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Sensitivities of seismic velocities to temperature, pressure and composition in the lower mantle

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Abstract

We calculated temperature, pressure and compositional sensitivities of seismic velocities in the lower mantle using latest mineral physics data. The compositional variable refers to the volume proportion of perovskite in a simplified perovskite-magnesiowüstite mantle assemblage. The novelty of our approach is the exploration of a reasonable range of input parameters which enter the lower mantle extrapolations. This leads to realistic error bars on the sensitivities. Temperature variations can be inferred throughout the lower mantle within a good degree of precision. Contrary to the uppermost mantle, modest compositional changes in the lower mantle can be detected by seismic tomography, with a larger uncertainty though. A likely trade-off between temperature and composition will be largely determined by uncertainties in tomography itself. Given current sources of uncertainties on recent data, anelastic contributions to the temperature sensitivities (calculated using Karato's approach) appear less significant than previously thought. Recent seismological determinations of the ratio of relative *S* to *P* velocity heterogeneity can be entirely explain by thermal effects, although isolated spots beneath Africa and the Central Pacific in the lowermost mantle may ask for a compositional origin. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Traditionally, velocity variations mapped by global seismic tomography have been attributed to temperature variations as documented by overviews of Ranalli (1996) and Yuen et al. (1996). Recently, some tomographic models found an anti-correlation between bulk and shear velocity anomalies in the lowermost mantle (Su and Dziewonski, 1997; Masters et al., 2000), which could be due to something else than temperature variations. Su and Dziewonski (1997) explained their result with an all-temperature model whilst Stacey (1998) favoured compositional effects. Observing a significant drop in radial correlation of Pvelocity anomalies together with a change of the relative ratio of bulk to shear wave speed, van der Hilst and Karason (1999) also argued for compositional heterogeneity in the bottom 1000 km of the lower mantle. Studies which mention compositional effects in the lower mantle do so using mostly qualitative arguments. The aim of this study is to be put these claims on a more quantitative footing.

A quantitative interpretation of seismic tomography needs several ingredients. Firstly, results from P and S wave tomography together with realistic error bars must be available. The latter are largely unknown, but

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essential to determine, for instance, how significant a drop in correlation is. Then, sensitivities of seismic velocities to the desired parameters have to be calculated. As we will show below, numerous assumptions need to be made in order to estimate these sensitivities leading to more uncertainties. Finally, given tomographic models and sensitivities together with their respective uncertainties, one can draw inferences on parameters such as temperature and composition, either by direct inversion or simple hypothesis testing.

The present work deals with the calculation of sensitivities of seismic velocities to temperature, pressure and composition and the corresponding error bars. The calculations are based on mineral physics data projected to lower mantle conditions via an equation-of-state (EOS) and a simplified model of the lower mantle consisting of perovskite and magnesiowüstite only. We assume that appropriate mixing of these minerals is able to represent the average Earth model PREM (Dzuewonski and Anderson, 1981) to a good degree of precision. The sensitivities are calculated for three parameters: temperature T, pressure P and composition X (the volumetric proportion of perovskite in the system). We included pressure for completeness and will discuss its importance below.

2. Elastic moduli, density and their T-P derivatives at mantle conditions

Most mineral physics data (density, bulk and shear moduli) are measured at modest temperature and pressure conditions compared to those in the lower mantle. An extrapolation to lower mantle conditions of these data needs to be done using an equation of state (EOS). There are many different types of EOS to choose from (Anderson, 1995). We opted for a third-order Birch-Murnaghan EOS which has extensively been used for modelling lower mantle composition (see Jackson, 1998, for a recent review). Recently, shortcomings of such an EOS have been pointed out and alternatives have been proposed (Stacey, 1998; Poirier and Tarantola, 1998). The question of an optimal EOS for the lower mantle is still open and we adopt here the pragmatic point of view that an EOS is valid, provided it gives a reasonable fit (defined below) to PREM. All EOSs contain some empirical element and testing against an earth model is their only way of assessment. It is then possible that different thermodynamic formulations lead to different parameters estimations (e.g. temperature and composition). We will briefly discuss this below.

Jackson (1998) has shown that third-order Eulerian isotherms and isentropes appear to be adequate for the strains encountered in the Earth's lower mantle. His preferred EOS is a combination of a Mie-Grüeneisen-Debye description of thermal pressure with the third-order Eulerian finite strain 300 K isotherm. Although this formalism is suitable to model the seismic parameter and density, the shear properties of the mantle cannot easily be included in that description. For our purposes, a hot isentropic compression is the most suitable. In order to calculate seismic sensitivities, we have to project elastic and density data, given at ambient conditions, to lower mantle temperatures and pressures. The least reliable measurements are found for the shear properties of lower mantle minerals. Particularly, the second pressure derivatives of the shear modulus are poorly constraint, so that we chose to use Stacey's (1992) observation instead which says that the shear modulus in the lower mantle varies linearly with incompressibility and pressure along an adiabatic compression. Although not an independent mineral physics constraint, this information will at least be compatible with the seismic data against which we test our extrapolations. The main difficulty to overcome is that the hot isentropic compression starts at some unknown high temperature $T_{\rm f}$, called foot of the adiabat, rather than 300 K.

