Partial melting in a thermo-chemical boundary layer at the base of the mantle

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Abstract

Seismological detections of complex structures in the lowermost mantle boundary layer (the D'' region) motivate a conceptual model of a compositionally stratified thermo-chemical boundary layer (TCBL) within which lateral temperature variations (sustained by large-scale mid-mantle flow) cause variations of partial melt fraction. Partial melt fractions of from 0 to 30% in the TCBL occur due to the eutectic of the boundary layer material lying below the high temperature at the core–mantle boundary (CMB), coupled with the presence of steep thermal gradients across the boundary layer. Regions of the TCBL with the highest temperatures have extensive partial melting, producing lateral chemical variations and strong effects on seismic velocities and boundary layer dynamics. This TCBL concept provides a relatively simple framework that can plausibly account for diverse seismological observations such as: predominance of large-scale volumetric elastic wave velocity heterogeneity in the boundary layer, laterally extensive, but intermittent abrupt shear and compressional velocity increases and decreases at the top of the D'' region, small-scale topography of D'' velocity discontinuities, thin ultra-low velocity zones at the CMB, widespread shear wave anisotropy in D'', bulk sound velocity anomalies detected in low shear velocity regions of D'', and large-scale upwellings from the most extensively melted regions of the boundary layer. Neutral or negative buoyancy of the partial melt in the TCBL is required, along with an increase in bulk modulus and some density increase of the boundary layer material relative to the overlying mantle. More complex models, in which the partially melted chemical boundary layer is laterally displaced by mid-mantle downwellings are also viable, but these appear to require additional special circumstances, such as a phase change, efficient segregation of slab crustal material, or abrupt onset of anisotropy, in order to account for rapid velocity increases at the top of D''. The precise nature of the compositional anomaly, or anomalies, in D'' and the eutectic composition of this zone are yet to be determined, but it appears likely that partial melting within the lowermost mantle plays a paramount role in the observed seismic velocity heterogeneity. Increased resolution geodynamic calculations of dense boundary layer structures with partial melting (and attendant viscosity reductions and chemical heterogeneity) are needed to quantify this TCBL concept.
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1. Introduction

Compositional stratification is a primary characteristic of all large planetary bodies. The great energy available during planetary accretion provides ample heat for partial or total melting of the growing body,

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which abets effective chemical differentiation and mineral or melt segregation in the presence of gravity. The Earth is compositionally stratified as a result of such processes (e.g., Anderson, 1987), with most of the densest materials having separated into the core and most of the lightest minerals having separated into the oceanic and continental crusts (the chemical partitioning coefficients of trace materials produce departures from strict density-driven stratification). Accretionary and core-formation scenarios for the Earth emphasize the likelihood that compositional layering is to be expected, unless subsequent mixing has disrupted it (e.g., Ruff and Anderson, 1980). Compositional stratification of Earth's mantle, either in the past or at present, has often been invoked to explain geochemical observations, with the historical focus being on possible upper mantle/lower mantle layering (see reviews by Hofmann, 1997; Hellfrich and Wood, 2001), and, more recently, on possible chemical stratification of the mid-mantle (e.g., Kellogg et al., 1999; van der Hilst and Kárason, 1999; Albarede and van der Hilst, 1999). While convection may play an important role in efficient transport of material of distinct composition to boundary layers where it can segregate and replenish the chemical boundary layer (CBL), the tendency toward chemical stratification of a planet is resisted by boundary layer instabilities, convective overturn of the interior, and viscous entrainment of buoyancy-segregated boundary layer materials. Our focus will be on possible compositional stratification in the lowermost mantle boundary layer.

Recognizing that the density and viscosity contrasts across Earth's core–mantle boundary (CMB) exceed those at the planet's surface, various scenarios for a thermo-chemical boundary layer (TCBL) at the base of the mantle (Fig. 1b–g) have been postulated, in some aspects mirroring that in the lithosphere (Fig. 1a). The lowermost few hundred kilometers of the mantle is called the D″ region because the seismic velocity gradients with depth tend to be low and there is stronger lateral velocity heterogeneity compared to the overlying mantle (e.g., Bullen, 1949; Young and Lay, 1987a; Wysession et al., 1998; Garnero, 2000). In this paper, we use D″ as a general label for the boundary layer in the lowermost mantle, whatever its precise nature or thickness.

