

## Mutually Consistent Estimates of Upper Mantle Composition from Seismic Velocity Contrasts at 400 km Depth

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*Abstract*—Seismologically determined properties of the 400 km discontinuity may be compared to experimentally determined properties of the associated phase transformation in order to place constraints upon upper mantle bulk composition. Disagreement among previous studies is commonly ascribed to differences in elastic equations of state (especially to assumptions about pressure and temperature derivatives) between studies. However, much of the disparity between studies is actually due to the selection of different seismic data functionals (*P*-wave velocity, *S*-wave velocity, etc.) for comparison to mineral elasticity calculations, rather than to the differences in elasticity data sets and equations of state. Within any given study, bulk sound velocity comparisons generally yield more olivine-rich compositional estimates than do *P*-wave velocity comparisons, which in turn indicate more olivine than *S*-wave velocities. Indeed, such variation in compositional estimates within a given study (arising from choice of data functional) exceeds the variation between studies (arising from elastic equation of state approximations). It can be argued that bulk sound velocities are better constrained seismologically than densities and, being independent of assumptions about shear moduli, should provide more reliable compositional estimates than *P*- or *S*-wave velocities.

Using recently measured bulk and shear moduli equations of state, mutually consistent estimates of upper mantle olivine content can be obtained from *P*-wave, *S*-wave, and bulk sound velocity contrasts at 400 km only if  $\partial \ln \mu / \partial T$  of  $\beta$  has a value of about  $-2 \times 10^{-4} \text{ K}^{-1}$ , yielding approximately 52% olivine by volume. A value of  $\partial \ln \mu / \partial T$  smaller in magnitude would require reassessment of several underlying assumptions.

**Key words:** Seismic discontinuities, phase transitions, elastic properties, equations of state, velocity contrasts.

### *Introduction*

The rapid increase in seismic velocity which has been found to occur near 400 km depth in the earth (e.g., BYERLY, 1926) is indicative of changes in the elastic properties of upper mantle materials. BERNAL (1936) proposed that such upper mantle velocity increases might be ascribed to an isochemical phase transformation of olivine to a spinel-like structure at depth. Subsequent high-pressure experimental investigations (e.g., RINGWOOD and MAJOR, 1966, 1970; AKIMOTO and FUJISAWA, 1968; KAWADA, 1977; SUIITO, 1977; YAGI *et al.*, 1979; KATSURA and ITO, 1989)

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and thermodynamic studies (e.g., AKAOGI *et al.*, 1984; NAVROTSKY and AKAOGI, 1984; BINA and WOOD, 1987; FEI *et al.*, 1991) confirmed that olivine undergoes a transformation from its usual “ $\alpha$ ” structure to a “ $\beta$ ” modified spinel structure, with an associated increase in density and seismic velocities, under conditions appropriate to approximately 400 km depth.

The 400 km seismic discontinuity can be characterized by abrupt changes in any of several seismic data functionals: density ( $\rho$ ),  $S$ -wave velocity ( $V_S$ ), bulk sound velocity ( $V_\phi$ ), or  $P$ -wave velocity ( $V_P$ ), the latter three being given by:

$$V_S \equiv (\mu/\rho)^{1/2}, \quad V_\phi \equiv (K_S/\rho)^{1/2}, \quad V_P \equiv ((K_S + \frac{4}{3}\mu)/\rho)^{1/2}, \quad (1)$$

where  $\mu$  is the shear modulus and  $K_S$  the adiabatic bulk modulus. If the 400 km seismic discontinuity is due to a phase transformation in material of uniform bulk composition, then the seismologically determined properties of the discontinuity may be compared with experimentally determined properties of phase transformations in minerals in order to place constraints upon that bulk composition.