Many high temperature extrapolation formulae have been advocated for thermoelastic properties (Anderson and Isaak, 1995). We chose to use the Anderson–Grüneisen parameter for incompressibility and assumed it to be constant at zero pressure. This is observed to be approximately true above the Debye temperature. In case of the shear modulus, we prefer a linear variation with temperature. For a given mineral, the density ρ , the adiabatic bulk modulus *K* and the shear modulus *G* at temperature $T_{\rm f}$ are then obtained from

$$\rho(T_{\rm f}, P=0) = \rho_0 \exp\left[-\int_{T_0}^{T_{\rm f}} \alpha(T) \,\mathrm{d}T\right],\tag{1}$$

$$K(T_{\rm f}, P=0) = K_0 \left[\frac{\rho(T_{\rm f}, P=0)}{\rho_0} \right]^{\delta_{S_0}}$$
(2)

and

$$G(T_{\rm f}, P = 0) = G_0 + (\partial G/\partial T)_P (T_{\rm f} - T_0),$$
 (3)

where the subscript '0' refers to ambient temperature and pressure conditions and the Anderson-Grüneisen parameter is given by $\delta_S = -1/(\alpha K)(\partial K/\partial T)_P$. Expressions (2) and (3) fit the measured data for MgO (Anderson and Isaak, 1995) remarkably well. We did not find any high temperature data for perovskite, but assumed that the same expressions would describe its high temperature elasticity best. Duffy and Anderson (1989) recommended an expression similar to (2) for the shear modulus. We also tried this in our modelling and found that the pressure and compressional derivatives remained unchanged, while the temperature sensitivities slightly increased. To evaluate $\rho(T_f, P = 0)$, the knowledge of the temperature dependence of the thermal expansivity is required. This is usually obtained from fitting laboratory data to the polynomial expansion

$$\alpha(T) = a + bT - cT^{-2}.$$
(4)

Other constants needed for the isentropic compression are the first pressure derivatives of the elastic moduli at constant entropy. Again these values are given at ambient temperature in the literature and need to be evaluated at $T_{\rm f}$. Since the second mixed T-P derivatives of elastic moduli are poorly constrained by laboratory measurements, we assumed that $K' = (\partial K/\partial P)_S$ and $G' = (\partial G/\partial P)_S$ are temperature independent at ambient pressure. It has been shown by Jackson (1998) that this is indeed a good approximation for the bulk modulus. The validity of this approximation for the shear modulus has not been established, but we took this into account by allowing a larger range of variation for this input parameter.

To extrapolate from $(T_f, P = 0)$ to (T, P), we make a Birch–Murnaghan adiabatic compression using

$$P = -(1 - 2\epsilon)^{5/2} (C_1 \epsilon + \frac{1}{2} C_2 \epsilon^2 + \frac{1}{6} C_3 \epsilon^3)$$
(5)

and

$$\rho(T, P) = \rho(T_{\rm f}, P = 0)(1 - 2\epsilon)^{3/2}, \tag{6}$$

where ϵ is the Eulerian strain of the mineral. The elastic moduli at the desired T-P conditions are

readily obtained from the following expressions for the compressional and shear wave speeds:

$$\rho V_P^2 = K + 4/3G$$

= $(1 - 2\epsilon)^{5/2} (L_1 + L_2\epsilon + L_3\epsilon^2/2)$ (7)

and

$$\rho V_S^2 = G = (1 - 2\epsilon)^{5/2} (M_1 + M_2\epsilon + M_3\epsilon^2/2).$$
(8)

We chose to truncate the Birch–Murnaghan equation to third-order which means that $C_3 = 0$ in Eq. (5). As emphasised before (Jackson, 1998), to ensure a self-consistent set of equations, L_3 and M_3 are different from zero. To evaluate the latter, we need to know the second pressure derivatives of the elastic moduli. These are also poorly constrained by laboratory measurements, but can fortunately be estimated since $K'' = (\partial^2 K / \partial P^2)_S$ is related to K' and K at zero pressure through the relation:

$$C_3 = 27K(T_f)\{K(T_f)K''(T_f) -K'(T_f)[7 - K'(T_f)] + 143/9\} = 0.$$
(9)

Along the lower mantle adiabat, we use Stacey's (1992) relation G = AK + BP, where A and B are readily calculated at zero pressure leading to

$$G''(T_{\rm f}) = AK''(T_{\rm f}).$$
(10)

