Abstract. Recent studies comparing density ($\rho$) 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 ($\sqrt{\mu}$) provides an important constraint upon proposed lower mantle compositions. Being independent of the shear modulus, $\sqrt{\mu}$ 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 $\rho$ or $S$-wave velocities. We have calculated $\rho$ and $\sqrt{\mu}$ 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 ($T_{3m}$) of 2000 K, we find that the $\rho$ data are most compatible with a lower mantle enriched in Fe, in agreement with previous studies. In addition, the $\sqrt{\mu}$ data require that silica enrichment accompany this Fe enrichment. Furthermore, increasing $T_{3m}$ increases both the required Fe and Si content. With a high assumed $T_{3m}$ (>2700 K), the $\rho$ data can be satisfied by low $X_{Mg}$ values, but even a pure perovskite lower mantle is too slow compared to $\sqrt{\mu}$. Thus, assuming no free SiO$_2$ in the lower mantle, this provides an upper bound on $T_{3m}$ 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}$K$^{-1}$, rather than 4.0$\times$10$^{-5}$K$^{-1}$, at high temperatures. Alternatively, but less probably, Fe and Si enrichment are not required if the average $\rho$ of the lower mantle is 1.0% less than given by PREM. The Si enrichment is not required if the average $\sqrt{\mu}$ 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 $T_{3m}$ $\approx$ 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; Maé 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 ($\rho$) 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 [1988] 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 [1985] 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 ($\sqrt{\mu}$), where $\sqrt{\mu}$ is its insensitivity to lateral heterogeneity. It is the simplest elastic property to measure in the laboratory. For a reasonable temperature estimate at the top of the lower mantle ($T_{3m}$) of 2000 K, we find that the $\sqrt{\mu}$ data are most compatible with a lower mantle enriched in Fe, in agreement with previous studies. In addition, the $\sqrt{\mu}$ data require that silica enrichment accompany this Fe enrichment. Furthermore, increasing $T_{3m}$ increases both the required Fe and Si content. With a high assumed $T_{3m}$ (>2700 K), the $\sqrt{\mu}$ data can be satisfied by low $X_{Mg}$ values, but even a pure perovskite lower mantle is too slow compared to $\sqrt{\mu}$. Thus, assuming no free SiO$_2$ in the lower mantle, this provides an upper bound on $T_{3m}$ 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}$K$^{-1}$, rather than 4.0$\times$10$^{-5}$K$^{-1}$, at high temperatures. Alternatively, but less probably, Fe and Si enrichment are not required if the average $\rho$ of the lower mantle is 1.0% less than given by PREM. The Si enrichment is not required if the average $\sqrt{\mu}$ 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 $T_{3m}$ $\approx$ 1700 K.

Conclusions

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; Maé 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 ($\rho$) 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 [1988] 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 [1985] 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.

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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 $2$. This implies that lateral heterogeneity in $\sqrt{\Phi}$ is an order of magnitude less than that in $V_p$ 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 $\rho$ 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]: $K_{Fe}^{per} = 0.10$, independent of pressure and temperature. We assumed an adiabatic temperature gradient in the lower mantle of 9.3 K/GPa [Akaogi et al., 1988].

We simplified the problem by characterizing candidate lower mantle compositions according to two variables, $X_{Mg}$ and $X_{Fe}$, 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 $(X_{Mg}, X_{Fe})$, we computed $\rho$ for the corresponding phase assemblage as a function of pressure 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 $\rho$ 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 $\sqrt{\Phi}$ and PREM. These misfit functions are contoured in the two-parameter compositional space in Figure 1. While the $\rho$ 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 $\rho$ 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 dependence on density. The regions of intersection of the contours define lower mantle compositions which satisfy the $\rho$ and $\sqrt{\Phi}$ data simultaneously. In agreement with the recent studies of Knittle et al. [1986] and Jeanloz and Knittle [1988], we find that the $\rho$ data are most compatible with a lower mantle enriched in Fe ($X_{Fe} = 0.86$) relative to pyrolite ($X_{Fe} = 0.77$). 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 ($X_{Mg} = 0.77$) than would be a pyrolite lower mantle ($X_{Mg} = 0.68$). 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].

**Table 1. Thermoelastic parameters used in this study**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>MgSiO₃</th>
<th>FeSiO₃</th>
<th>MgO</th>
<th>FeO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase</td>
<td>pv</td>
<td>pv</td>
<td>mw</td>
<td>mw</td>
</tr>
<tr>
<td>$V_p$ (km/s)</td>
<td>24.4³</td>
<td>25.4⁴</td>
<td>11.2⁵</td>
<td>12.2⁵</td>
</tr>
<tr>
<td>$K_{30}$ (GPa)</td>
<td>269⁴</td>
<td>269⁴</td>
<td>102.7⁴</td>
<td>179.7⁴</td>
</tr>
<tr>
<td>$K_{\phi}$</td>
<td>4.0⁴</td>
<td>4.0⁴</td>
<td>4.1⁴</td>
<td>3.6⁴</td>
</tr>
<tr>
<td>$\rho$</td>
<td>2.7⁴</td>
<td>2.7⁴</td>
<td>3.0⁴</td>
<td>3.0⁴</td>
</tr>
<tr>
<td>$\rho_0$ (10²⁴cm⁻¹)</td>
<td>4.0⁴</td>
<td>4.0⁴</td>
<td>4.0⁴</td>
<td>4.8⁴</td>
</tr>
</tbody>
</table>

Phases are perovskite (pv) and magnesiowüstite (mw); $V_p$, $K_{30}$, $K_{\phi}$ are at 300 K and zero pressure; $\rho$ is independent of pressure and temperature; $\rho_0$ is mean zero-pressure value between 300 and 1300 K. ³Jeanloz and Thompson [1983]. ⁴Knittle and Jeanloz [1987]. ⁵Knittle et al. [1986]. ⁶Bukowski and Wolf [1989]. ⁷Sumino and Anderson [1984]; Jeanloz and Thompson [1989].