Such comparisons have been performed in a number of studies. For example, WEIDNER (1986) suggested that upper mantle compositions containing 40–70% olivine by volume would be in agreement with seismologically determined velocity profiles. On the other hand, BINA and WOOD (1987) arrived at a range of 66–74% olivine by volume, while DUFFY and ANDERSON (1989) obtained a compositional range of 35–53% olivine by volume and suggested a preferred value of 40% olivine. Such disparate results have led to controversy (cf. ITA and STIXRUDE, 1992) over whether upper mantle compositions more closely resemble an olivine-rich peridotite, such as the “pyrolite” (RINGWOOD, 1970) model, or an olivine-poor (< 50%) “piclogite” (BASS and ANDERSON, 1984).

It is commonly assumed that such variation in compositional estimates is due largely to differences in the equations of state, especially in the values of the pressure and temperature derivatives of the elastic moduli, assumed for the high pressure phases (ANDERSON, 1988). However, it is also clear that significant variation can arise simply due to choice of seismic data functional: the BINA and WOOD (1987) estimates, for example, are based largely upon bulk sound velocities while those of DUFFY and ANDERSON (1989) are based largely upon  $S$ -wave velocities. Indeed, DUFFY and ANDERSON (1989) pointed out that  $V_P$  calculations were indicative of upper mantle compositions about 10% richer in olivine than corresponding  $V_S$  calculations, and BINA and WOOD (1987) noted that  $V_\phi$  profiles suggest an even more olivine-rich mantle than either  $V_P$  or  $V_S$  calculations.

Here we obtain upper mantle compositional estimates from all four seismic data functionals for each of three published studies incorporating widely differing elastic equations of state. We thus are able to compare the relative magnitudes of variations in compositional estimates arising solely from differences in equations of state to those due solely to choice of seismic data functional. Finally, we make use of recently published equation-of-state data to determine what conditions must

hold for all four seismic data functionals to yield mutually consistent compositional estimates.

### *Method*

The calculation of absolute velocity and density profiles requires estimates of mineral proportions and elastic properties as functions of depth throughout the transition zone (cf. ITA and STIXRUDE, 1992). Given the uncertainties associated with extrapolating the elastic properties of several mantle minerals to high pressures and temperatures (cf. WEIDNER and ITO, 1987), we simplify the problem by comparing only the relative parameter increases across the 400 km discontinuity with the relative parameter increases across the  $\alpha \rightarrow \beta$  transition in olivine at transition zone pressures and temperatures. Thus, we obtain estimates of upper mantle olivine content while afflicted with only those uncertainties attendant upon extrapolating the elastic properties of the  $\alpha$  and  $\beta$  phases of olivine to transition zone pressures and temperatures. This approach assumes that no other mineralogical transformations contribute significantly to rapid velocity increases at 400 km depth. This assumption is justified because the other major phase transition to occur in the upper mantle—the eclogite-garnetite transition, in which pyroxene dissolves into the garnet structure with increasing pressure to form a garnet-majorite solid solution—has been shown by experimental studies (e.g., AKAOGI and AKIMOTO, 1977; AKAOGI, 1978; IRIFUNE *et al.*, 1986) and thermodynamic analyses (e.g., BINA and WOOD, 1984; AKAOGI *et al.*, 1987) to occur over a very broad depth interval, thus failing to generate rapid seismic velocity increases over narrow depth ranges in the upper mantle. We shall not address further the implications of either the sharpness of the 400 km discontinuity or the topography thereon since these issues are discussed elsewhere (cf. BINA and HELFFRICH, 1993).

To facilitate comparisons between and within studies, we must adopt representative values of the changes in seismic data functionals across the 400 km discontinuity. Regional waveform modeling studies have given values of  $\Delta V_p^{400 \text{ km}}$  (from models T7 of BURDICK and HELMBERGER (1987), K8 of GIVEN and HELMBERGER (1980), GCA of WALCK (1984), CAPRI of LEVEN (1985), CJF of WALCK (1985), S25 of LEFEVRE and HELMBERGER (1989), and NWB-1 of BOWMAN and KENNETT (1990)) ranging from 3.9% to 6.0% (mean 5.0%,  $\sigma$  0.7%) and values of  $\Delta V_s^{400 \text{ km}}$  (from models SNA and TNA of GRAND and HELMBERGER (1984)) of 4.6%. As representative parameter increases, we here adopt a value for  $\Delta V_p^{400 \text{ km}}$  of 4.9%, from models GCA (Gulf of California) and S25 (Canadian Shield), and a value for  $\Delta V_s^{400 \text{ km}}$  of 4.6%, from models TNA and SNA (Tectonic and Shield North America, respectively). The velocity profiles GCA and TNA have frequently been used in this context in previous studies (e.g., BINA and WOOD, 1986, 1987; WEIDNER, 1985, 1986; WEIDNER and ITO, 1987; AKAOGI *et al.*, 1987; DUFFY and

