for heat capacity and thermal expansivity are used in the data base of Piazzoni et al.
736 (2007).

737 An important difference is that the formalism used by Jacobs and de Jong (2005, 2007) incor-
738 porates more details of the phonon spectrum than the Debye formalism allows.

739 Such details are essential because the Debye model was shown to result in insufficient accuracy
740 in the heat capacity from 0 K up to the melting point of forsterite (Jacobs and de Jong, 2005a).
741 That compelled them to employ Kieffer's (1979) model to represent the experimental data associated
742 with the vibrational density of state (VDoS), such as vibrational frequency-temperature-pressure
743 measurements derived from Raman and infrared spectroscopy. Kieffer's model appeared also to be
744 required for other minerals such as MgSiO_3 perovskite.

745 Secondly, the formalism of Jacobs and de Jong (2005, 2007) incorporates intrinsic mode an-
746 harmonicity. These data became available for a number of mantle materials, such as forsterite,
747 perovskite and akimotoite through the work of Gillet et al. (1991), Gillet et al. (2000) and Rey-
748 nard and Rubie (1996) respectively. Jacobs and de Jong (2005, 2007) demonstrated that intrinsic
749 anharmonicity significantly affects slope and position of phase boundaries in the magnesium-olivine
750 and magnesium-pyroxene system.

751 Thirdly the formalism is constructed in such a way that, at zero Kelvin, static lattice properties
752 are calculated, which can be constrained by or compared with ab initio methods.

753 The fourth difference is that the phonon-thermodynamic formalism incorporates electronic and
754 magnetic properties, which is shown by Jacobs and de Jong (2009) to be a requirement for accu-
755 rate representation of Fe bearing mantle materials. They showed that the vibrational formalism
756 is suitable to predicting mixing properties in olivine. Their incorporation of iron in the system
757 $\text{MgO} - \text{SiO}_2$ is work in progress. Because the phonon-thermodynamic model incorporates more
758 physical properties relative to polynomial models used by e.g. Fabrichnaya (1998), Holland and
759 Powell (1998), Saxena (1996), Jacobs et al. (2005b), the thermodynamic description of substances
760 is more unambiguously constrained.

761 **A.2 Computation of thermophysical parameters with the phonon-thermodynamic** 762 **model**

763 The central equation of the phonon-thermodynamic model is the expression for the Helmholtz energy
764 of a material. For insulating materials such as present in the system $\text{MgO} - \text{SiO}_2$, The Helmholtz

765 energy is written as:

$$766 \quad A(T, V) = U^{ref}(V_0^{st}) + U^{st}(V) + A^{vib}(T, V) \quad (6)$$

767 All thermodynamic properties are derived from the Helmholtz energy by applying classical ther-
768 modynamic theory. The system MgO – SiO₂ contains insulator materials and for such case the
769 Helmholtz energy is expressed as the sum of a static lattice and a vibrational contribution:

770 The first term on the right-hand side of eqn. (6) is a reference energy contribution at zero Kelvin
771 and zero pressure for a substance in which no vibrational motion is present. The molar volume of
772 this static lattice is denoted by V_0^{st} . The second term represents the change in energy resulting from
773 the change in volume of the static lattice from V_0^{st} to V . This term is calculated by applying an
774 equation of state, such as a third order Birch-Murnaghan equation of state or the universal equation
775 of state developed by Vinet et al. (1987). The last term represents the vibrational contribution to
776 the Helmholtz energy and is expressed in vibrational mode frequencies and their mode Grüneisen
777 parameters. Taking the isothermal volume derivative of eqn. (6) results in the expression for the
778 equation of state, which is expressed as the sum of the static lattice and vibrational (thermal)
779 contribution:

$$780 \quad P(T, V) = P^{st}(V) + P^{vib}(T, V) \quad (7)$$

781 At a selected condition of pressure and temperature the molar volume of the material is solved
782 numerically from (7). Density, ρ , in (3) is then calculated from the molar volume using the molar
783 masses of the endmembers. Once the volume is known, all other thermodynamic properties follow
784 by taking the appropriate differential of eqn. (6).

785 The calculation of the heat capacity, c_P , in (5) is more involved and proceeds in several steps by
786 making use of the well-known thermodynamic relation:

$$787 \quad c_P = c_V + \alpha^2 KVT \quad (8)$$

788 The explicit expressions for the heat capacity at constant volume, c_V , isothermal bulk modulus, K ,
789 and thermal expansivity, α , are derived from eqn (6) by taking the appropriate differentials:

$$790 \quad c_V = T \left(\frac{\partial S}{\partial T} \right)_V = -T \left(\frac{\partial^2 A}{\partial T^2} \right)_V \quad (9)$$

$$791 \quad K = -V \left(\frac{\partial P}{\partial V} \right)_T = V \left(\frac{\partial^2 A}{\partial V^2} \right)_T \quad (10)$$

$$792 \quad \alpha = \frac{1}{K} \left(\frac{\partial P}{\partial T} \right)_V = -\frac{1}{K} \left(\frac{\partial}{\partial T} \left[\frac{\partial A}{\partial V} \right]_T \right)_V \quad (11)$$

793 All differentiations in (9,10,11) can be derived analytically from the explicit expression for the
794 Helmholtz energy (Jacobs and de Jong, 2007).