The uncertain laboratory measurements of the second derivatives of the elastic moduli are thus replaced by constraints from Eqs. (9) and (10). This ensures that our system of equations is consistent without injecting any information incompatible with seismic data. The constants C_i , L_i and M_i are calculated from the elastic moduli and their isentropic pressure derivatives (full expressions can be found in Jackson (1998)). Assuming the pressure P to be known at all depths from PREM, we compute the Eulerian strain ϵ from Eq. (5) using a Newton–Raphson method. Expressions (6)-(8) allow to evaluate density and the elastic moduli of a given mineral at the desired temperature and pressure. To calculate the sensitivities we need to specify the end-temperature and the adiabatic temperature gradient. The gradient is given by

$$\left(\frac{\partial T}{\partial P}\right)_{S} = \frac{\gamma T}{K}.$$
(11)

In the quasi-harmonic approximation, the Grünesien parameter γ only depends upon density as $-d \ln \gamma / d \ln \rho = q$ which, upon integration with constant q, yields

$$\gamma = \gamma_0 \left(\frac{\rho_0}{\rho}\right)^q.$$
 (12)

This allows to calculate the end-temperature using

$$T = T_0 \exp\left[\frac{(\gamma_0 - \gamma)}{q}\right].$$
 (13)

The T-P derivatives for individual mineral properties are readily calculated numerically. First, we make a compression to a final pressure P as given by PREM. This corresponds to some final temperature T from Eq. (13). We now make another compression to the same final P, but a slightly different end-temperature T + dT (where $dT \ll T$). This is achieved by starting the extrapolation from a slightly different adiabat. Numerical differentiation then gives the temperature derivatives at constant pressure of the elastic constants and density. We checked that such an evaluation of derivatives is numerically stable (i.e. independent of dT). Similarly, we can calculate the pressure derivatives at constant entropy by making a compression to P + dP (where $dP \ll P$) starting this time from the same initial foot temperature. The pressure derivatives at constant temperature may then be evaluated from the thermodynamic identity

$$\left(\frac{\partial Z}{\partial P}\right)_T = \left(\frac{\partial Z}{\partial P}\right)_S - \left(\frac{\partial T}{\partial P}\right)_S \left(\frac{\partial Z}{\partial T}\right)_P, \quad (14)$$

where Z stands for any thermodynamic parameter.

3. From individual minerals to mantle properties

As mentioned before, we assume the mantle to be composed of two minerals only. The density of the mantle $\bar{\rho}$ is then simply the volumetric average of the density of perovskite (pv) and magnesionwüstite (mw) which corresponds to a relaxed state Reuss average:

$$\bar{\rho} = \rho_{\rm mv} + X(\rho_{\rm pv} - \rho_{\rm mv}) \tag{15}$$

Our compositional variable is X, the relative volume proportion of perovskite in the system. The elastic

moduli of the mantle are more appropriately obtained from a Voigt–Reuss–Hill average (Watt et al., 1976) using the following expressions:

$$M^{\rm V} = M_{\rm mw} + X(M_{\rm pv} - M_{\rm mw})$$
 (16)

$$M^{\rm R} = \frac{M_{\rm pv}M_{\rm mw}}{M_{\rm pv} - X(M_{\rm pv} - M_{\rm mw})}$$
(17)

$$\bar{M} = \frac{1}{2}(M^{\rm V} + M^{\rm R})$$
 (18)

where M means bulk or shear modulus. The seismic velocities in the mantle may then be evaluated using

$$V = \left(\frac{\bar{C}}{\bar{\rho}}\right)^{1/2} \tag{19}$$

where the *P* wave speed is given by $\bar{C} = \bar{K} + 4/3\bar{G}$ and the *S* wave speed by $\bar{C} = \bar{G}$. The sensitivities of the seismic velocities are simply obtained by differentiation of (19)

$$\left(\frac{\partial \ln V}{\partial \xi}\right) = \frac{1}{2\bar{\rho}V^2} \left[\left(\frac{\partial \bar{C}}{\partial \xi}\right) - V^2 \left(\frac{\partial \bar{\rho}}{\partial \xi}\right) \right]$$
(20)

where ξ stands for T, P or X. $\partial \bar{\rho} / \partial \xi$ and $\partial \bar{C} / \partial \xi$ are readily obtained by differentiating Eqs. (15)-(18). Expression (20) only contains temperature and pressure derivatives of individual mineral properties since the compositional derivatives of individual minerals are zero (i.e. you do not change the bulk modulus of perovskite by adding more or less perovskite to the system). The separate adiabatic compressions of different minerals from a common foot temperature to a common pressure will yield different end-temperatures. The system needs then to relax to a common final temperature before calculating the properties of the mixture (Stacey, 1998). This leads to non-zero quantities $(\partial X/\partial P)$ and $(\partial X/\partial T)$. We adopted a different approach, starting from different foot temperatures to a common end-temperature. This is easily achieved numerically and ensures that $(\partial X/\partial P) = (\partial X/\partial T) = 0$, in expression (20).

4. Input parameters

The calculations outlined previously are very dependent on the thermodynamic reference state of

the lower mantle, many assumptions and the numerical values of the elastic parameters at ambient conditions. We propose to test a whole range of input parameters rather than somehow choose as has been done in previous studies. We can thus analyse the effect of each parameter on the computed derivatives and estimate error bars.