ANDERSON, 1969). Taken together, these values give a  $\Delta V_{\phi}^{400 \text{ km}}$  value of 5.1%. None of the more recent studies having addressed the question of upper mantle density profiles, we adopt a value for  $\Delta \rho^{400 \text{ km}}$  of 3.9% from the average-earth model 1066B of GILBERT and DZIEWONSKI (1975).

As a representative sample, we consider here three published studies incorporating widely differing elastic equations of state: those of WEIDNER (1986) (model "DW"), BINA and WOOD (1987) (model "BW"), and DUFFY and ANDERSON (1989) (model "DA"). Using the respective equations of state given in each of these studies, we have computed the following seismic data functionals:

$$\begin{aligned} \Delta \rho^{\alpha \rightarrow \beta} &\equiv \frac{\rho^{\beta} - \rho^{\alpha}}{\rho^{\alpha}}, & \Delta V_S^{\alpha \rightarrow \beta} &\equiv \frac{V_S^{\beta} - V_S^{\alpha}}{V_S^{\alpha}}, \\ \Delta V_{\phi}^{\alpha \rightarrow \beta} &\equiv \frac{V_{\phi}^{\beta} - V_{\phi}^{\alpha}}{V_{\phi}^{\alpha}}, & \Delta V_P^{\alpha \rightarrow \beta} &\equiv \frac{V_P^{\beta} - V_P^{\alpha}}{V_P^{\alpha}}, \end{aligned} \quad (2)$$

for the  $\alpha$ - $\beta$  transition in pure olivine of composition  $(\text{Mg}_{0.9}\text{Fe}_{0.1})_2\text{SiO}_4$  (cf. RINGWOOD, 1975) under pressure and temperature conditions appropriate to 400 km depth. The results for each of the three models are shown in Table 1. We then divided each of these computed functionals for the phase transition, from Table 1, into the respective representative data functionals for the 400 km discontinuity, denoted by row "S" in Table 2, to obtain the respective estimate of upper mantle olivine content, shown in Table 3. For these calculations we assumed pressures of 13 GPa and temperatures of 1700 K at 400 km depth; raising the assumed temperature to 2000 K alters the values in Table 1 by less than 0.5% and those in Table 3 by less than 5%.

Table 1

*Parameter increases across the  $\alpha \rightarrow \beta$  transition at 400 km depth computed from elasticity data sets of various studies*

Model	$\Delta \rho^{\alpha \rightarrow \beta}$	$\Delta V_S^{\alpha \rightarrow \beta}$	$\Delta V_{\phi}^{\alpha \rightarrow \beta}$	$\Delta V_P^{\alpha \rightarrow \beta}$
BW	5.9%	9.3%	6.6%	7.6%
DW	6.1%	10.2%	6.9%	8.2%
DA	5.8%	12.7%	7.5%	9.7%
TS	6.7%	8.9%	9.6%	9.3%

Computed for  $(\text{Mg}_{0.9}\text{Fe}_{0.1})_2\text{SiO}_4$  at 13 GPa and 1700 K. References for BW, DW, and DA are given in the text. TS is This Study.

Table 2

*Representative seismologically determined parameter increases at 400 km depth*

Model	$\Delta \rho^{400 \text{ km}}$	$\Delta V_S^{400 \text{ km}}$	$\Delta V_{\phi}^{400 \text{ km}}$	$\Delta V_P^{400 \text{ km}}$
S	3.9%	4.6%	5.1%	4.9%

References for S are given in the text.