795 In Kieffers (1979) model the directionally averaged longitudinal and transverse sound velocities
796 are related to the angular vibrational frequency $\omega_{i,max}$ by:

$$797 \quad u_i = \frac{1}{4} \left(\frac{4\pi ZV}{3N_A} \right)^{1/3} \omega_{i,max} \quad (12)$$

798 In (12) u_1 and u_2 represent the sound velocities of the transverse (shear) waves and u_3 that of the
799 Voigt-Reuss-Hill longitudinal wave. The shear wavespeed is calculated according to:

$$800 \quad v_s^2 = \frac{G}{\rho} = \frac{3}{4} (u_3^2 - v_B^2) = \frac{3}{4} \left(u_3^2 - \frac{K_S}{\rho} \right) \quad (13)$$

801 The P - T phase diagram for a specific composition in the MgO – SiO₂ system is derived from the
802 Gibbs energy of each mineral phase. The Gibbs energy determines the stability of the phase and is
803 derived from the Helmholtz energy as:

$$804 \quad G(P, T) = A(T, V) + P \cdot V \quad (14)$$

805 As stated above, the volume of the mineral phase at a specific pressure and temperature is derived
806 from (7) resulting in a value for the $P \cdot V$ term in (14). This value combined with the value for the
807 Helmholtz energy derived from (6) results in the value of the Gibbs energy of each phase. From
808 the Gibbs energy values of each phase and applying general rules of classical thermodynamics it is
809 straightforward to derive which phase assemblage is stable at given (P, T) , (Connolly, 2005).

810 A.3 Computational aspects

811 The model equations (1),(2) and (5) are solved on a two dimensional quarter circle cylindrical
812 domain covering the full depth of the mantle, using finite element methods based on the SEPRAN
813 finite element package (Segal and Praagman, 2000).

814 Free slip impermeable boundaries are prescribed for the Stokes equation (2). We apply carte-
815 sian coordinates and local transformations to implement the mechanical boundary conditions on
816 the curved boundaries (Cuvelier et al., 1986). Temperature is prescribed at the bottom and top
817 horizontal surfaces with a driving temperature contrast $\Delta T = 3500$ K. Zero heatflux symmetry
818 conditions apply on the radial boundaries.

819 Approximately $2 \cdot 10^5$ nodal points are used spanning 64000 quadratic elements for the velocity
820 field using 227 and 567 nodal points in the radial and horizontal direction respectively. A fourfold
821 subdivision is applied on the vertices of the 7-point velocity elements to obtain linear temperature
822 elements for the energy equation (van den Berg et al., 1993). Grid refinement is applied with nodal
823 point spacing reduced to approximately 6 km in the depth interval containing the transition zone.

824 An integrated finite element method in terms of the velocity and pressure fields is combined with
825 a direct solver for the solution of the Stokes equation where renumbering of the degrees of freedom
826 is applied to reduce the profile of the stiffness matrix.

827 The energy equation is integrated in time with a predictor-corrector method, applying a Courant
828 type time step control (van den Berg et al., 1993).

829 Necessary thermo-physical properties density, thermal expansivity and specific heat, are com-
830 puted through a general interface procedure using equidistant tabulation and bi-linear interpolation
831 of these properties in the P, T domain relevant for the mantle $300 \text{ K} < T < 4000 \text{ K}$, $\delta T = 2 \text{ K}$, 0
832 $< P < 140 \text{ GPa}$, $\delta P = 0.066 \text{ GPa}$. This represents a flexible and efficient tool that facilitates the
833 use of alternative thermodynamic data bases (van den Berg et al., 2002, Jacobs et al., 2006).

834 P, T domain tabulation is essential since pointwise calculation of thermo-physical properties is
835 not feasible in view of the large number of evaluations of these properties. This becomes clear
836 from the following assessment of the number of evaluations involved per integration time step, for a
837 general model case with N_e stokes elements.