One of the basic paradigms for the D″ region is that it must include a thermal boundary layer (TBL), con-

ducting heat out of the core (Fig. 1b). There is general agreement that long-term sustainability of the Earth's geodynamo requires heat flux from the core into the mantle (most calculations are in the range 2–10 TW (e.g., Buffett et al., 1996; Labrosse et al., 1997; Anderson, 2002; Buffett, 2002; Labrosse, 2002), compared to a total surface heat flux of about 44 TW), so D″ must certainly function as a TBL at the base of the mantle to some extent. Higher estimates of heat flow out of the core (>2–3 TW) suggest rapid inner core growth, and improbably high core temperatures in the early Earth unless heat sources are added to the core (e.g., Buffett, 2002). The low viscosity of the outer core material ensures that the CMB itself must be nearly isothermal, at a temperature somewhere between 3300 and 4800 K, and there is possibly a superadiabatic temperature increase of 1000–2000 K across the boundary layer (e.g., Williams, 1998; Boehler, 2000; Anderson, 2002). Reducing the heat flux and temperature increase estimates below the above values requires either the presence of superadiabatic thermal gradients shallower in the mantle (at 670 km depth, or in the mid-mantle), which have not yet been demonstrated to exist, or dramatic and unexpected melting point depression of iron by its lighter alloying constituent. A large temperature increase across the TBL is expected to reduce seismic velocities and radial seismic velocity gradients in D″ (e.g., Stacey and Loper, 1983), but the effects of high pressure should reduce temperature dependence of seismic velocity. This effect, and any attempt to calculate heat flux across the boundary layer on the basis of observed velocity structure, strongly depend on the boundary layer material properties.

As the mantle convection system has likely not approached a steady state, viscosity reduction of several orders of magnitude at the base of the D″ TBL may be present due to the temperature-dependence of viscosity, possibly complementary to the viscosity increases across the lithospheric TBL (e.g., Balachandar et al., 1995; Tackley, 1996; Solomotov and Moresi, 2002). While the evolution of convective systems tends to diminish the viscosity contrasts across hot thermal boundary layers with time, cooling of the interior by subducted downwellings may allow large viscosity ratios to persist. Any viscosity reduction in D″ is superimposed on the overall high viscosity of the lower mantle, which is one to two orders of magnitude greater than that of the upper mantle (e.g., Forte and

a) Surface tectonics and deep mantle observables

b) TBL Model   c) CBL Model   d) Dregs Model

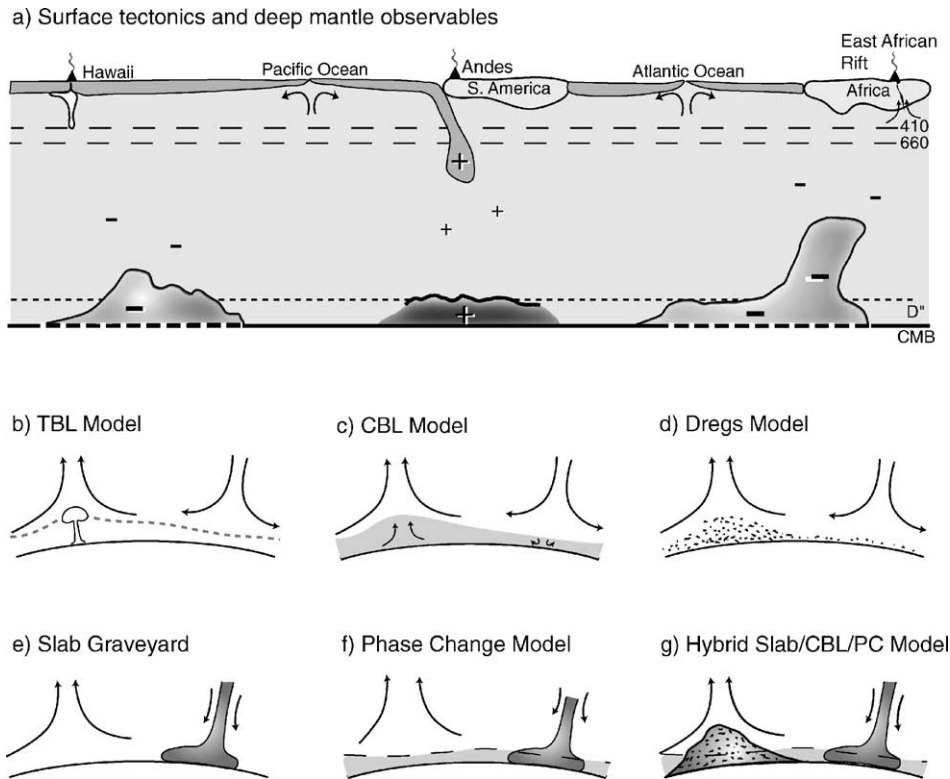e) Slab Graveyard   f) Phase Change Model   g) Hybrid Slab/CBL/PC Model