Table 3

*Estimates of upper mantle olivine content computed from parameter increases at 400 km depth for various models*

Model	Upper Mantle Olivine Content from:			
	$\Delta\rho$	$\Delta V_S$	$\Delta V_\phi$	$\Delta V_P$
BW	66%	49%	77%	64%
DW	64%	45%	74%	60%
DA	67%	36%	68%	51%
TS	58%	51%	53%	53%

Values are percent olivine by volume, obtained by dividing the entries of Table 2 by the corresponding entries of Table 1. References for BW, DW, and DA are given in the text. TS is This Study.

### *Results and Discussion*

If each model were internally consistent and the seismologically determined data functionals accurate for the earth, a given model would yield the same upper mantle compositional estimate regardless of which functionals were compared. In other words, all entries should be the same within any given row of Table 3, differences between rows being due to the differing elastic equations of state of the various models. Clearly, none of these models yields consistent compositional estimates. The variation in compositional estimates within any given model ( $\sigma_{\text{rms}}$  about 13% olivine), due to choice of data functional, exceeds the variation between different models ( $\sigma_{\text{rms}}$  about 5% olivine), due to differences in equations of state. For example, DUFFY and ANDERSON (1989) used the parameter  $\Delta V_S$  to estimate an upper mantle olivine content of about 40% (computed as 36% in Table 3), noting that use of the parameter  $\Delta V_P$  caused this estimate to rise to about 50% (51% in Table 3). Had they also examined the parameters  $\Delta\rho$  or  $\Delta V_\phi$ , they would have obtained even greater estimates of 65–70% olivine (67% and 68%, respectively, in Table 3). Thus, within a given study we obtain significantly different estimates of upper mantle olivine content from each of the four seismic data functionals we have considered, suggesting possible problems with the assumed equations of state in each of these studies.

Uncertainties in computed functionals across the phase transition arise primarily from the extrapolation of mineral bulk and shear moduli to the high pressures and temperatures of the upper mantle. Since density and bulk sound velocity depend only upon the bulk modulus while  $P$ - and  $S$ -wave velocities are dependent upon the bulk and shear moduli, and since seismologically inferred bulk moduli should be less sensitive to attenuative dispersion and lateral heterogeneity than shear moduli, it can be argued (cf. BINA and SILVER, 1990) that the bulk sound velocity should provide the best constrained compositional estimate amongst the functionals.

Similarly, since seismic velocities are additionally constrained by body-wave travel time data while density profiles utilize only free oscillation data and are globally averaged, the density contrast should yield a relatively poorly constrained compositional estimate.