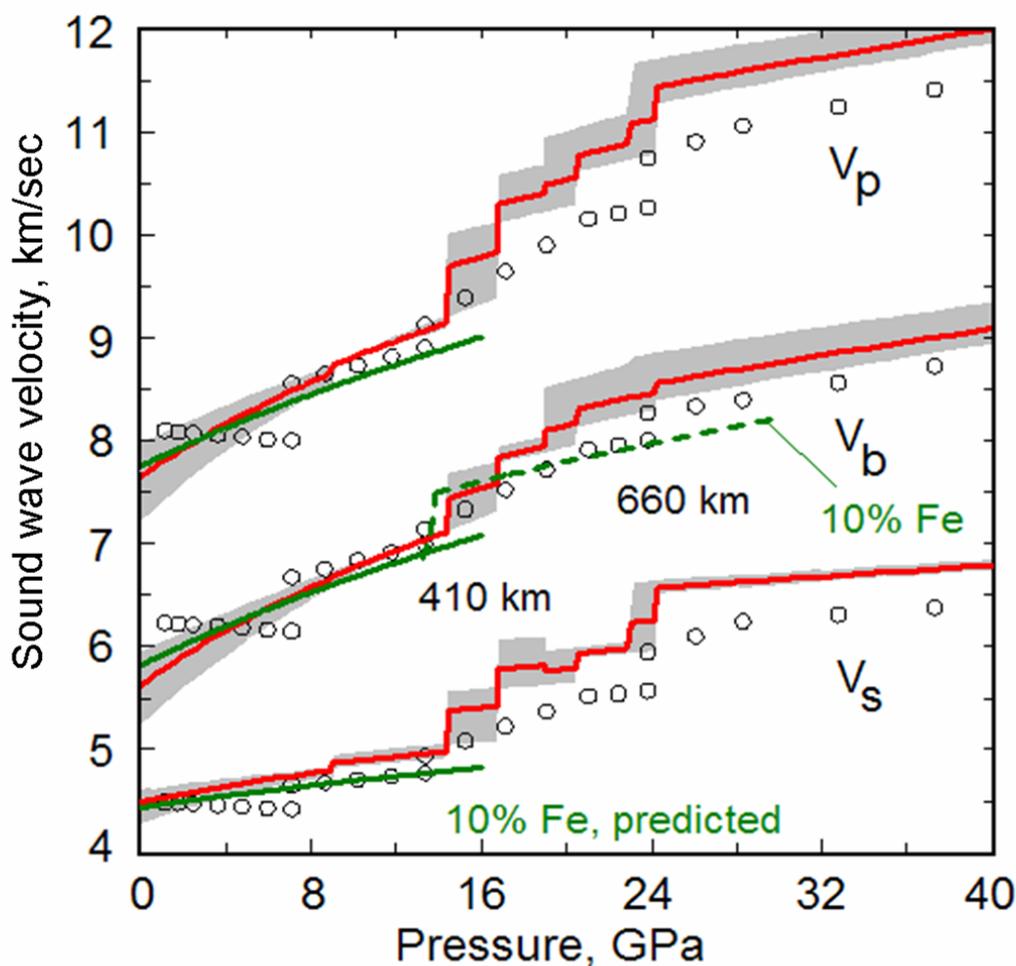
838 For the Stokes equation only ρ needs to be computed. For the energy equation the values of
839 ρ , c_P and α must be computed (factor 3 in (15)). A four times higher number of elements is used

840 for the energy equation (factor 4 in (15)). $n_g = 7$ gauss integration points are used per element.
841 These evaluations are repeated two times per integration time step in a predictor/corrector scheme,
842 resulting in the following number of thermo-table evaluation per time step.

$$843 \quad N_{eval} = (N_{stokes} + N_{energy}) \times 2 = (N_e \times n_g + 3 \times N_e \times 4 \times n_g) \times 2 = 26 \times N_e \times n_g \quad (15)$$

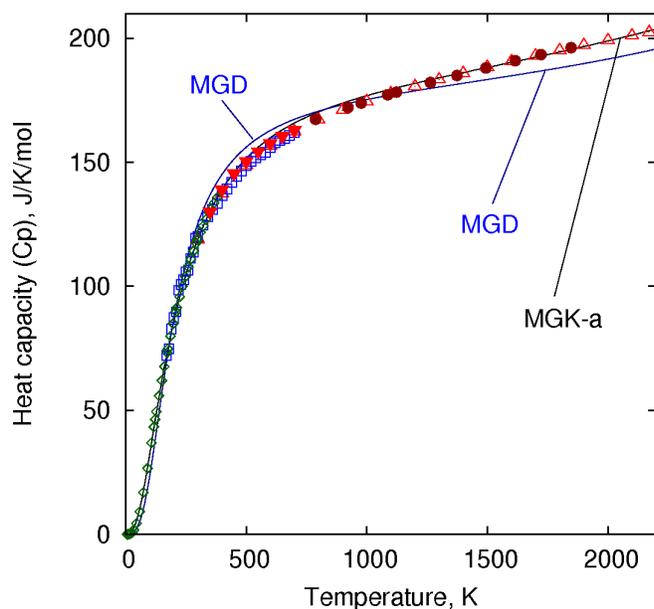
844 This amounts to $N_{eval} = 1.2 \cdot 10^7$ table evaluations per integration time step for the finite element
845 mesh size used in our model calculations where $N_e = 64000$.