4.1. Foot of the adiabat

Density and seismic velocities are computed along an adiabatic temperature profile, for which a foot temperature (at P = 0) has to be chosen. This foot temperature strongly depends, for instance, on the dynamics of the whole mantle system, on the presence of boundary layers or chemical differentiation within the mantle. To avoid these difficult debates, a large range of foot temperatures for the lower mantle adiabat is explored, ranging between 1500 and 2500 K.

4.2. Pressure profile

We need to know the spherically averaged pressure to calculate the strain at a given depth (Eq. (5)). It is natural to take the pressure from PREM, but it should be kept in mind that this pressure is somewhat uncertain due to assumptions (e.g. adiabacity) not constrained by seismic data. To explore the effect of pressure variations on the computed derivatives, we allow up to 1% variations on the PREM pressure at all depths.

4.3. Average composition of the lower mantle

It is generally assumed that (Mg, Fe)SiO₃ perovskite and (Mg, Fe)O are the major components of the lower mantle, representing at least 80% of the lower mantle composition. Ca- and Al-rich phases could be minor components of the lower mantle. The calcium rich phase must be found as an independent CaSiO₃ perovskite (Kesson et al., 1998), whereas the aluminium rich phase could form either a separated garnet (O'Neil and Jeanloz, 1994), at least to a modest depth, or be included in the (Mg, Fe)SiO₃ perovskite structure (Irifune, 1994). In the present study we neglect these secondary phases, and consider average

proportions of perovskite of 50–100% complemented by magnesiowüstite.

4.4. Bulk iron content

This parameter depends on the degree of mantle differentiation: a mantle convecting as a single layer would result in a lower mantle containing about 10% of iron (the upper mantle value); a stratified convection would correspond to a different lower mantle iron content. We study here variations of the bulk iron content of the lower mantle ranging between 5 and 15% in volume.

4.5. Iron partitioning

The relative proportions of the minerals and the bulk iron content are not sufficient to define the composition of the lower mantle: the iron partitioning between perovskite and magnesiowüstite K_{Fe} must also be defined:

$$K_{\rm Fe} = \frac{(X_{\rm Fe}/X_{\rm Mg})_{\rm pv}}{(X_{\rm Fe}/X_{\rm Mg})_{\rm mw}}$$
(21)

Experimental studies of this parameter have suggested values between 0.2 and 0.5 (Katsura and Ito, 1996; Martinez et al., 1997). But it has also been proposed that $K_{\rm Fe}$ might change significantly with temperature, pressure and composition; Wood and Rubie (1996) suggest that a small amount of Al₂O₃ can increase $K_{\rm Fe}$ to a value of unity (equal partitioning of iron between perovskite and magnesiowüstite), and Mao et al. (1997) found variations between 0.04 and 0.29 for a different temperature, pressure and starting composition. Kesson et al. (1998), however, performed experiments for a pyrolite lower mantle, and found no evidence of such variations, but a fairly constant value of K_{Fe} around 0.45. We test values between 0.2 and 0.5, which are all consistent with our chosen bulk composition.

4.6. Thermo-elastic parameters

The values of the thermo-elastic parameters used for perovskite and magnesiowüstite are listed in Table 1. The compressional parameters for perovskite are taken from Jackson (1998). He gives four possible data sets,

	Perovskite				Magnesiowüstite
ρ (g/cm ³)	4.109+1.03 X _{Fe}				3.584+2.28 X _{Fe}
K (GPa)	264.0				162.5+11.5 X _{Fe}
K'	3.97	3.95	3.77	3.75	4.13
$(\partial K/\partial T)_P$ (GPa/K)	-0.011	-0.015	-0.010	-0.015	-0.0145^{b}
γ	1.31	1.39	1.33	1.41	1.41
<i>q</i>	1	2	1	2	1.3
G (GPa)	175.0 ^c				130.8 -75.6 X _{Fe}
G'	$1.8 (0.4)^{c}$				2.5 ^d
$(\partial G/\partial T)_P$ (GPa/K)	$-0.029 (0.003)^{c}$				-0.024^{e}
$a (10^{-5} \text{ K}^{-1})$ in Eq. (4)	$1.19 (0.17)^{\rm f}$				3.681 ^g
$b (10^{-8} \text{ K}^{-2})$ in Eq. (4)	$1.20 \ (0.10)^{\rm f}$				0.9283 ^g
<i>c</i> (K) in Eq. (4)	0.0^{f}				0.7445 ^g

Table 1 Thermoelastic parameters of the lower mantle^a

^a All data are from Jackson (1998) unless otherwise stated. Where available, measurement errors are in parentheses.

^b Stacey (1998).

^c Sinelnikov et al. (1998).

^d Duffy and Ahrens (1992).

e Zhao and Anderson (1994).

f Fiqued et al. (1998).

