

CONSTRAINTS ON LOWER MANTLE COMPOSITION AND TEMPERATURE
 FROM DENSITY AND BULK SOUND VELOCITY PROFILES

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Abstract. Recent studies comparing density (ρ) from the seismological model PREM to that predicted for various perovskite and magnesiowüstite phase assemblages under lower mantle conditions suggest that the lower mantle is a few percent denser than reasonable candidates for upper mantle composition such as pyrolite. This has been interpreted as evidence for an iron-enriched lower mantle. In addition to density, bulk sound velocity ($\sqrt{\Phi}$) provides an important constraint upon proposed lower mantle compositions. Being independent of the shear modulus, $\sqrt{\Phi}$ has several desirable characteristics. Experimentally, it can be determined in the laboratory by density measurements under static compression; seismologically, it is not affected by attenuative dispersion and is expected to be much less laterally heterogeneous than P- or S-wave velocities. We have calculated ρ and $\sqrt{\Phi}$ along lower mantle adiabats, as functions of iron-magnesium content (X_{Mg}) and silica content (X_{Si}), and compared them to values obtained from PREM. For a reasonable temperature estimate at the top of the lower mantle (T_{lm}) of 2000 K, we find that the ρ data are most compatible with a lower mantle enriched in Fe, in agreement with previous studies. In addition, the $\sqrt{\Phi}$ data require that silica enrichment accompany this Fe enrichment. Furthermore, increasing T_{lm} increases both the required Fe and Si content. With a high assumed T_{lm} (>2700 K), the ρ data can be satisfied by low X_{Mg} values, but even a pure perovskite lower mantle is too slow compared to $\sqrt{\Phi}$. Thus, assuming no free SiO₂ in the lower mantle, this provides an upper bound on T_{lm} of approximately 2700 K. Finally, conclusions regarding the composition and temperature of the lower mantle are strongly dependent upon uncertainties in estimated thermoelastic parameters and upon choice of a seismological model. Most importantly, neither Fe nor Si enrichment is required if the zero-pressure volume coefficient of thermal expansion of perovskite is about $2.5 \times 10^{-5} \text{K}^{-1}$, rather than $4.0 \times 10^{-5} \text{K}^{-1}$, at high temperatures. Alternatively, but less probably, Fe and Si enrichment are not required if the average ρ of the lower mantle is 1.0% less than given by PREM. The Si enrichment is not required if the average $\sqrt{\Phi}$ of the lower mantle is 0.5% slower than PREM, closer to the value given by the body-wave model derived from the Jeffreys-Bullen tables, or if the lower mantle is anomalously cold, with $T_{lm} \approx 1700$ K.

Introduction

Constraints on lower mantle bulk composition and temperature have a major bearing upon investigations into the bulk composition and internal dynamics of the Earth, the chemical stratification of the mantle, and the presence of thermal boundary layers in the mantle [Silver et al., 1985, 1988]. It has been known for some time that such constraints may be obtained by comparing seismic profiles with the measured elastic properties of candidate mantle compositions [Birch, 1952]. Important advances during the last fifteen years — the construction of density profiles of the Earth from free-oscillation data [Jordan and Anderson, 1974; Gilbert and Dziewonski, 1975], the discovery of silicate perovskite [Liu, 1974; Liu and Ringwood, 1975; Mao et al., 1977], and the recognition that silicate perovskite is probably the most abundant mineral in the lower mantle [Knittle and Jeanloz, 1987] — have greatly improved the precision attainable through such comparisons. Recent comparisons

have focused on the density (ρ) profile of the lower mantle, because it is the simplest elastic property to measure in the laboratory. For example, Knittle et al. [1986] and Jeanloz and Knittle [1989] calculated the densities of various perovskite and magnesiowüstite phase assemblages under lower mantle conditions. Comparison of their calculated density profiles to the lower mantle profile from Dziewonski and Anderson's [1981] seismological model PREM suggested that the lower mantle is a few percent denser than reasonable candidates for upper mantle composition, such as pyrolite [Ringwood, 1975]. This difference has been interpreted as evidence for an iron-enriched lower mantle.