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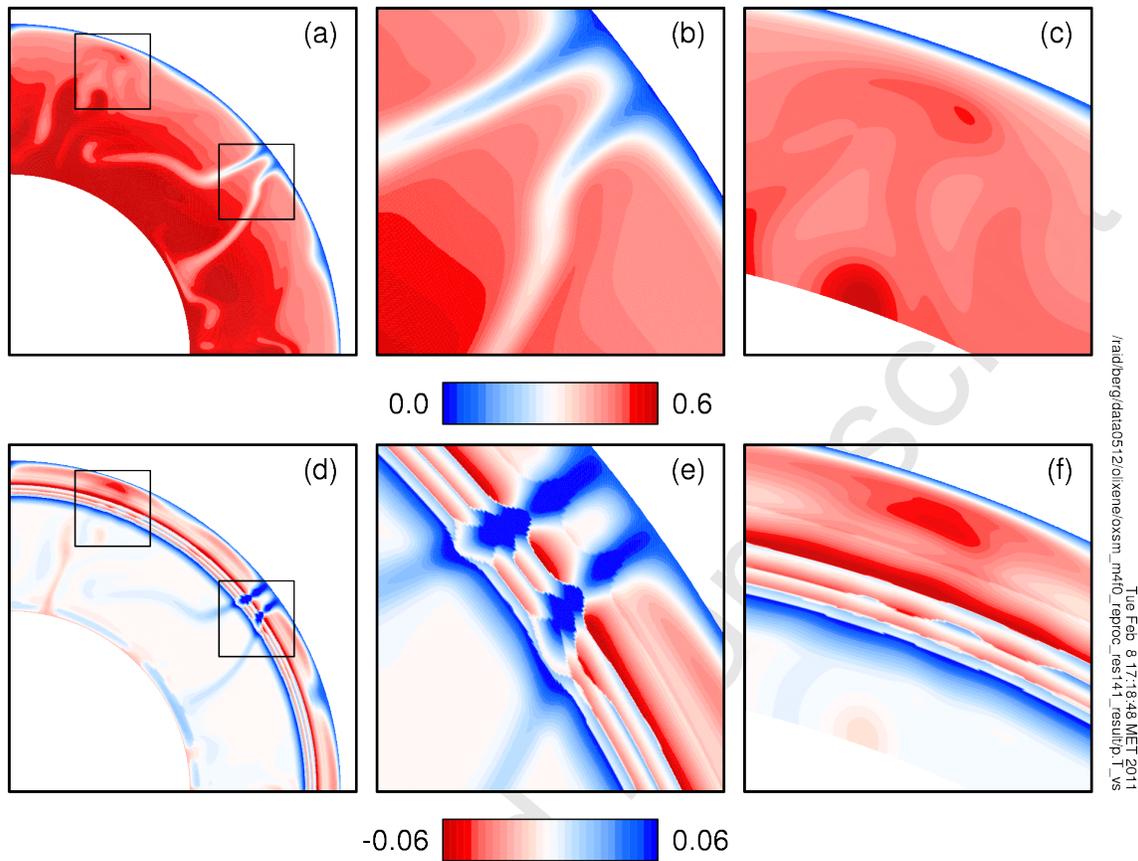
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Figure 1: Pressure-depth dependence of the seismic, longitudinal (v_p), shear (v_s) and bulk (v_b) wavespeeds, after (Jacobs and de Jong, 2009). Solid red curves are model predictions for mantle adiabats (1420 K) and a similar mineral composition as in our present model. Grey fields represent wavespeeds for compositions ranging from Mg_2SiO_4 to MgSiO_3 . Green curves represent a model with $(\text{Mg}_{0.9}\text{Fe}_{0.1})_2\text{SiO}_4$. The dashed green curve is from a model based on calphad type parameterizations for the same olivine composition (Jacobs and de Jong, 2005b). Discrete symbols represent the PREM model.