Fig. 1. Schematic characteristics of the mantle system and proposed scenarios for the lowermost mantle boundary layer. (a) Mantle cross-section showing key structural elements of the near-surface thermo-chemical boundary layer involved in plate tectonics and the distribution of large-scale features of lower mantle structure inferred from seismology. Cycling oceanic lithosphere, part of the mantle convection system, involves combined thermal and chemical boundary layers which are eventually subducted. Continental lithosphere involves more permanent thermal and chemical boundary layers that translate on the surface. Globally extensive phase transitions exist at depths near 410 and 660 km. The deep mantle has large scale regions of relatively low (minus signs) or high (plus signs) elastic velocities, with the strongest patterns located in the D″ region (below the dotted line). Relatively strong velocity increases are seen at the top of high velocity regions of D″ (thick line), and relatively well-developed ultra-low velocity zones are observed at the CMB below low velocity regions (dashed areas). (b) Thermal boundary layer (TBL) (dotted line) model for a homogeneous composition lower mantle with large scale circulation and small scale boundary layer instabilities. (c) Chemical boundary layer (CBL) of a globally extensive, dense, hot D″ region, modulated by mid-mantle flow and having small-scale convection within a double-thermal boundary layer. The CBL may involve ancient materials from accretion or replenishing sources of heterogeneity associated with core–mantle reaction products or downwelling slab heterogeneities. (d) Localized, dense chemical heterogeneities concentrated beneath upwellings are envisioned in the dregs model. (e) Subducted lithospheric slabs accumulating in a slab graveyard may result in ephemeral thermal/chemical heterogeneities in D″ that will eventually upwell. (f) A phase transition may occur in a homogenous composition lower mantle, affecting both downwelling and upwelling material. (g) A conjectured hybrid model combining notions of slab graveyard, laterally displaced CBL, and phase change (PC) models to explain diverse seismic observations only partly explained by models (b)–(f).

Mitrovica, 2001). Thermal boundary layer instabilities at the CMB are often invoked as a source of localized upwelling plumes in the mantle (Fig. 1b). For a simple TBL, such instabilities would produce large excess mantle temperatures in ascending plumes, which may only be partially diminished by entrainment (e.g.,

Farnetani and Richards, 1995; Farnetani, 1997). The overall dynamics of the hot D″ thermal boundary layer are expected to differ from the cold boundary layer at the surface. For example, the downwelling sheets formed by cold, high-viscosity surface boundary layer instabilities appear to be influenced by the slab

strength and the viscosity increase and phase changes between the upper and lower mantles (e.g., Bunge et al., 1996), and will likely have no counterpart in the hot D″ boundary layer. The large uncertainties of heat flux out of the core and of key material properties within D″ such as the thermal expansion coefficient (e.g., Chopelas, 1996) yield large uncertainty about the relative role of large-scale circulation in the deep TBL versus any small-scale plume instabilities.

The dynamics of the D″ boundary layer may be strongly impacted if partial melting takes place in the rapid thermal increase at the base of the mantle, as a result of attendant viscosity reduction in the layer. While it appears that end-member $(Mg,Fe)SiO_3$-perovskite and $(Mg,Fe)O$ ferropericlase have melting temperatures higher than the upper bound on CMB temperature (e.g., Zerr and Boehler, 1993, 1994), the mixture of minerals in the lower mantle is likely to involve a eutectic system, with much lower melting temperature than for the end-member minerals. Extrapolation of a lower mantle pyrolite solidus experimentally determined by Zerr et al. (1998) down to the CMB gives a solidus temperature of about 4300 K (Boehler, 2000), within the range of CMB temperature estimates. This raises the possibility that partial melting may occur in D″, even for a simple thermal boundary layer at the base of a homogeneous composition mantle. Although the chemistry of eutectic melts under D″ condition is essentially unconstrained, any enrichment within D″ of components outside of the typical $CaO–MgO–FeO–Al_2O_3–SiO_2$ mantle compositional system is anticipated to depress the solidus temperature from that of the (presumably compositionally simpler) overlying mantle (e.g., Wen et al., 2001). In this sense, if D″ is notably enriched in hydrogen or carbon (through downward segregation of melts, or sequestration of subduction-related material), reduced iron or silicon (through core interaction), or even elements such as alkalis or titanium that are incompatible near Earth's surface (again, likely through magmatic segregation or, in the case of Ti, through stratification produced at accretion), then we would expect the eutectic temperature to be depressed relative to that within the overlying mantle. The effects of such additional components on the eutectic temperature in the lowermost mantle is difficult to assess: since melting point depression depends on the molar abundance of the impurity within the liquid, hydrogen is (on a per mass basis) likely to be the most effective element at depressing the melting temperature under D″ conditions. Unsurprisingly, this mirrors hydrogen's effects at shallower depths within the planet.