Thus, we may proceed by using recently measured bulk moduli equations of state to obtain a compositional estimate from the bulk sound velocity contrast. We may then use recently measured shear moduli equations of state to determine the value of the unmeasured  $\partial\mu/\partial T$  for the  $\beta$  phase necessary for the  $P$ - and  $S$ -wave velocity contrasts to yield mutually consistent estimates of upper mantle olivine content. For  $(\text{Mg}_{0.9}\text{Fe}_{0.1})_2\text{SiO}_4$  olivine in the  $\alpha$  phase, we adopt  $K$  (129 GPa),  $\partial K/\partial P$  (4.56),  $\mu$  (77.6 GPa), and  $\partial\mu/\partial P$  (1.71) from the measurements of ZAUG *et al.* (1993) to 12.5 GPa, and  $\partial K/\partial T$  ( $-0.0157$  GPa/K) and  $\partial\mu/\partial T$  ( $-0.0135$  GPa/K) from the measurements of ISAAC *et al.* (1989) to 1700 K. For the  $\beta$  phase, we adopt  $K$  (174 GPa),  $\partial K/\partial P$  (4.0), and  $\partial K/\partial T$  ( $-0.027$  GPa/K) from the measurements of FEI *et al.* (1992) to 26 GPa and 900 K;  $\mu$  (1.10 GPa) from the measurements of SAWAMOTO *et al.* (1984) and WEIDNER *et al.* (1984), and  $\partial\mu/\partial P$  (1.7) from the measurements of GWANMESIA *et al.* (1990) to 3 GPa. We apply Eulerian finite strain equations of state (cf. BINA and HELFFRICH, 1992), using the Suzuki-type thermal expansion formulation of FEI *et al.* (1991). We find that, in order for the three seismic velocity contrasts to yield mutually consistent compositional estimates at 400 km depth (13 GPa and 1700 K), we require a value of  $-0.022$  GPa/K for  $\partial\mu/\partial T$  for phase  $\beta$ , a value which falls between that of MgO ( $-0.024$  to  $-0.026$  GPa/K) and that of phase  $\alpha$  ( $-0.014$  GPa/K) and which is near that of  $\text{Al}_2\text{O}_3$  ( $-0.021$  to  $-0.024$  GPa/K) (ANDERSON *et al.*, 1992). These results are shown in row "TS" in Tables 1 and 3. Thus, we obtain mutually consistent compositional estimates of approximately 52% olivine by volume if  $\partial \ln \mu/\partial T$  of  $\beta$  has a value of about  $-2.0 \times 10^{-4} \text{ K}^{-1}$ , a value nearer that of rocksalt oxides ( $-2.2 \times 10^{-4} \text{ K}^{-1}$ ) than that of average silicates ( $-1.4 \times 10^{-4} \text{ K}^{-1}$ ) according to the systematics of ANDERSON (1988).

### Conclusions

In conclusion, the seismologically determined properties of the 400 km discontinuity may be compared to experimentally determined properties of the associated phase transformation in order to place constraints upon upper mantle bulk composition. Disagreement among the conclusions of previous studies is commonly assumed to arise largely from differences in the assumed equations of state. However, much of the disparity can in fact be ascribed to which seismic data functionals are chosen for comparison with mineral elasticity calculations. Indeed, the variation in compositional estimates within any given model due to choice of data functional exceeds the variation between different models due to differences in

equations of state. The three studies examined herein do not yield mutually consistent compositional estimates for all three seismic velocity functionals: bulk sound velocity calculations at 400 km indicate a more olivine-rich upper mantle than do  $P$ -wave velocity calculations, which in turn indicate a greater olivine content than do  $S$ -wave velocity calculations, indicating possible problems with the assumed equations of state in each of these studies. It can be argued that bulk sound velocities are better constrained seismologically than densities and, being independent of assumptions about shear moduli, should provide more reliable compositional estimates than  $P$ - or  $S$ -wave velocities.

Using recently measured bulk and shear moduli equations of state, mutually consistent estimates of upper mantle olivine content can be obtained from  $P$ -wave,  $S$ -wave, and bulk sound velocity contrasts at 400 km only if  $\partial \ln \mu / \partial T$  of  $\beta$  has a value of about  $-2 \times 10^{-4} \text{ K}^{-1}$ . Such a value yields mutually consistent compositional estimates of about 52% olivine by volume. Hence, measurement of such a value would indicate that the magnitude of the 400 km seismic discontinuity is consistent with the isochemical occurrence of the  $\alpha$ - $\beta$  phase transformation in an upper mantle of an olivine-rich peridotite composition such as pyrolite.

If  $\partial \mu / \partial T$  for the  $\beta$  phase is shown experimentally not to have as large a value as predicted herein, how might it still be possible to obtain mutually consistent compositional estimates? One possibility would be that the magnitude of the velocity contrast at 400 km is not well characterized seismologically, so that the numbers in Table 2 are not representative. (Variation of the numbers in Table 2 by  $\pm 0.5\%$  results in a corresponding variation of  $\pm 5\%$  in Table 3.) A second possibility would be that another phase transition progresses significantly over the narrow depth interval of the 400 km discontinuity, undermining our assumption that the entire observed velocity contrast is due to the  $\alpha \rightarrow \beta$  transition. Finally, a third possibility would be to invoke discontinuities in the bulk chemical composition of the mantle (e.g., BULLEN, 1937; ANDERSON and BASS, 1986).

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