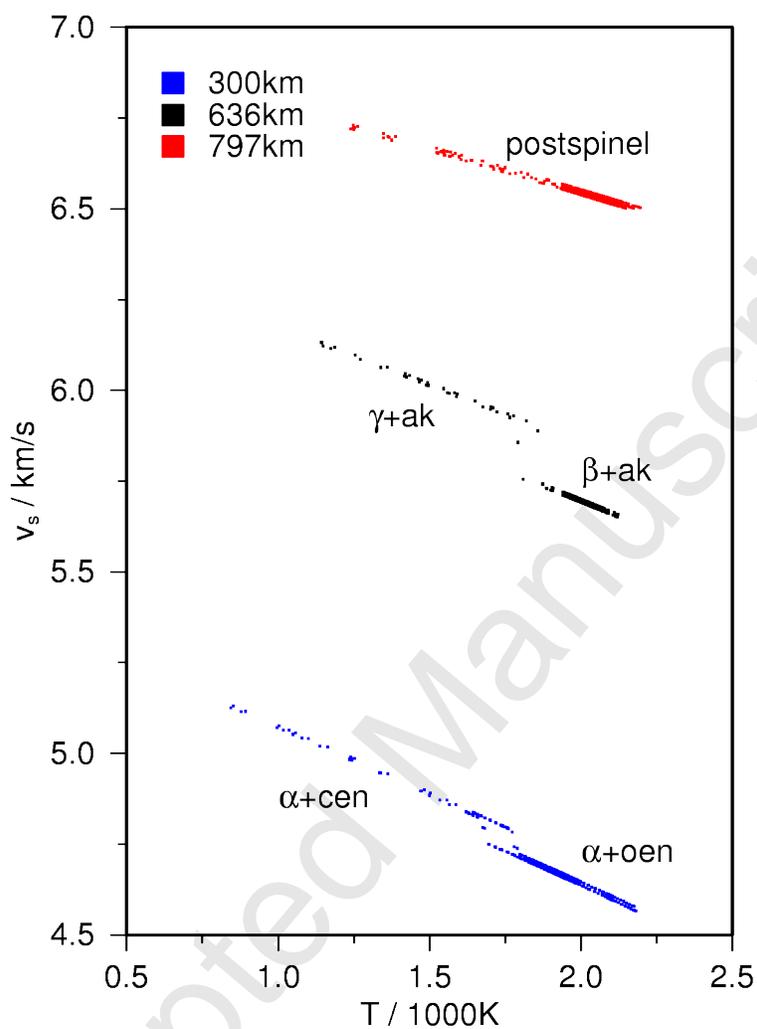
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Figure 2: Heat capacity of forsterite at 1 bar pressure from alternative mineral physics models compared with observational data. The curve labeled MGK-a corresponds to the model of Jacobs and de Jong (2007) that includes a Kieffer type VDoS and intrinsic anharmonicity. The curve labeled MGD is obtained from the Mie-Grneisen-Debye model employed by Stixrude and Lithgow-Bertelloni (2005). Experimental data are from Orr (1953), triangles, Robie (1982), squares, Watanabe (1982), diamonds, Ashida et al. (1987), inverted triangles, Gillet et al. (1991) filled circles.



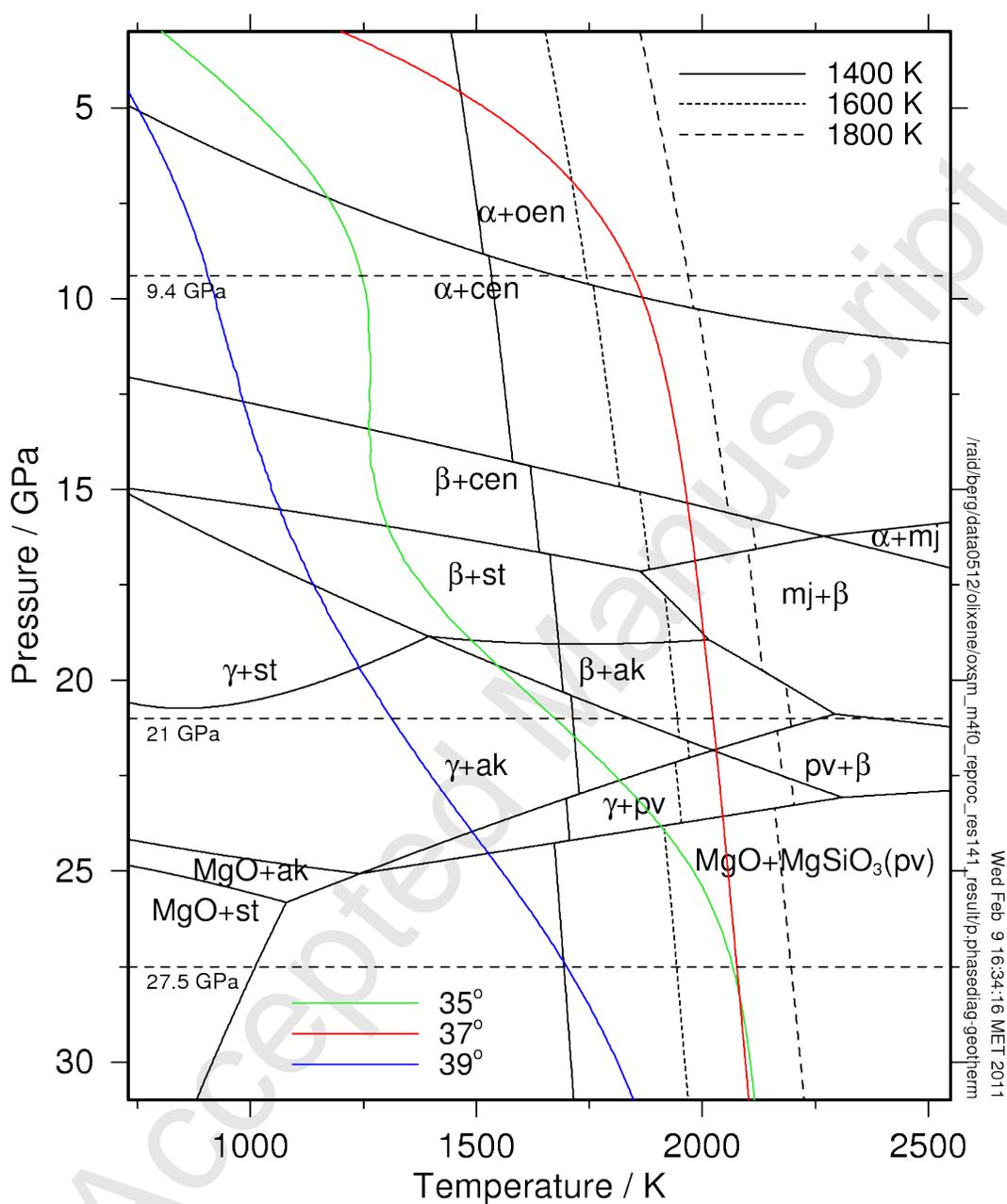
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Figure 3: (a) Full domain temperature snapshot showing two colliding cold downwellings and a hot mantle upwelling. Black boxes represent zoom-in windows corresponding to frames (b,c). (b) zoom-in temperature of the cold downwellings flow. (c) zoom-in temperature of the shallow head of a hot upwelling. (d) Full domain distribution of the lateral variation of the shear wavespeed δv_s with respect to the smooth background profile. (e) zoom-in of δv_s of the cold downwelling. (f) zoom-in of δv_s of the hot mantle plume head.