^g Fei et al. (1992).

all consistent with various available P-V-T experimental data (see references therein). We use all four data sets to model the effects of experimental uncertainties on computed partial derivatives. Concerning the shear parameters of perovskite, we use the recent experimental data of Sinelnikov et al. (1998) and vary their values within their error bars. Thermal expansivity for perovskite and its uncertainties are taken from Fiqued et al. (1998), which combines their P-V-Tdata up to 57 GPa and 2500 K with previous data. It is generally thought that parameters for magnesiowüstite are better constrained than those of perovskite (Zhao and Anderson, 1994). To avoid too big an increase in the number of varying parameters, they are assumed perfectly known. In summary, for perovskite, K_0 and G_0 are constant and all other input parameters vary. For magnesiowüstite, no explicit variations are made, but changes occur in K_0 and G_0 through the variations in iron content (X_{Fe}) (see Table 1). At ambient conditions, the Anderson-Grüneisen parameter also varies implicitly. We do not choose this parameter, but it is directly calculated from its definition. Given the range of respective input parameters, the variation is 2.45 < $\delta_{\rm S}(300 \,{\rm K}, P = 0) < 4.22$ for perovskite and 2.78 < $\delta_S(300 \text{ K}, P = 0) < 2.86$ for magnesiowüstite. This large range should cover most restrictions implied by

assuming the Anderson–Grüneisen to be temperature independent at zero pressure.

5. Results

Density, seismic velocities and their derivatives are calculated for all possible combinations of the input parameters described above. This generated more than 1.5 million cases. Many of these predictions are unrealistic from a seismic point of view. We only kept cases for which the average prediction of density and seismic velocities over depth matched those of PREM within one percent. In the lower mantle, typical rms-velocity anomalies are around the 0.5% level. The 1% tolerance is intended to also cover eventual biases in PREM and seems realistic given the velocity anomalies found by current tomographic models. All our calculations are performed over a depth range between 1000 and 2600 km. This is to avoid boundary layers where adiabacity might be questionable. This left us with approximately 2000 different combinations of input parameters compatible with PREM. We averaged the sensitivities of the velocities over all compatible cases. The results are shown in Fig. 1 and given as a polynomial expansion for depth in Table 2. The errors of the sensitivities



Fig. 1. Sensitivities of P wave velocities and S wave velocities to temperature (top), pressure (middle) and composition (bottom), as a function of depth. Each profile corresponds to the average of 2000 cases for which calculated radial velocities and density gave a good fit to PREM. Error bars correspond to 1 S.D. around the average.

correspond to one standard deviation around the average and are also given as a polynomial expansion.

Temperature derivatives decrease quite steeply with increasing depth due to the sharp decrease of the thermal expansivity with pressure. V_S has a higher sensitivity to temperature than V_P because $|\partial G/\partial T| > |\partial K/\partial T|$ for both phases. An average lateral temperature variation of 100 K at the top of the lower mantle increasing to an average temperature anomaly of 200 K at the bottom can explain currently observed rms-velocity anomalies which are fairly constant over most parts of the lower mantle (0.006 for d ln V_S and 0.003 for d ln V_P are average values from most recent tomographic models (Masters et al., 2000). Velocities, are thus, sensitive to fairly small temperature variations. P and S anomalies highly correlate with a correlation factor of 0.8 (Masters et al., 2000). They could hence be explained by a single temperature effect throughout the mantle. This assumes that extrinsic (volume dependent) temperature effects dominate. For a detailed discussion on intrinsic versus extrinsic effects, see Anderson (1989). We roughly estimated intrinsic temperature sensitivities and found that they reach up to 50% of our calculated sensitivities. If we want to infer temperature variations from tomography, we also need to worry about errors. This is best done by evaluating the relative error on temperature as a function of depth. Fig. 2 shows the contribution from errors in sensitivities alone. This is a lower bound since the errors in seismic tomography will add to the ones shown. The relative errors on inferred temperature variations increase slightly with depth, but stay below 15%. Precision from S waves is slightly better than that from P waves. If seismic tomography induced errors stay within reasonable



Fig. 2. Relative errors as a function of depth for temperature and compositional variations due to errors in sensitivities alone.

	a	$b(\times 10^3)$	$c(\times 10^7)$	
$\partial V_P^{\rm qh}/\partial T \ (10^{-5} {\rm K}^{-1})$	-5.03 (0.47)	2.22 (-0.13)	-3.52 (0.23)	
$\partial V_{\rm s}^{\rm qh}/\partial T \ (10^{-5} {\rm K}^{-1})$	-7.82 (0.75)	3.27 (-0.31)	-4.88(0.55)	
$\partial V_P^{\text{an}}/\partial T (10^{-5} \text{ K}^{-1})$	-0.68 (0.27)	0.22 (-0.09)	-0.32(0.14)	
$\partial V_{\rm S}^{\rm an}/\partial T \ (10^{-5}{\rm K}^{-1})$	-1.55 (0.62)	0.43 (-0.18)	-0.58(0.25)	
$\partial V_P / \partial P \ (10^{-3} \mathrm{GPa}^{-1})$	5.23 (0.31)	-2.39(-0.19)	3.85 (0.35)	
$\partial V_S / \partial P \ (10^{-3} \mathrm{GPa}^{-1})$	4.44 (0.43)	-2.04 (-0.24)	3.32 (0.41)	
$\partial V_P / \partial X \ (10^{-1})$	1.72 (0.24)	-0.98 (-0.04)	1.44 (0.08)	
$\partial V_S / \partial X \ (10^{-1})$	1.50 (0.37)	-1.43 (-0.09)	1.92 (0.19)	