**Fig. 1. Individual lower mantle RMS % misfit contours between the seismological model PREM and the $\rho$ (solid) and $\sqrt{\Phi}$ (dotted) profiles calculated for varying $X_{Mg}$ and $X_{Fe}$ 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%.

**Fig. 2. Effect of temperature: net lower mantle RMS % misfit contours between PREM and the $\rho$ and $\sqrt{\Phi}$ profiles calculated for varying $X_{Mg}$ and $X_{Fe}$ 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 thermelastic data with the seismological models PREM [Gilbert and Dziewonski, 1975], JB [Jeffreys and Bullen, 1940], and LASPR (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 1068B 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, 1985, 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 LASPR was constructed to fit global absolute body-wave travel times; it averages 0.1% slower and 0.4% 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 $T_p$ that depend only on $\sqrt[3]{\gamma}$ (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 thermelastic parameters in Table 1. For example, the $K_{S2}$ value for perovskite in Table 1 [Knuttlee 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 $K_{S2}$ for perovskite yields nearly identical results provided that $K_{S2}^p$ is increased to about 4.5 in value.

Furthermore, the value of $\delta_2$ for perovskite in Table 1 [Knuttlee 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 4.4x10^{-10} K^{-1} predicted by Hemley et al. [1989] from lattice dynamical measurements, such thermal expansivity measurements involve heating meta-stable perovskite samples under atmospheric pressure, and it is possible that some degree of retrograde transformation may occur upon heating leading to possible overestimation of $\delta_2$ at high temperature. Severe twinning of single-crystal perovskite upon heating was noted by Ross and Hazen [1980]. The possibility that $\delta_2$ for perovskite may be lower than 4.0x10^{-10} K^{-1} has been suggested by Hall and Jackson [1990] based upon the poor fit of the Knittle et al. [1989] data to a Mie-Gruneisen formulation; they suggest a range of 2.0 to 4.0x10^{-10} K^{-1} based upon high-temperature studies of analogues ScAlO$_3$ perovskite. The effect of adopting a lower value of $\delta_2$ for perovskite of 2.5x10^{-10} K^{-1} is shown in Figure 4; Fe-enrichment relative to pyrolite is no longer required in order to match the $\rho$ data, and a slight Si-depletion relative to pyrolite is indicated by the $\sqrt[3]{\gamma}$ data.

![Fig. 4. Effect of varying thermelastic parameters: net lower mantle RMS % misfit contours between PREM and the $\sqrt[3]{\gamma}$ profiles calculated for varying $X_{Me}$ and $X_{Mg}$ along a 2000 K adiabat. Triangle denotes pyrolite. Thermelastic parameters used are those of Table 1 (solid), low perovskite $\delta_2$ (dotted), high perovskite $\delta_2$ (dashed), and low $\delta_0$ with high $\delta_2$ (dot-dashed). Only 0.5% contours are shown.](image)

Finally, no experimental measurements of the Anderson-Gruneisen parameter $\delta_2$ (which represents the $P$-dependence of $\alpha$ or, equivalently, the $T$-dependence of $K_{S2}$) are yet available for perovskite, the $\delta_2$ value in Table 1 having been obtained from the thermodynamic estimates of Bukowinski and Wolfe [1990]. Anderson [1988] suggested, on the basis of systematics of analogue compounds, that $\delta_2$ for silicate perovskite should be closer to 4.0 in value. Chopelas and Boehler [1988] have suggested an even larger value of 5.5, based upon expansivity-volume systematics. The effect of adopting a higher value of $\delta_2$ 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 $\rho$ data, but an even greater Si-enrichment relative to pyrolite is indicated by the $\sqrt[3]{\gamma}$ data. The effect of adopting both a lower $\delta_0$ and a higher $\delta_2$ 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 $\delta_0$ of about 2.5x10^{-10} K^{-1} (perhaps in combination with a higher $\delta_2$ value) or, less probably, a mantle density that is 1.0% less than that given by PREM. Reducing $T_{lim}$ from 2000 to 1700 K removes the requirement for Si enrichment and reduces that for Fe enrichment. Variations in other parameters alone --- $K_{S2}$, $\delta_0$, or the seismologically determined $\sqrt[3]{\gamma}$ --- 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 $\sqrt[3]{\gamma}$, may place further constraints upon this problem.

Acknowledgments. We thank A. Chopelas, M. Bukowski, R. Hemley, I. Jackson, R. Jeanloz, and B. Kennett for preprints. We
also thank R. Hemley, I. Jackson, and H.-K. Mao for discussions of their experimental results. Finally, we thank D. L. Anderson, I. Jackson, B. Kennett, A. E. Ringwood, and I. S. Sacks for thoughtful comments on the manuscript. This material is based upon work supported by G. K. Gilbert postdoctoral fellowship from the Carnegie Institution of Washington (CRB) and by the Department of Terrestrial Magnetism (PGS).

References


(Rceived July 31, 1989; accepted March 1, 1990.)