COMPOSITION OF THE UPPER MANTLE: GEOPHYSICAL TESTS
OF TWO PETROLOGICAL MODELS

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Abstract. The elastic properties of candidate mantle phases are used to test the viability of olivine-rich (pyrolitic) and $CaO + Al_2O_3$-rich (eclogitic) assemblages for the mantle. High temperature adiabats for each phase of interest are constructed and compared to mantle seismic properties. Both pyrolitic and eclogitic assemblages satisfy the seismic properties between ~200 and 400 km. Between 400 and 670 km depth an eclogitic assemblage yields a superior match to velocities and velocity gradients. The 400 km seismic discontinuity may represent a chemical boundary between pyrolite and picritic eclogite ("piclogite") or phase transformations in the olivine + orthopyroxene components of a piclogitic assemblage containing about 16% olivine. High velocity gradients in the transition zone may be explained by the transformation of Ca-rich cpx to majorite garnet. Seismic properties at the top of the lower mantle are consistent with pyrolite, piclogite or perovskite, implying that the 670 km discontinuity may be a chemical boundary.

Comparisons of laboratory elasticity data with seismic velocity profiles have been used in many studies to constrain the composition of the Earth's mantle. With few exceptions, it has been assumed a priori that the dominant minerals throughout the mantle are olivine (ol) and orthopyroxene (opx), coexisting with a small quantity of garnet (gt) and clinopyroxene (cpx). However, it remains to be demonstrated that ol-rich assemblages provide either a unique or the most satisfactory fit to the seismic data. Anderson (1976, 1979), Liu (1979), Lees et al. (1983), and Jeanloz and Thompson (1983) have discussed the difficulties of explaining the discontinuity at 670 km and the velocities in the transition region on the basis of phase relations in the ol and opx systems. A conclusion of the above studies is that the 670 km discontinuity may represent a chemical boundary. Differences in the Fe and/or Si (opx) content of the upper and lower mantle have been suggested, and Anderson (1979) proposed that the mantle between 220-670 km depth is dominated by gt + cpx (eclogite) rather than ol + opx. It is clearly desirable to test the viability of the gt-cpx hypothesis by direct comparison of the high pressure-high temperature velocities for such an assemblage with mantle velocity and density profiles. Although the stability fields and elastic properties of CaO- and Al_2O_3-rich high-pressure phases are less well constrained than those of ol and opx, sufficient information exists for silicates and analog compounds to examine the plausibility of an eclogitic region. In this paper we calculate the compressional (V_p) and shear (V_s) velocities, and density (ρ) of olivine, pyroxenes, garnets, and their polymorphs, at elevated temperatures and pressures. The properties of assemblages dominated by gt + cpx or ol + opx are then compared to observed mantle velocities and densities.

Data Base

Although elasticity data for silicates and oxides has been steadily accumulating, a number of important phases remain uncharacterized. We have therefore relied on systematics to estimate the properties of some high-pressure phases. Data on analog compounds for all pertinent crystal structures are available and they yield consistent elasticity patterns. Bulk modulus (K) and rigidity (μ) are estimated from mean atomic weight or molar volume systematics and elastic constants of analog compounds. A complete discussion of our data base including T- and P-derivatives will be presented elsewhere (Bass and Anderson, in preparation).

The elastic and thermal properties and densities of ol, opx, gt, majorite (mj), (Mg,Fe)O, perovskite (pv), corundum and stishovite have been summarized previously (O. L. Anderson, et. al., 1968; Jeanloz and Thompson, 1983; and references therein). Elasticity data are also available for jadeite (e.g., Hughes and Nishitake, 1963; β and γ spinels (Weidner et al., 1984; Sawamoto et al., 1984) and diopside (Levien et al., 1979). For some phases only static compression results are available (e.g. mj, $MgSiO_3$-pv) and in these cases measured values of K were used with velocity systematics to define μ for a given compound. In the absence of other constraints, both K and μ were estimated by velocity systematics. We note that perovskite-structure compounds exhibit well defined elasticity trends (Liebermann et al., 1977). For garnet-structures K (~170 GPa) and V_p/V_s (~1.79) are virtually independent of composition and this has been assumed to apply to majorite (K = 220 GPa). Jadeite (jd), diopside (di), and opx, form majorite-garnet type solid solutions (Ringwood and Major, 1966, 1971). Molar volumes of the (hypothetical) majorite end-members are estimated to be 101.0 (jd) and 122.6 cc/mole (di) by assuming ideal mixing in solid solution. The post-majorite phase of jd-di solutions is thought to have a perovskite structure with end-member volumes of 32.1 ($CaSiO_3$, Ringwood and Major, 1971) and 24.9 cc/mole ($NaAlSi_2O_6$, Reid and Ringwood, 1975).