The density contrast at the CMB, the history of extensive chemical transport across the CMB, and the location of D″ between mantle and core convection regimes (stratified, or otherwise), make it likely that chemical heterogeneities denser than typical mantle material and less dense than typical core material have concentrated in D″ over time. Thus, it is logical that a chemically distinct layer could exist at the base of the mantle (e.g., Ruff and Anderson, 1980; Anderson, 1987, 1998), in what is almost certainly the hottest portion of the silicate Earth. This leads to the notion of a chemical boundary layer at the base of the mantle (Fig. 1c). While the presence of a CBL will modify heat transport across the CMB, it does not negate the need for heat flux out of the core to sustain the geodynamo, so a TBL must also be present. For an enduring CBL that resists erosion by entrainment over long times and persists as a coherent layer, a density increase of at least 3–6% from overlying mantle has often been found to be required in fluid dynamics models (e.g., Christensen, 1984; Sleep, 1988; Kellogg and King, 1993; Kellogg, 1997; Sidorin and Gurnis, 1998; Montague and Kellogg, 2000). A ratio of chemical to thermal buoyancy, B, greater than 1 is generally inferred to be necessary to keep the layer stable. Smaller density anomalies, of about 2%, may survive for geologically long times without replenishment, but it is commonly asserted that it is unlikely that a distinct layer can survive with such a small density increase, and the dense heterogeneity will concentrate into patches below upwellings (e.g., Davies and Gurnis, 1986; Hansen and Yuen, 1989; Tackley, 1998; Davaille, 1999; Gonnermann et al., 2002).

This common finding that several percent or stronger density increase in the boundary layer is required for long-term survivability is now coming under fire. Zhong and Hager (2003) find that for a 1000 km thick layer of the lower mantle with a net negative buoyancy of approximately 1%, more than 90% of the dense material can survive for 4.5 Gyr. Part of the difference from earlier results is that one must appropriately scale the buoyancy parameters for a layered system, and earlier work overestimated the stabilizing density increase by using the Boussinesq

approximation. Increasing pressure has a strong effect of reducing thermal expansion, so early calculations tend to err on the side of overly large density anomalies to overcome thermal expansion effects. If D″ has thinned over time, achieving its current thickness today, it may involve only a small density increase of 1% or less, and still endure as a global layer. Another factor is that low viscosity of the boundary layer may also diminish entrainment efficiency, as found numerically (e.g., Kellogg and King, 1993; Schott et al., 2002) and in laboratory experiments for mixing between viscous layers (Namiki, 2003). Stiffer overlying flow is simply ineffective at entraining less viscous material below it, and Namiki (2003) argues that the volume of D″ could have remained unchanged since it formed.

It is also possible that chemical heterogeneity in D″ could be continuously generated by processes such as core–mantle chemical reactions (e.g., Knittle and Jeanloz, 1989, 1991; Goarant et al., 1992; Poirier, 1993; Song and Ahrens, 1994; Dubrovinsky et al., 2001) or by segregation of crustal components in subducted lithosphere (e.g., Hofmann and White, 1982; Christensen and Hofmann, 1994; Wysession, 1996; Coltice and Ricard, 1999). Dispersed chemical heterogeneities in D″ may be in the form of "dregs" (Fig. 1d), which, over time, will concentrate under upwellings if their chemical buoyancy suffices to resist entrainment (e.g., Manga and Jeanloz, 1996; Kellogg, 1997; Montague et al., 1998; Forte and Mitrovica, 2001; Schott et al., 2002; Gonnermann et al., 2002). This can result in hot dense piles, with large temperature contrasts across the CBL. Sheared tendrils of entrained material could cause small-scale heterogeneity at shallower depths (e.g., Schott et al., 2002).