Table 2 Polynominal fits to the partial derivatives^a

^a The sensitivities are expressed as $\partial V/\partial \xi = a + bz + cz^2$ where z is the depth in km. Given are the constants for sensitivities and in brackets the ones for the corresponding errors. In case of temperature, the superscript 'qh' stands for the quasi-harmonic part and 'an' for the anelastic part.

bounds, we can expect to infer lower mantle temperature variations with a good degree of precision.

Pressure derivatives are generally one order of magnitude too low for pressure to play a major role in the observed seismic velocity variations. Typical rms-velocity anomalies give lateral pressure variations in the range of 1-4 GPa. Although these variations only represent a few percent of the hydrostatic reference pressure, an order of magnitude calculation for a convective mantle, where buoyancy forces are balanced by pressure gradients only, give lateral pressure variations an order of magnitude smaller. This is also confirmed by convective flow calculations (Cadek, personal communication). Still, it is worth to be interested in lateral pressure variations. If we have the means to infer lateral temperature and pressure variations (as small as those might be) from tomography, we should, for instance, be able to put tighter constraints on inferences of lower mantle viscosity using seismic tomography.

The most interesting are the compositional derivatives. These derivatives are due to differences in elastic moduli and density between the two minerals. There is no simple intuitive way to understand the results, since there is a complicated interplay between the input measurements and the reference model parameters, such as the iron content and the geotherm. The main characteristics are as follows. Firstly, typical rms-velocity variations give perovskite variations of a few percent, except where the compositional sensitivities are close to zero. Here, the relative error is also unacceptably high (Fig. 2) so that composition remains undetermined. We note that in the upper part of the lower mantle compositional changes are reasonably well constrained by P wave tomography, whereas in the lower part S wave tomography is the constraint. Relative errors on composition are higher than those for temperature and represent again a lower bound. From shallow mantle studies, we know that seismic velocity variations are quite insensitive to compositional changes (Goes et al., 2000). In contrast, P and S velocity variations together are able to detect small changes in composition throughout the lower mantle. Secondly, the compositional sensitivities have opposite signs for P and S in most parts of the lower mantle. Should we then expect an anti-correlation between Pand S wave tomography? Only if compositional effects are dominant. Masters et al. (2000) have shown that P and S velocity variations correlate well (0.8)throughout the lower mantle. This is more of an indication that temperature plays the dominant role. Compositional variations have however an influence on the magnitude of the inferred temperature variations. To see this, imagine a slab penetrating deep in the lower mantle (van der Hilst et al., 1997). Assume further that d ln $V_S = 0.006$ and d ln $V_P = 0.003$, typical rms values we took throughout this work. It is straightforward to invert the P and S anomalies for temperature and compositional variations within the slab. At each point of the slab we solve the perfectly well determined system:

$$d \ln V_P = \frac{\partial \ln V_P}{\partial T} dT + \frac{\partial \ln V_P}{\partial X} dX$$

$$d \ln V_S = \frac{\partial \ln V_S}{\partial T} dT + \frac{\partial \ln V_S}{\partial X} dX$$
(22)

The temperature variations vary from $-126(\pm 12)$ K at the top to $-188(\pm 18)$ K at the bottom of the lower mantle. The compositional change is constant at $-0.012(\pm 0.006)$. In the top of the lower mantle, the temperature estimates are close to estimates from S anomalies alone. In the bottom part, they are close to results from P anomalies alone. In the mid-mantle, they are in between the two. This is understandable if we recall that for compositional variations it is the other way around. The compositional change shows a depletion in perovskite. Although the error is high with 50%, the sign is robust. This result agrees with inferences from phase transformations in a pyrolitic mantle compared to those in subducting lithosphere (Ringwood, 1991). Ringwood (1991) argued for an approximate depletion of 10% of perovskite in slabs. This is much higher than what we find here, but the rms values we used for velocities are low compared to what is found in actual slab images.

6. Discussion

We presented results for temperature, pressure and compositional derivatives of seismic velocities together with error bars due to various input parameters.