An important additional constraint upon lower mantle composition is provided by the bulk sound velocity ($\sqrt{\Phi}$), where Φ equals K_S/ρ or, equivalently, $V_P^2 - \frac{4}{3}V_S^2$. (Here K_S is the adiabatic bulk modulus, V_P P-wave velocity, and V_S S-wave velocity.) Earlier studies used both ρ and $\sqrt{\Phi}$ to argue for lower mantle compositions enriched in iron [Anderson and Jordan, 1970], silica [Burdick and Anderson, 1975], or both [Anderson, 1970] relative to the upper mantle, under the assumption that the lower mantle consisted of mixed oxides. Davies [1974] used these two elastic parameters to evaluate the tradeoff between composition and assumed mantle temperatures. More recently, Jackson [1983] has explored tradeoffs between composition, temperature, and thermal expansion by interpretation of ρ and K_S parameters obtained by adiabatic decompression of the seismological model PEM [Dziewonski et al., 1975]. In view of the advances discussed above and other recent seismological and thermoelastic studies, a reexamination of $\sqrt{\Phi}$, which has traditionally been central to seismology/mineral physics comparisons, is warranted — with particular emphasis upon the uncertainties in seismological data and thermal equations of state.

Its independence of the shear modulus makes $\sqrt{\Phi}$ an especially useful parameter in making such comparisons. Values of $\sqrt{\Phi}$ at high pressures can be obtained in the laboratory by the differentiation of third-order Eulerian finite strain isothermal compression curves:

$$\Phi \equiv \frac{K_S}{\rho} = \left(\frac{\partial P}{\partial \rho} \right)_S = \left(\frac{\partial P}{\partial \rho} \right)_T \cdot (1 + T\alpha\gamma), \quad (1)$$

where P is pressure, S entropy, T temperature, α the volume coefficient of thermal expansion, and γ the Grüneisen parameter. These Φ values may be corrected to high temperatures:

$$\frac{\Phi(T)}{\Phi(T_0)} = \exp \left[\int_{T_0}^T \alpha(1 - \delta_S) dT' \right] \approx [1 + \bar{\alpha}(1 - \delta_S)\Delta T], \quad (2)$$

where δ_S is the adiabatic Anderson-Grüneisen parameter (assumed to be independent of temperature), ΔT the difference $T - T_0$, and $\bar{\alpha}$ the mean value of α from T_0 to T (obtained from its zero-pressure value $\bar{\alpha}_0$ by integration of $-\delta_T/K_T$). Thus $\sqrt{\Phi}$, while more difficult to measure than ρ , is simpler to determine than V_P and V_S at high pressures, the latter two being dependent upon the shear modulus.

At the same time, $\sqrt{\Phi}$ should be better constrained seismologically than ρ , as it can be determined from both free-oscillation and body-wave travel time data. In addition, as nearly all dissipation in the mantle occurs in the shear modulus [Dziewonski and Anderson, 1981], $\sqrt{\Phi}$ will not experience attenuative dispersion in the seismic band, allowing for the direct comparison of free-oscillation and body-wave data sets. Furthermore, laboratory measurements — typically made at frequencies well outside the seismic band — may be compared to seismic observations with greater confidence.

Another important feature of $\sqrt{\Phi}$ is its insensitivity to lateral heterogeneity. For nearly all manifestations of lateral heterogeneity

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that have been observed in the mantle — lateral variations in the continental upper mantle [Wickens and Buchbinder, 1980], variations associated with subducted slabs [Jordan, 1977; Creager and Jordan, 1984], localized lower mantle anomalies [Lay, 1983], and large scale velocity variations in the mantle [Woodhouse and Dziewonski, 1987] — the ratio $d \ln V_S / d \ln V_P$ has been found to be about 2 in value. This implies that lateral heterogeneity in $\sqrt{\Phi}$ is an order of magnitude less than that in V_S for a Poisson's ratio of 0.25. Thus, the use of $\sqrt{\Phi}$ reduces the possible bias arising from inadequate sampling of various regions of the Earth.