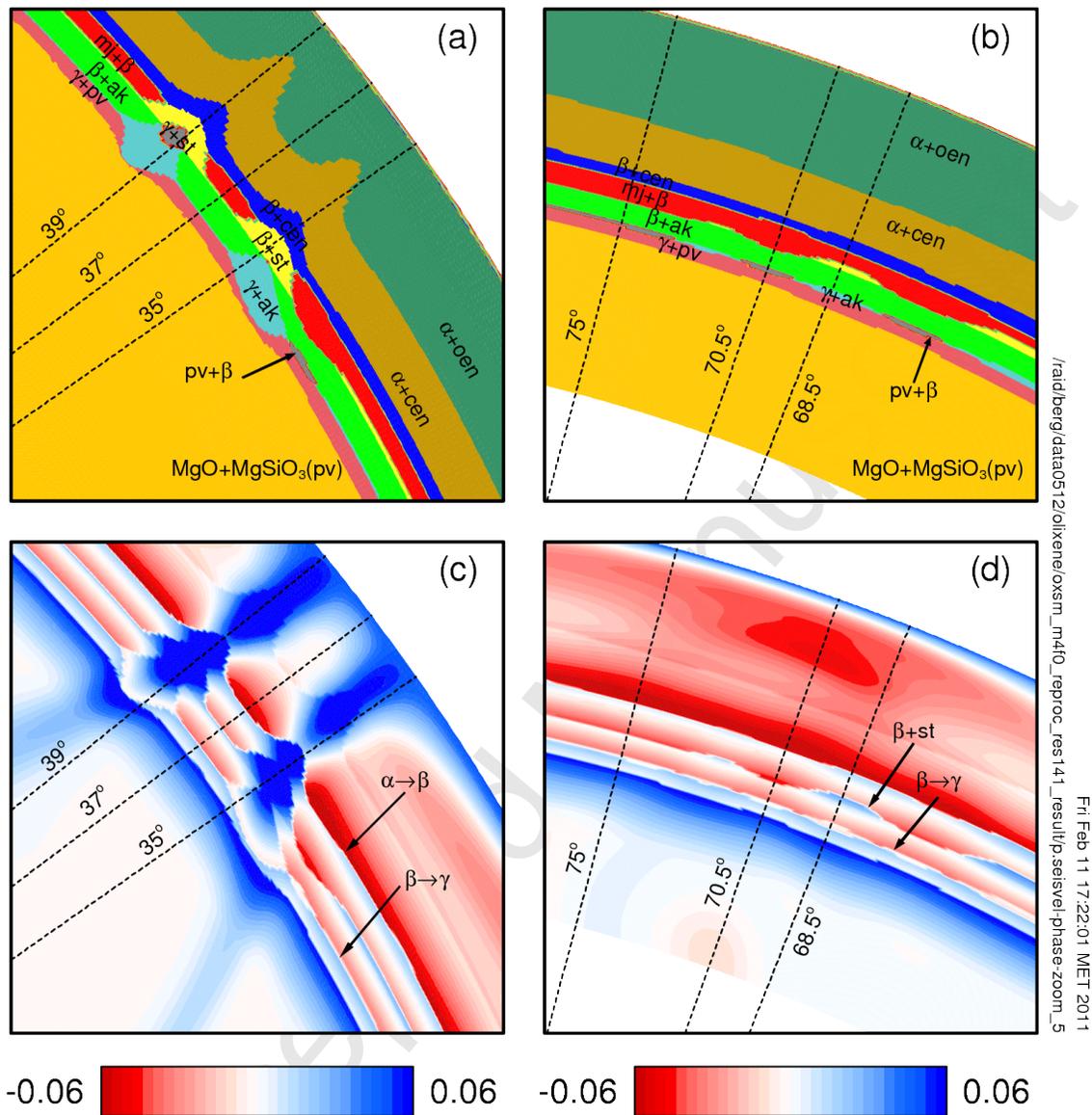
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Figure 4: Isobaric wavespeed-temperature data samples taken from the model output shown in Fig. 1. Samples correspond to finite element grid points in 20 km deep zones centered at 300, 636 and 797 km depth. Curve labels indicate the mineral associations that correspond to the stability fields in the phase diagram shown in Fig. 5. Sampling depths indicated in the plot labels correspond to model pressure values of 9.4, 21 and 27.5 GPa respectively.