We believe that temperature and pressure derivatives are particularly well constraint since they are obtained by numerical differentiation. This ensures that most influences of the reference state are of second-order. Compositional derivatives are more sensitive to the average properties of the mantle (elastic moduli, average composition, temperature, etc.), and hence, depend to first-order on all input parameters in our calculations. This is well reflected by the inferred error bars. If uncertainties on seismic tomography stay within reasonable bounds, these error bars show that temperature variations can be inferred within a good degree of precision throughout the mantle. Compositional variations can also be inferred, but with a lower degree of precision. This is quite different to the situation in the uppermost mantle (before phase transitions occur), where it appears that velocity variations are largely insensitive to compositional effects. Some trade-off is likely between temperature and compositional effects. This trade-off will largely be determined by the magnitude of uncertainties in tomography. It is hoped that the inclusion of other geophysical data in this interpretation problem will mainly decrease the uncertainties in composition and thus reduce any expected trade-off.

We would like to remind the reader that many assumptions went into these calculations. For instance, it could be argued that the allowed variation for $\partial K / \partial T$ is too narrow. Indeed, for iron baring perovskites much lower values have been observed (Wang et al., 1994), even though these authors classified their result as suspect. We found furthermore if we allowed $\partial K / \partial T$ to be much lower than -0.0015, the thermal expansivity quickly became negative as a function of depth. We thus decided to use only magnesium perovskite data for this parameter. We neglected Ca and Al in our lower mantle description. This is probably acceptable for the average properties of the lower mantle, but may be a shortcoming in the study of compositional derivatives, especially since these particular elements behave relatively incompatibly during upper mantle melting of peridotide, leading to a significant depletion in the lower mantle. It is certainly possible to define different compositional parameters than the one used in the present study. Our main purpose was to show on a simple case how mineral physics and seismic data can be quantitatively combined to learn more about the composition of the lower mantle. The higher sensitivity to temperature of the shear velocity depends mainly on the value of $\partial G/\partial T$ for magnesium perovskite. We chose a value measured in a very difficult experiment (Sinelnikov et al., 1998). Jackson (1998) argues for an absolute value 30% smaller for a suitable mantle assemblage, but elasticity systematics (Zhao and Anderson, 1994) and Stacey (1998) favour a value close to what we used. These few remarks serve as a reminder that as new mineral physics data will become available, the conclusions of the present study will be modulated as a consequence.

Only temperature derivatives have previously been studied by different authors. Fig. 3 shows the temperature derivatives of Karato (1993) and Stacey (1998) compared to ours. Shown is only Karato's anharmonic part to make a comparison possible. It is clear that his sensitivities are much smaller than the others. These differences are most likely explained by the improvement of mineral physics data over recent years. Stacey's results are much closer to ours, but only his estimates for P waves agree within our error bars. There are two main differences between Stacey's and



Fig. 3. Comparison of the temperature derivatives (elastic term only) of P wave velocities (top) and S wave velocities (bottom). Shown are results from the study of Karato (1993) and Stacey (1998).

our calculations. He included higher order anharmonic effects while we used the quasi-harmonic approximation. This has a direct baring on γ and more importantly on q. As a result, his $\delta_S = -1/(\alpha K)(\partial K/\partial T)_P$ deviates up to 20% and his $\epsilon = -1/(\alpha G)(\partial G/\partial T)_P$ up to 50% from our estimates. Stacey's results depend to first-order on these quantities whereas our difference scheme only to second order. Stacey further uses a different equation of state, a variable not tested here. What exactly causes the differences needs to be explored in future work, but this is probably an example how different thermodynamic formulations can lead to different parameter estimations.

Since Karato's (1993) work it is widely accepted that anelastic effects are important in the calculation of temperature sensitivities. Recently, measurements for lower mantle minerals have become available which ask for a reexamination of his estimates. Following Karato's approximations, the anelastic contribution is written as

$$\frac{\partial \ln V_{\text{anel}}}{\partial T} = \frac{F(\beta)}{\pi Q} \frac{E}{RT^2}$$
(23)

 β expresses the frequency dependence of the quality factor Q and the function $F(\beta) = \pi \beta / 2(\pi \beta / 2)$. E is the activation energy and R the gas constant. The parameters needed for Eq. (23) are rather uncertain for the lower mantle which led us again to adopt a search within bounds. Seismic studies find values for β ranging between 0.1 and 0.4 (Romanowicz and Durek, 2000). This is compatible with experimental values (Jackson, 2000). Recent shear quality factors in the lower mantle vary between 300 and 360 (Romanowicz and Durek, 2000). We further assume that bulk attenuation is negligible. Until recently, no experimental data were available concerning the attenuation of lower mantle minerals. Gettting et al. (1997) conducted the first experiments measuring attenuation and dispersion in MgO. They found a rather low attenuation with an activation energy E =230 kJ/mol. The frequency dependence of attenuation was also obtained, with $\beta = 0.3$. Not much is known about the activation energy in (Mg, Fe)SiO₃, but measurements on other members of the perovskite family (some of which have been used as analogues) give values for E about twice that of MgO (Poirier, 1995) and very recently Webb et al. (2001) measured even higher values. We, therefore, varied E between 230 and 730 kJ/mol. The last important parameter is temperature. Our adiabatic compressions fitting PREM gave a geotherm varying from $T = 2260 \pm 267$ K at a depth of 1000 km and $T = 2435 \pm 322$ K at a depth of 2600 km. This is close to the geotherm obtained by Stacey (1998), but hoter than the temperature profile corresponding to the preferred mineral assemblage of Jackson (1998). The anelastic term of Eq. (23) can now be computed and results are shown in Fig. 4. All different parameter combinations we tried lead to modest amplitudes, on average of the order of the error bars of the quasi-harmonic contribution. Karato (1993) estimates the activation energy using