Results and Discussion

In Figure 1 we show V_p, V_s and ρ for the low and high pressure phases of each component in our model mineral assemblages. The 1400°C adiabats were constructed using third-order Eularian finite strain theory (Sammis et al., 1970). All Fe-Mg silicates contain 10% Fe^{2+} component, except garnet (~20% almandite). Also shown are Earth model PREM (Dziewonski and Anderson, 1981) and other recent profiles (Grand and Helmberger, 1984; Walck 1984; Given and Helmberger, 1980). A common feature is the high velocity gradient between 400 and about 670 km depth. The transition zone gradients are inconsistent with adiabatic compression of a homogeneous mineral assemblage and a broad phase transition is implied. The depth and breadth of the inferred phase change is an important constraint on the mineralogy in this region.
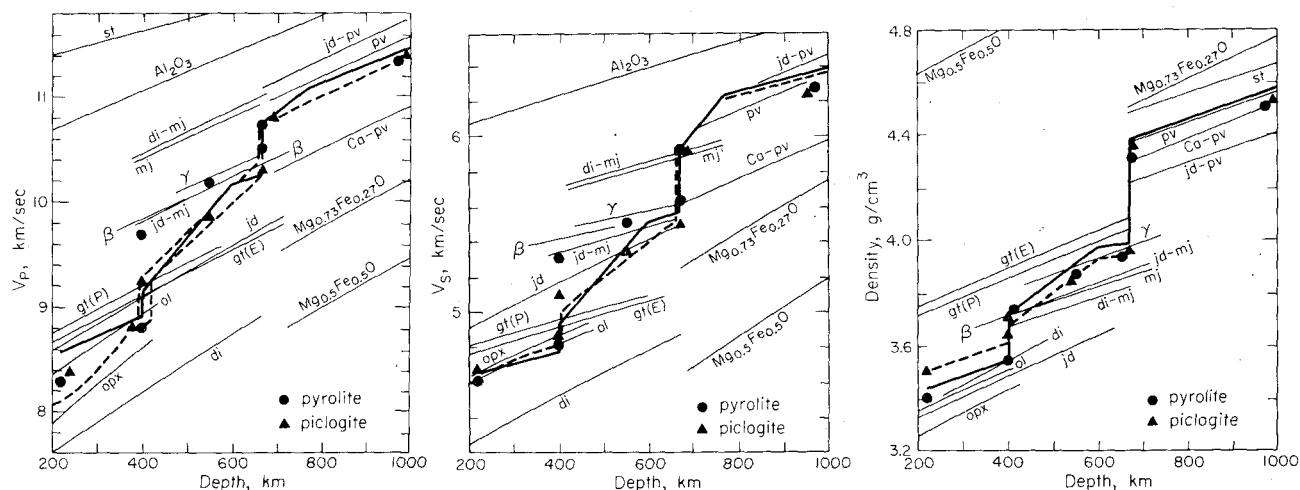
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Fig. 1: V_p, V_s and density for various minerals. Earth model PREM is shown (heavy solid line) along with a range of velocities from other studies (dashed lines). The dashed density profile is a perturbation of PREM which has the same mean upper mantle + transition zone density. Adiabats are initiated at $1400\,^\circ C$ (P = O). Circles and triangles indicate the properties of pyrolite and piclogite, respectively. The seismic profiles are substantially lower than pyrolite velocities (predominately β or γ, + mj) between 400-670 km, but are well matched by piclogite. Velocity jumps for pyrolite do not satisfy the 400 km discontinuity. (ol, olivine; opx, orthopyroxene; di, diopside; jd, jadeite; gt(E,P), garnet (eclogite, pyrolite); mj, opx majorite; di- or jd-mj, diopside or jadeite majorite; pv, $Mg_{0.9}Fe_{0.1}SiO_3$-perovskite; jd- or Ca-pv, jadeite or $CaSiO_3$ perovskite; st, stishovite).