In this study, we investigate the structure of the problem of constraining lower mantle composition by calculating ρ and $\sqrt{\Phi}$ profiles along lower mantle adiabats and comparing them to the model PREM. By contouring, as functions of iron-magnesium and silica content, the misfit between our calculated mantle properties and those obtained from PREM, we place constraints upon acceptable lower mantle compositions and temperatures. We also analyze the sensitivity of these constraints to choice of reference seismological model and to uncertainties in the mineral thermoelastic parameters.

Method and Results

The thermoelastic parameters used in this study are given in Table 1 along with their references. The coefficient of Fe-Mg partitioning between perovskite and magnesiowüstite was taken from Bell et al. [1979] and Ito and Yamada [1982]: $K_{FeMg}^{FeMg} = 0.10$, independent of pressure and temperature. We assumed an adiabatic temperature gradient in the lower mantle of 9.3 K/GPa [Akaogi et al., 1989].

We simplified the problem by characterizing candidate lower mantle compositions according to two variables, X_{Mg} and X_{Pv} , given by the molar ratios $Mg/(Mg+Fe)$ and $Si/(Mg+Fe)$, respectively. (This parameterization neglects other cations — such as calcium, whose effects should be small [Mao et al., 1989], and aluminum, whose effects are unknown.) For each composition, given by (X_{Mg}, X_{Pv}) , we calculated ρ for the corresponding phase assemblage as a function of depth along a lower mantle adiabat, assuming a temperature at the top of the lower mantle (T_{lm}) of 2000 K, a value suggested by experimental results on the temperatures of upper mantle phase transitions [Akaogi et al., 1989; Ito and Takahashi, 1989; Jeanloz and Knittle, 1989]. For each such composition, we then computed the root-mean-square percent (RMS %) misfit over the lower mantle between our calculated ρ profile and that of PREM. For each composition we also calculated Voigt-Reuss-Hill-averaged [Watt et al., 1976] $\sqrt{\Phi}$ along the adiabat and computed the RMS % misfit between our calculated profile and PREM. These misfit functions are contoured in the two-parameter compositional space in Figure 1. While the ρ and $\sqrt{\Phi}$ misfit functions may be combined in an RMS fashion to give a single net RMS % misfit, we have left them uncombined in Figure 1 so as to better illustrate their individual compositional dependences.

It is apparent from the major axes of the contours in Figure 1 that ρ is primarily sensitive to iron content, through the molar mass and molar volume; $\sqrt{\Phi}$, on the other hand, is sensitive to both silica content, through the bulk modulus, and to iron content, through its

Table 1. Thermoelastic parameters used in this study

Parameter	MgSiO ₃	FeSiO ₃	MgO	FeO
Phase	pv	pv	mw	mw
V_0 (cm ³)	24.46 ^a	25.49 ^a	11.25 ^a	12.25 ^a
K_{S0} (GPa)	269. ^b	269. ^b	162.7 ^a	179.7 ^a
K_{S0}'	4.0 ^b	4.0 ^b	4.1 ^a	3.6 ^a
δ_S	2.7 ^d	2.7 ^d	3.0 ^c	3.0 ^c
$\bar{\alpha}_0$ (10 ⁻⁵ K ⁻¹)	4.0 ^c	4.0 ^c	4.0 ^a	4.8 ^a

Phases are perovskite (pv) and magnesiowüstite (mw); V_0 , K_{S0} , K_{S0}' are at 300 K and zero pressure; δ_S is independent of pressure and temperature; $\bar{\alpha}_0$ is mean zero-pressure value between 300 and 1300 K. ^aJeanloz and Thompson [1983]. ^bKnittle and Jeanloz [1987]. ^cKnittle et al. [1986]. ^dBukowinski and Wolf [1989]. ^eSumino and Anderson [1984]; Jeanloz and Thompson [1983].