The notion of accumulation of slab material in D″, as a 'slab graveyard' (Fig. 1e) invokes the combined thermal and chemical heterogeneity of lithospheric slabs to account for structure in D″ (e.g., Wysession, 1996; Grand et al., 1997; Garnero and Lay, 2003). Recycling of oceanic crust is often appealed to by geochemists as a source of chemical heterogeneity in the mantle (e.g., Hofmann, 1997; Coltice and Ricard, 1999). If high viscosity features such as slabs are present in mid-mantle downwellings, they may play a role in plowing aside CBL material, perhaps spawning instabilities on the margins of the downwellings (e.g., Tan et al., 2002).

A globally extensive phase transformation (Fig. 1f) has also been proposed for the base of the mantle, possibly modulated by cold downwelling slabs (e.g., Nataf and Houard, 1993; Sidorin et al., 1999a), but a candidate transition has not yet been identified (see discussion by Wysession et al., 1998). Indeed, the mere presence of the sole possible mantle material that has been observed to undergo a phase transition at near CMB conditions, SiO_2 (Murakami et al., 2003), implies the presence of a compositional boundary, as silica-saturated compositions do not typically occur in pyrolitic or peridotitic compositions. A phase transformation would presumably be observed as a global feature, although lateral variations in temperature and flow stresses could produce large-scale topography on the boundary.

The current trend in characterizations of the D″ region is toward complex hybrid models (Fig. 1g), involving a combination of effects of a TBL, an enduring CBL, ponding of slabs in or on top of the boundary layer, and superimposed (unspecified) phase changes (e.g., Sidorin et al., 1999b; Tackley, 2000; Wen et al., 2001; Tan et al., 2002; Ni and Helmberger, 2003a,b). This complexity stems from attempts to reconcile seismological observations and their inferred geodynamical behavior. Given that the surface boundary layer involves a combination of thermal, chemical, and phase changes in an active dynamic system (Fig. 1a), such complex scenarios for D″ (Fig. 1g) are not intrinsically unrealistic and have gained some currency in the community. However, the goal in the current paper is to develop a relatively simple TCBL concept for D″ that naturally gives rise to complex structural manifestations as a result of partial melting in the hot boundary layer. Salient observations from seismology pertinent to formulation of the conceptual model will be summarized first, then consideration of partial melting effects will lead to presentation of the new TCBL model.

2. Seismological constraints on the boundary layer

Seismology provides most available constraints on structure of the deep mantle, with many observations contributing to characterization of the boundary layer. Several recent reviews outline the full suite of seismological investigations (e.g., Garnero, 2000; Lay et al., 1998a; Gurnis et al., 1998; Loper and Lay, 1995).

Here we briefly recap the major findings pertinent to the fundamental nature of the D″ region which we then incorporate into our new conceptual model for the TCBL.

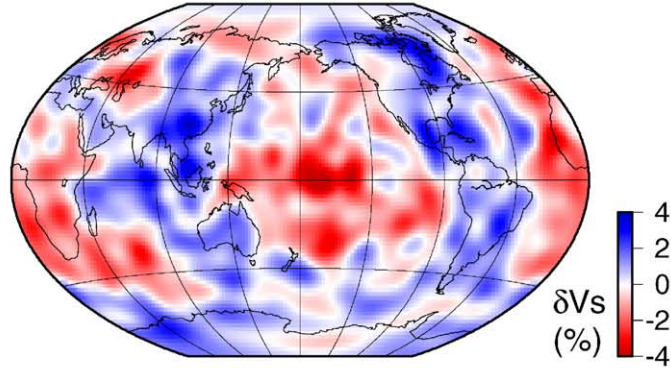## 2.1. Large-scale velocity heterogeneity