We compare two model mineral assemblages with the mantle data: one is pyrolite, which is predominately ol with minor opx > gt ~ cpx (Ringwood, 1975), and the other is eclogitic, with gt ≈ omphacitic cpx (jd + di) > ol or opx. The pyrolite assemblage is 57% (by weight) ol, 17% opx, 14% gt and 12% di. The proportions of the eclogite phases were adjusted to give a good fit of ρ, V_p and V_s with the seismic data between 220 km and 670 km. Jadeite is an important component of mantle eclogite and serves to decrease the density and increase the velocity of the cpx-component of the mantle. A small amount of ol and opx is required to match the densities and velocities throughout the transition region, and phase changes in these components make it possible to satisfy the properties of the 400 km discontinuity as well. The overall chemistry of both assemblages does not change with depth but the phase chemistry, of course, does. The resulting eclogite composition has a low-pressure mineralogy of 23% di, 21% jd, 37% gt, 16% ol and 3% opx, and is thus a picritic-eclogite, or "piclogite" in composition. The piclogite gt contains slightly more Fe^{2+} than the pyrolite gt, consistent with eclogite gt from kimberlites.

We have assumed that across the 400 km discontinuity all ol is converted to β, and opx is dissolved in the gt phase as mj. At 550 km, 60% of the cpx has transformed to mj, which coexists with γ and opx-mj. At the bottom of the transition region all pyroxene is present as mj; below 670 km γ and gt-mj transform into pv-bearing assemblages. Although the phase relations for mineral compositions appropriate to our pyrolite and piclogite assemblages are not well determined, the above sequence of phase transformations is consistent with the results of Jeanloz and Thompson (1983), Akaogi and Akimoto (1979) and Liu (1980). An important point is that di and jd are stable over a broader pressure range than opx. Phase changes in ol are very narrow relative to the width of the transition zone.

The results of our velocity (Voigt-Reuss-Hill averaging) and density calculations for piclogite and pyrolite are shown in Figure 1 and Table 1. Between 200-400 km depth, both pyrolite and piclogite satisfy the mantle properties. The pyrolitic assemblage may be slightly preferred because V_s of piclogite is about 2% high at a depth of 400 km. However, the differences in velocity between pyrolite and piclogite are small from 200-400 km and we consider both models to fit the velocity data in this region.

Within the transition region (400-670 km depth), where we presume β and γ to be stable and the opx → mj reaction complete, the densities of both assemblages compare well with the density of the mantle. However, the velocities of pyrolite and piclogite are quite different. Pyrolite yields S-velocities 3-7% higher and P-velocities 4-5% higher than the seismic values. By contrast, V_p and V_s for piclogite provide a close match to the seismic velocity.

The variation of density with depth is poorly determined with available data but the average mantle density between 220 and 670 km is well constrained (Jordan and Anderson, 1974). The average densities of pyrolite and piclogite assemblages are both within 1% of PREM over this depth interval indicating that density does not provide a basis for distinguishing the two compositional models. Between 400 and 670 km depth pyrolite and piclogite are similar and slightly lower than PREM suggesting that PREM is too dense in this region. The dashed line in Fig. 1 shows a modification of PREM with the same average density between 220-670 km.

Phase changes in pyrolite cannot explain the 400 and 670 km discontinuities (Table 1). It is traditional to refer to the 400 km discontinuity as the "olivine-spinel" phase change but the calculated velocity jumps in olivine are more than twice as high as observed. At 670 km the observed velocity increases by 5% and the boundary is sharp, rather than diffuse as predicted for an ol or opx phase change (Jeanloz and Thompson, 1983).

It is difficult to match the high velocity gradients observed between 400 and 670 km with a pyrolitic model. The transition zone gradients are much higher than is charac-

Table 1. Compressional velocity, V_p, shear velocity, V_s, and density, ρ, for three mineral assemblages and the Earth's mantle. Velocity in km/sec; ρ in g/cm³.