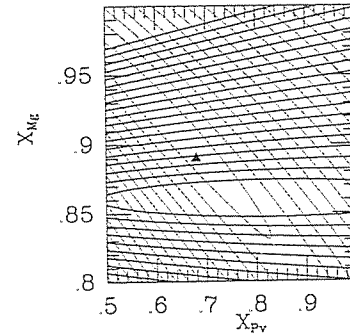


Fig. 1. Individual lower mantle RMS % misfit contours between the seismological model PREM and the ρ (solid) and $\sqrt{\Phi}$ (dotted) profiles calculated for varying X_{Mg} and X_{Si} along a 2000 K adiabat. Contours suggest Fe and Si enrichment relative to the petrological model pyrolite (triangle). Contour interval is 0.2%; innermost contours are 0.4%.

dependence on density. The regions of intersection of the contours define lower mantle compositions which satisfy the ρ and $\sqrt{\Phi}$ data simultaneously. In agreement with the recent studies of Knittle et al. [1986] and Jeanloz and Knittle [1989], we find that the ρ data are most compatible with a lower mantle enriched in Fe ($X_{Mg} \approx 0.86$) relative to pyrolite ($X_{Mg} \approx 0.89$). However, we also find that the $\sqrt{\Phi}$ data require that silica enrichment accompany such iron enrichment, leading to a lower mantle which is richer in silicate perovskite ($X_{Pv} \approx 0.77$) than would be a pyrolite lower mantle ($X_{Pv} \approx 0.68$). Furthermore, as demonstrated in Figure 2, as the assumed value of T_{lm} is increased, both the iron and silica contents must be increased as well, in agreement with the previous study of Jackson [1983]. (The presence of a mildly superadiabatic gradient in the lower mantle, suggested by some lines of evidence [Silver et al., 1988], would have essentially the same effect as raising T_{lm} by about 200 K.) A T_{lm} of 2700 K, consistent with the possible existence of a thermal boundary layer at the top of the lower mantle [Jeanloz and Morris, 1986], is compatible with the ρ data for low X_{Mg} (< 0.83). However, even a pure perovskite lower mantle ($X_{Pv} = 1$) is too slow compared to the $\sqrt{\Phi}$ data. Thus, assuming no free SiO₂, a pure perovskite lower mantle provides an upper bound on T_{lm} of approximately 2700 K.

Discussion and Conclusions

Thus, direct comparison of the thermoelastic data of Table 1 with the seismological model PREM indicates that the lower mantle is richer in both iron and silica than upper mantle pyrolite compositions. The expected uncertainty in average lower mantle density is less than 0.5% [Silver et al., 1988], and there is little variation in

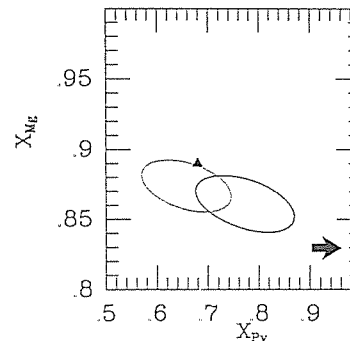


Fig. 2. Effect of temperature: net lower mantle RMS % misfit contours between PREM and the ρ and $\sqrt{\Phi}$ profiles calculated for varying X_{Mg} and X_{Si} along 1700 K (dotted), 2000 K (solid), and 2700 K (dashed, arrow off-scale) adiabats. Triangle denotes pyrolite. For clarity, only 0.5% contours are shown.