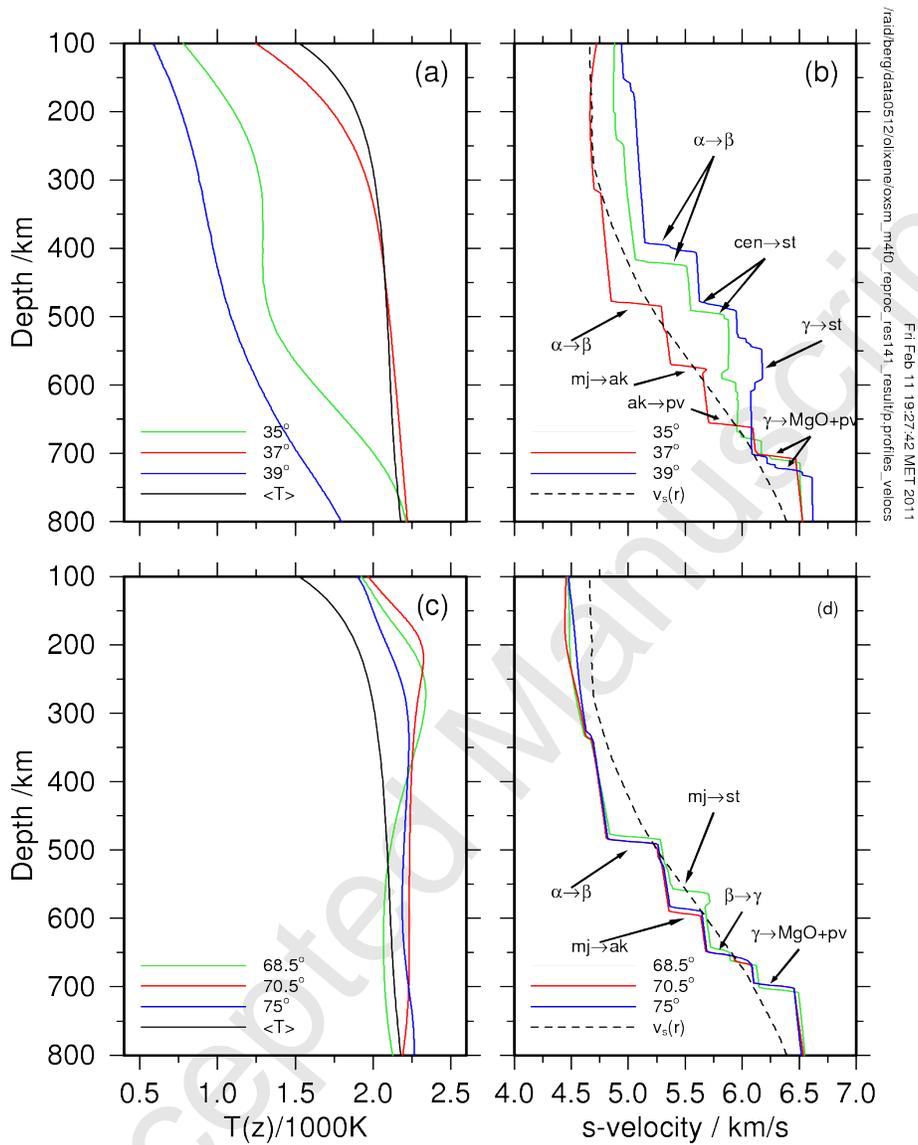
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Figure 5: Phase diagram of the olivine-pyroxene magnesium endmember model used in the convection model. Adiabats of potential temperature T_p between 1400 and 1800 K are plotted for reference. Solid curves represent radial temperature profiles, with angular position shown in the legend, and corresponding to the dashed lines in Fig. 6a. Horizontal dashed lines, labeled with a pressure value, correspond to the isobaric cross sections shown in Fig. 4.