Depth (km)	Piclogite			Pyrolite			Perovskite $Mg_{0.9}Fe_{0.1}SiO_3$			Earth		
	V_p	V_s	ρ	V_p	V_s	ρ	V_p	V_s	ρ	V_p	V_s	ρ
220	8.35	4.67	3.50	8.27	4.60	3.40				8.35	4.64	3.44
400−	8.82	4.86	3.65	8.80	4.81	3.54				8.82	4.77	3.54
400+	9.24	5.10	3.70	9.68	5.31	3.72				9.24	5.00	3.72
550	9.85	5.35	3.86	10.17	5.51	3.87				9.90	5.37	3.91
670−	10.29	5.50	3.96	10.50	5.63	3.95				10.26	5.56	3.99
670+	10.73	5.90	4.36	10.70	5.92	4.32	10.92	6.01	4.37	10.75	5.95	4.38
971	11.35	6.25	4.53	11.32	6.27	4.50	11.51	6.33	4.55	11.42	6.38	4.56

teristic of adiabatic compression of a homogeneous medium. The γ phase (Fo_{90}) is stable from about 475 to 670 km and with an ol-rich assemblage most of the transition region would be characterized by shallow velocity gradients. However, Akaogi and Akimoto (1979) show that dissolution of Ca-rich cpx into a gt-mj phase occurs over a pressure range that encompasses the transition zone. The stability field of gt-mj is also very broad for Al_2O_3-rich assemblages. Our calculations show that the gradual transformation of CaO- and Al_2O_3-rich cpx to mj can explain the high velocity gradients in the transition region. Thus, the available elasticity and phase stability data tend to favor a piclogitic mineral assemblage in the transition zone. Lees et al. (1983) were also unable to satisfy the seismic data for this region with an ol-opx assemblage.

In the lower mantle pyrolite, piclogite and $(Mg_{0.9}Fe_{0.1})SiO_3$ (pv) give comparable velocities and densities although the latter gives the best overall fit. The presence of a thermal boundary layer at 670 km would increase the temperature at the top of the lower mantle and this would favor the pure pv assemblage.

We conclude that piclogite (44% cpx, 37% gt, 16% ol, 3% opx) is a more satisfactory candidate mineral assemblage than is pyrolite for the transition zone, even though pyrolite may not be outright rejected due to uncertainties in material properties. Jd is an important component of our piclogite and eclogite cpx from kimberlite pipes. Because pyrolite and piclogite have similar properties under shallow mantle and lower mantle conditions, neither model can be excluded for these regions, although a lower mantle assemblage closer to perovskite or pyrolite is cosmochemically more acceptable. Thus, either or both the 400 and 670 km discontinuities may be chemical boundaries. The seismic properties between ~200 km and 400 km are generally consistent with piclogite. If piclogite is adopted then the 400 km discontinuity would be due to phase changes in the ol and opx components of the assemblage and any chemical boundary between pyrolite and piclogite would be shallower.

At transition zone and lower mantle depths both piclogite and pyrolite have comparable densities. If the 670 km discontinuity is a chemical boundary, then there must be a density contrast of several percent to maintain the transition zone and lower mantle as chemically distinct regions. The persistence of a piclogite transition zone and a peridotite or pv lower mantle would require that the mj-gt to pv transition in piclogite occur at a substantially higher pressure than the γ-spinel to pv and/or mj-gt to pv transitions in a Ca- and Al-poor pyrolitic assemblage. The work of Akaogi and Akimoto (1979), Jeanloz and Thompson

(1983) and Liu (1979) indicate that di-mj and Al_2O_3-rich gt may be stable to greater pressure than their Mg-Fe and low-Al_2O_3 counterparts. More experimental work is required to clarify the effect of Ca, Na, and Al on these phase changes. The velocities and densities of piclogite and pyrolite are slightly less than the lower mantle values. If a thermal boundary layer exists at 670 km then temperatures may be in excess of those used here and a pv lower mantle would be favored, strengthening the arguments for a chemical discontinuity. A chemical boundary at 670 km would also help explain the sharpness of the 670 km discontinuity. Jd-pv, $CaSiO_3$-pv and Al_2O_3-rich perovskites all appear to be less dense than $(Mg,Fe)SiO_3$-perovskite and the mantle at 670+ km. It is therefore unlikely that eclogite would sink into the lower mantle even if transformed to a perovskite bearing assemblage.

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