lower mantle density profiles among various published seismological models (less than 0.2% between various models based upon free oscillations). However, there are significant discrepancies among bulk sound velocity profiles. In Figure 3, we have calculated RMS % misfit contours for comparisons of the thermoelastic data with the seismological models PREM, 1066B [Gilbert and Dziewonski, 1975], JB [Jeffreys and Bullen, 1940], and IASPR (B. Kennett, personal communication, 1989). The model PREM was constructed using free-oscillation data and both absolute and relative body-wave travel times; its implications for lower mantle composition have been discussed above. Model 1066B was constructed using free-oscillation data alone; it averages 0.1% slower and 0.1% less dense than PREM through the lower mantle and implies compositions slightly less Fe-enriched than does PREM. Model JB was constructed using absolute body-wave travel times alone; it averages 0.5% slower than PREM and implies compositions substantially less Si-enriched than does PREM, requiring no silica enrichment relative to pyrolite. (Incorporating the Bullen-A-i density profile [Bullen, 1965, pp. 231-235], model JB averages 1.4% denser than PREM and thus implies substantially more Fe-rich compositions; however, such high density values are not in accord with subsequent studies incorporating free oscillation data.) Model IASPR was constructed to fit global absolute body-wave travel times; it averages 0.1% slower and 0.2% less dense than PREM and implies compositions slightly less Fe- and Si-rich. Thus, conclusions regarding lower mantle composition, especially with respect to silica content, are significantly dependent upon which seismological model is used for comparison.

These velocity discrepancies are significant, resulting in travel time variations of a second or more. They cannot be ascribed to attenuative dispersion and are probably not due to lateral heterogeneity, as discussed in the introduction; thus, they must represent other sources of uncertainty, such as tradeoffs with upper mantle structure. Tighter constraints on lower mantle bulk sound velocity can be obtained by reexamination of the free oscillation data, by inversion for V_p and V_s models for the same region, or by direct measurement of acoustic travel times T_o that depend only on $\sqrt{\Phi}$ (P. Silver and C. Bina, in preparation, 1990).

In addition to the uncertainty in lower mantle velocities, there are considerable uncertainties associated with the experimentally determined thermoelastic parameters in Table 1. For example, the K_{S0} value for perovskite in Table 1 [Knittle and Jeanloz, 1987] is close to the value of 273 GPa obtained by Mao and Hemley (personal communication, 1989), but other studies [Kudoh et al., 1987; Yeganeh-Haeri et al., 1989] have yielded significantly lower values of about 245 GPa. Adopting such a lower value of K_S for perovskite yields nearly identical results provided that K_{S0}' is increased to about 4.5 in value.

Furthermore, the value of $\bar{\alpha}_0$ for perovskite in Table 1 [Knittle et al., 1986] is a matter of active inquiry. While this value is in good agreement with that measured by Mao and Hemley (personal communication, 1989) and falls within the range of 2.7 to $4.4 \times 10^{-5} \text{K}^{-1}$ predicted by Hemley et al. [1989] from lattice dynam-

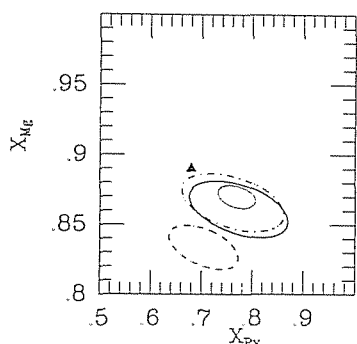


Fig. 3. Effect of choice of seismological model: net lower mantle RMS % misfit contours between seismological models PREM (solid), 1066B (dotted), JB (dashed), and IASPR (dot-dashed) and the ρ and $\sqrt{\Phi}$ profiles calculated for varying X_{Mg} and X_{Si} along a 2000 K adiabat. Triangle denotes pyrolite. (JB $\sqrt{\Phi}$ is matched with Bullen-A-i ρ .) Only 0.5% contours are shown (1.0% for JB).