One of the important and surprising discoveries of global seismic tomography is the existence of large-scale patterns of seismic velocity heterogeneity in the lowermost mantle boundary layer. One might have anticipated a very white heterogeneity spectrum within a hot, relatively inviscid boundary layer. The predominance of large-scale structure is observed for both shear and compressional velocities, with representative recent models of D″ seismic velocities being shown in Fig. 2. Shear waves (Fig. 2a) are characterized by relatively high velocities (V_s) beneath the circum-Pacific, with relatively low velocities under the central Pacific and south Atlantic/Africa (e.g., Grand, 2002; Gu et al., 2001; Mégnin and Romanowicz, 2000; Masters et al., 2000; Castle et al., 2000; Kuo et al., 2000; Ritsema et al., 1999). The recent models have shear velocity fluctuations ranging over ±2–3% within D″ and there is quite good overall consistency of the large-scale features between different models. Compressional wave velocities (V_p) (Fig. 2b) are characterized as having a range of ±1% fluctuations, with low velocity areas beneath the southern Pacific and south Atlantic/Africa and high velocities under eastern Eurasia (e.g., Zhao, 2001; Fukao et al., 2001; Karáson and van der Hilst, 2001; Boschi and Dziewonski, 1999, 2000; Bijwaard et al., 1998; Vasco and Johnson, 1998). The strength of estimated compressional velocity heterogeneity is sometimes stronger by factors of 3–10 for models that seek to invert for CMB topography in combination with a 20–300 km thick boundary layer (e.g., Sze and van der Hilst, 2003; Garcia and Souriau, 2000; Doornbos and Hilton, 1989), so the large-scale tomographic models may well be heavily smoothed images that underestimate even large scale velocity fluctuations. In general, the consistency amongst V_p models is less than between V_s models in D″, possibly due to the weaker heterogeneity for V_p and/or the additional spatial sampling provided by ScS and SKnS phases for V_s determinations. The inhibition of thermal expansion by pressure expected in the mantle suggests that accounting for the seismic velocity heterogeneity by thermal effects alone will be very difficult, favoring interpretation as chemical and anisotropic effects.

Some studies find good correlation between V_p and V_s structures (e.g., Masters et al., 2000), however, this correlation appears to break down in certain regions, such as beneath the northern Pacific, where V_p anomalies tend to be positive and V_s anomalies tend to be negative (Fig. 2). A south-to-north decrease in the V_p/V_s ratio has also been found using diffracted waves traversing D″ below the northern Pacific (Wysession et al., 1999). V_s models show markedly stronger increases in RMS velocity heterogeneity in the lowermost 300 km of the mantle than do V_p models (Fig. 2c), although the various models do differ in the extent to which shear velocity heterogeneity is concentrated toward the CMB. Even for well-correlated V_p and V_s models (e.g., Masters et al., 2000), this raises the possibility of distinct behavior for V_p and V_s due to competing thermal and chemical variations, coupled with the possible presence of low degrees of partial melting. Indeed, the variability in V_p/V_s ratios and occasional decorrelation of V_p and V_s anomalies alone provide strong evidence that thermal effects alone cannot explain the seismic observations (Anderson, 1987).