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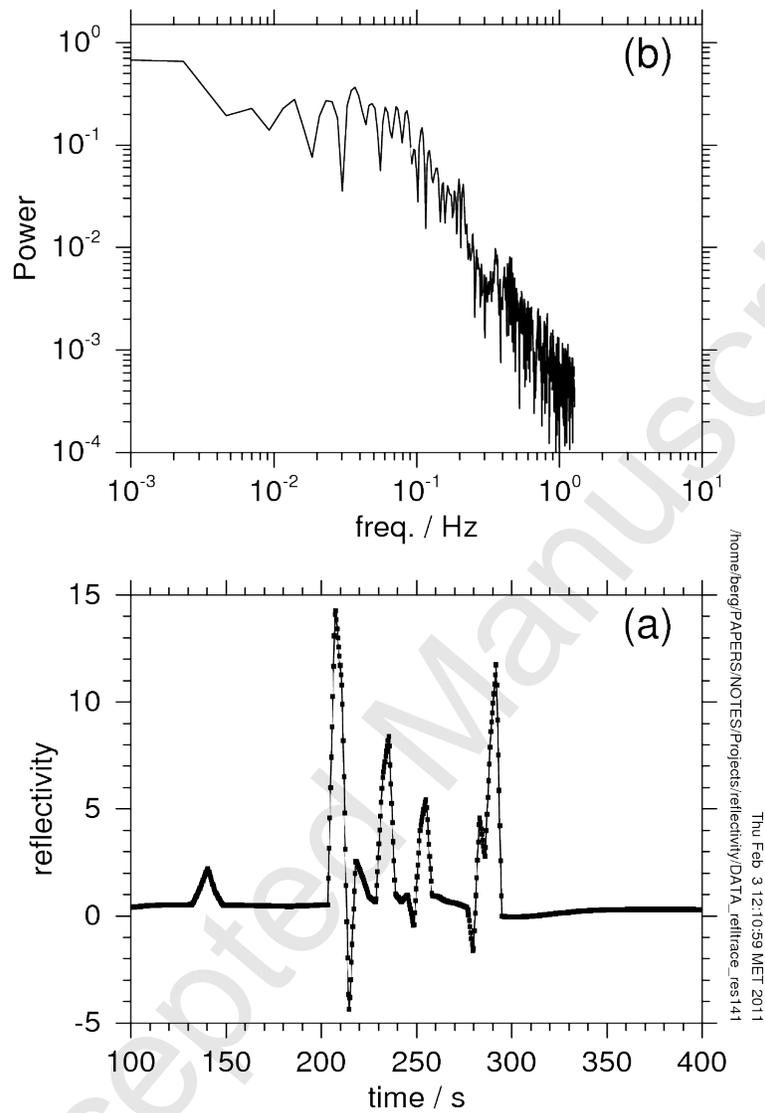
Figure 6: (a) Zoom-in on the spatial mineral phase distribution near the cold downwelling shown in Fig. 3b,e. Dashed lines indicate the position of radial profiles. (b) Similar zoom-in as in (a) near the hot mantle region shown in 3c,f. Individual mineral domains in (a,b) have been labeled according to the phase diagram shown in Fig. 5. Frames (c,d) show the lateral variation of the shear wavespeed, δv_s for the same zoom-in windows as in (a,b) respectively.



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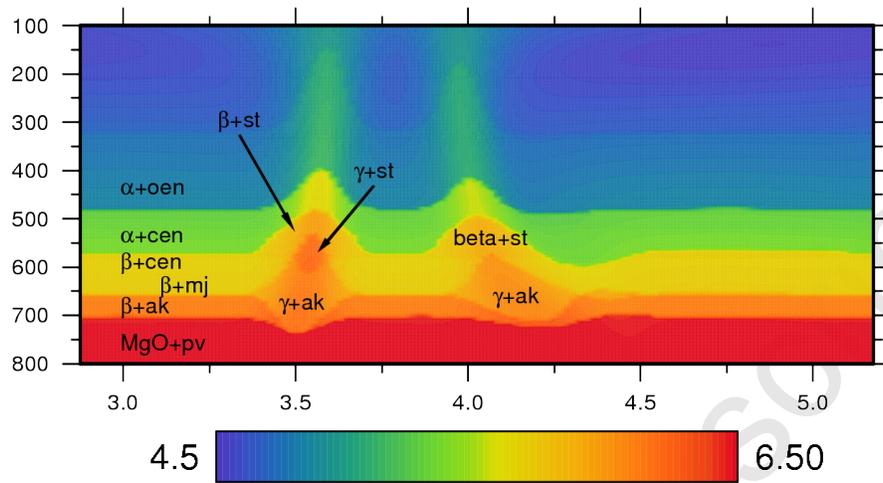
Figure 7: Radial profiles in zoom-in windows of Fig. 6. Temperature (left) and shear wavespeed (right). The (global) laterally averaged temperature is plotted for reference as a black curve in frames (a,c). The dashed curve in the frames (b), (d) represents the smoothed background wavespeed profile. Sharp transitions in the velocity profiles are labeled by the corresponding phase transitions that can be identified in the profiles drawn in Fig. 6.



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Figure 8: Spectral analysis of a single unfiltered reflectivity time trace plotted shown in frame (a), corresponding to the highlighted red trace in Fig. 9(a). (b) powerspectrum of the time trace in (a), showing that the peak power is below the frequency of 0.1 Hz, corresponding to wavelength's from 50 to 60 km in the transition zone.



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Figure 10: Shear wavespeed, in km/s, distribution for the zoom-in window of Fig. 6a,c. Labeled regions of contrasting shear wavespeed correspond to the contrasting mineral phase regions in Fig. 6. The wavespeed contrasts of the different mineral phase domains are closely correlated with the 'signal phases' of the reflectivity sections shown in Fig. 9.