ics, such thermal expansivity measurements involve heating metastable perovskite samples under atmospheric pressure, and it is possible that some degree of retrograde transformation may occur upon heating leading to possible overestimation of α at high temperatures. Severe twinning of single-crystal perovskite upon heating was noted by Ross and Hazen [1989]. The possibility that $\bar{\alpha}_0$ for perovskite may be lower than $4.0 \times 10^{-5} \text{K}^{-1}$ has been suggested by Hill and Jackson [1990] based upon the poor fit of the Knittle et al. [1986] data to a Mie-Grüneisen formulation; they suggest a range of 2.0 to $4.0 \times 10^{-5} \text{K}^{-1}$ based upon high-temperature studies of analogue ScAlO_3 perovskite. The effect of adopting a lower value of $\bar{\alpha}_0$ for perovskite of $2.5 \times 10^{-5} \text{K}^{-1}$ is shown in Figure 4; Fe-enrichment relative to pyrolite is no longer required in order to match the ρ data, and a slight Si-depletion relative to pyrolite is indicated by the $\sqrt{\Phi}$ data.

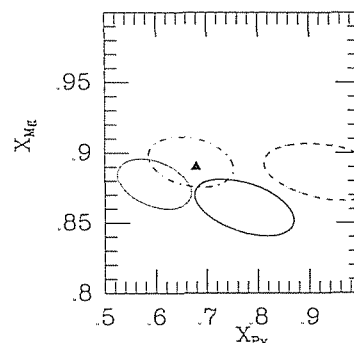


Fig. 4. Effect of varying thermoelastic parameters: net lower mantle RMS % misfit contours between PREM and the ρ and $\sqrt{\Phi}$ profiles calculated for varying X_{Mg} and X_{Si} along a 2000 K adiabat. Triangle denotes pyrolite. Thermoelastic parameters used are those of Table 1 (solid), low perovskite $\bar{\alpha}_0$ (dotted), high perovskite δ_S (dashed), and low $\bar{\alpha}_0$ with high δ_S (dot-dashed). Only 0.5% contours are shown.

Finally, no experimental measurements of the Anderson-Grüneisen parameter δ_S (which represents the P -dependence of α or, equivalently, the T -dependence of K_S) are yet available for perovskite, the δ_S value in Table 1 having been obtained from the thermodynamic estimates of Bukowinski and Wolf [1990]. Anderson [1988] suggested, on the basis of systematics of analogue compounds, that δ_S for silicate perovskite should be closer to 4.0 in value. Chopelas and Boehler [1989] have suggested an even larger value of 5.5, based upon expansivity-volume systematics. The effect of adopting a higher value of δ_S for perovskite of 4.0 is also shown in Figure 4; Fe-enrichment relative to pyrolite is no longer required in order to match the ρ data, but an even greater Si-enrichment relative to pyrolite is indicated by the $\sqrt{\Phi}$ data. The effect of adopting both a lower $\bar{\alpha}_0$ and a higher δ_S is also depicted in Figure 4; in this case neither Fe- nor Si-enrichment is required by the seismological data.

In conclusion, the experimental and seismological data taken at face value argue for a lower mantle enriched in both iron and silica and a temperature at the top of the lower mantle of less than 2700 K. However, there are combinations of parameters, within present uncertainties, that allow for a homogeneous mantle: in particular, a lower perovskite $\bar{\alpha}_0$ of about $2.5 \times 10^{-5} \text{K}^{-1}$ (perhaps in combination with a higher δ_S value) or, less probably, a mantle density that is 1.0% less than that given by PREM. Reducing T_{lm} from 2000 to 1700 K removes the requirement for Si enrichment and reduces that for Fe enrichment. Variations in other parameters alone — K_S , δ_S , or the seismologically determined $\sqrt{\Phi}$ — can remove the enrichment in either Fe or Si, but not both. Work in progress, involving the consistency of various compositional models with the observed radial derivative of $\sqrt{\Phi}$, may place further constraints upon this problem.

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