Fig. 4. Anelastic part of the temperature derivatives for P wave velocities (top) and S wave velocities (bottom) as a function of depth. Shown are averages and standard deviation from approximately 1000 individual calculations within given ranges. Results from Karato (1993) are shown for comparison, as well as our elastic results for a magnitude comparison.

 $E = gRT_m$. From the given references, we estimate his activation energies to lie between 750 and 1980 kJ/mol outside our range. Further measurements, the inclusion of a proper absorption band model for Q and the investigation into possible non-temperature activated processes (see Anderson, 1989) are however needed to coroborate our suggestion.

Robertson and Woodhouse (1996a) measured the ratio of relative S to P wave velocity heterogeneity in the lower mantle. Assuming a purely thermal origin for the anomalies, they made an interpretation of their

measurements (Robertson and Woodhouse, 1996b) and proposed that the Anderson-Grüneisen parameter δ_S had to be close to unity around a depth of 1900 km. Stacey (1998) calculated this parameter for all depths and found values substantially higher (similar to earlier estimates of Anderson (1989)), leading him to the conclusion that thermal anomalies alone cannot explain the facts. He proposed that seismic tomography is more sensitive to compositional effects in the lower mantle. Masters et al. (2000) recently presented evidence that the strong monochromatic increase of the ratio based on traveltime data (Robertson and Woodhouse, 1996a; Bolton and Masters, 1999) is not a general feature of the lower mantle, but rather due to some privileged sampling of some isolated spots in the lower mantle beneath Africa and the Central Pacific. The determination of the same ratio including surface waves and normal mode data shows a more modest increase (Masters et al., 2000). Fig. 5 shows the ratio of relative S to P velocity heterogeneity calculated from our temperature sensitivities together with seismic and previous mineral physics determinations. For



Fig. 5. Ratio of *S* to *P* wave velocity heterogeneity obtained in this study from temperature sensitivities (quasi-harmonic and anelastic part). For comparison, the results of Karato (1993) and Stacey (1998) and the observations of Robertson and Woodhouse (1996a) and Masters et al. (2000) are also shown.

completeness, we included the anelastic effect in our calculation, although it only increased the ratio by 0.1. The main change was an increase of the error bars. The ratio is rather flat due the fact that the sensitivities are averages from thousands of individual cases. It is of interest to note that our average value is very close to a recent first principle calculation for MgO (Karki et al., 1999). All ratios, except those from traveltime data alone fall within our error bars. This means that most velocity heterogeneity in the lower mantle can be explained by a thermal origin. Does this leave any scope for a chemical influence? Certainly, the large ratios from a depth of 2000 km due to very slow S anomalies below Africa and the Central Pacific cannot be explained by thermal effects alone. Knowing that seismic velocity anomalies are indeed sensitive to compositional changes, it is most likely that chemical heterogenities are responsible for the observed high ratios in these particular places. We, thus, subscribe to Stacey's proposal, but only in isolated spots of the lower mantle.

In this work we only investigated variations of input parameters to a given equation of state. In future work it will be interesting to understand the influence of the EOS itself on calculated sensitivities. Deviations from adiabacity of the temperature profile and full anharmoncity need to be investigated as well. Finally, it will certainly become necessary to refine the compositional variable.

7. Conclusion

We calculated sensitivities of seismic velocities in the lower mantle to temperature, pressure and composition, where composition is the volume proportion of perovskite in a perovskite–magnesiowüstite assemblage. We used the latest mineral physics data and explored a large range of input parameters leading to realistic error bars on the sensitivities.

We find temperature sensitivities comparable to previous determinations. The error bars are such that we can expect a good degree of precision on the determination of temperature variations, provided the errors on tomography stay within reason. We also calculated compositional sensitivities. As opposed to the uppermost mantle, seismic velocities are sensitive to modest changes in composition in the lower mantle. Error bars for composition are large, but *P* and *S* tomography together should be able to infer some compositional changes throughout the lower mantle with some confidence. Even, if the lower mantle is mainly thermally driven, composition will have an important effect on the magnitude of the temperature variations.

Given current sources of uncertainties, anelastic contributions (calculated using Karato's approach) to the temperature derivatives are fairly modest. Discrepancies of the ratio of relative S to P wave velocity heterogeneity between seismological observations and temperature dependent laboratory measurements seem to be localised in the lowermost mantle below Africa and the Central Pacific. Compositional effects could explain this discrepancy. In most parts of the lower mantle, however, the ratio is compatible with a thermal origin.

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