Simultaneous inversions of P and S data have been performed in an attempt to isolate bulk sound velocity variations from shear velocity variations (e.g., Robertson and Woodhouse, 1996; Su and Dziewonski, 1997; Kennett et al., 1998; Masters et al., 2000), but there are significant discrepancies between these models, perhaps as a consequence of incompatible resolution of V_p and V_s structures on a global basis. Direct comparisons of P and S travel time anomalies on specific paths support the possible decorrelation of these elastic velocities for localized regions within D″ (e.g., Saltzer et al., 2001), as well as reaffirming the greater variations in V_s than V_p (e.g., Tkalcic and Romanowicz, 2001; Simmons and Grand, 2002). Global tomography inversions to date lack detailed resolution of structure in D″, with particularly limited resolution of radial velocity gradients; however, there is no question that large-scale patterns of velocity variations dominate in the boundary layer, with at least some spatial correlation with the upper mantle and mid-mantle dynamic systems.
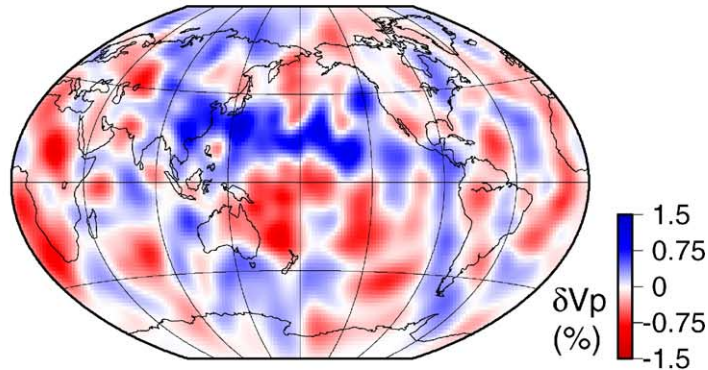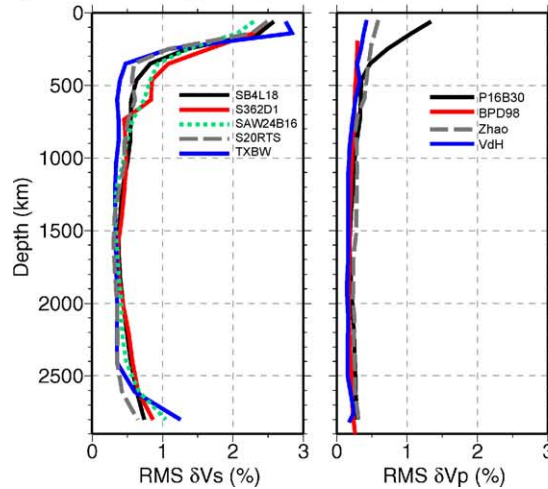
Fig. 2. Representative results of large-scale mantle tomography for velocity structure at the base of the mantle. (a) Map of shear velocity variations at a depth of 2750 km relative to a 1-D reference model obtained by Mégnin and Romanowcz (2000). Note the long-wavelength patterns of high velocities beneath the circum-Pacific and low velocities beneath the central Pacific and Africa. Variations of ±3% are imaged by this and other models with similar spatial patterns. (b) Map of compressional velocity variations at a depth of 2750 km relative to a 1-D reference model obtained by Zhao (2001). Long-wavelength patterns dominate, with substantial overall correlation with shear velocity variations, but clear regions of decorrelation (as in the mid-Pacific). Variations of ±1.0% are observed. (c) RMS velocity fluctuations at various depths in the mantle shear velocity models SB4L18 (Masters et al., 2000), S362D1 (Gu et al., 2001), SAW24B16 (Mégnin and Romanowicz, 2000), S20RTS (Ritsema and van Heijst (2000), and TXBW (Grand, 2002) and in the compressional velocity models P16B30 (Bolton, 1996), BPD98 (Boschi and Dziewonski, 1999), Zhao (Zhao, 2001), and VdH (Karáson and van der Hilst, 2001).

2.2. D″ discontinuities

An important feature of the D″ region that is not yet resolved in global tomography inversions is the intermittent presence of a rapid velocity increase several hundred kilometers above the CMB. This feature, found in both S- and P-wave investigations, is often called the D″ discontinuity (e.g., Wysession et al., 1998), and representative shear velocity profiles obtained by waveform modeling are shown in Fig. 3. These models, obtained for distinct regions of D″, involve a 2.5–3% shear velocity increase at depths from 130 to 300+ km above the CMB that is present laterally over intermediate-scale (500–1000 km) regions. Wysession et al. (1998) review the many studies of this feature, noting that there are substantial variations in depth of the discontinuity, greater consistency amongst S wave reflections/triplications from the discontinuity than for P waves, and typically larger inferred V_s increases than V_p increases, with the latter usually being 0.5–1.0%, though some models do have 3% V_p increases (e.g., Wright et al., 1985; Weber and Davis, 1990). The increase in velocity at the top of D″ may be distributed over up to a few tens of kilometers in depth, or it may be very sharp (e.g., Lay and Helmberger, 1983a; Young and Lay, 1987b).

The regions with the strongest evidence for a V_s discontinuity are highlighted in Fig. 4a. Wysession et al. (1998) show individual data sampling in greater detail. Some of these areas also have evidence for a V_p discontinuity, but in some regions, such as under Alaska and Central America, any V_p discontinuity must be at or below the detection threshold of about 0.5% (Young and Lay, 1989; Ding and Helmberger, 1997; Reasoner and Revenaugh, 1999). Stacking of array data is necessary to detect such small discontinuities, and many 'non-observations' reported for individual seismograms must be viewed as inconclusive. The S wave observations tend to be longer period than the P wave data used to look for the discontinuity, so it is viable that a transition zone several tens of kilometers thick can explain the absence of high frequency pre-critical P reflections. Note in Fig. 4a that most areas with strong evidence for an S reflector are in the high velocity regions of Fig. 2; the primary exception is under the central Pacific, where a V_s discontinuity is observed in a region of low D″ shear velocities (e.g., Garnero et al., 1993b; Russell et al., 2001).
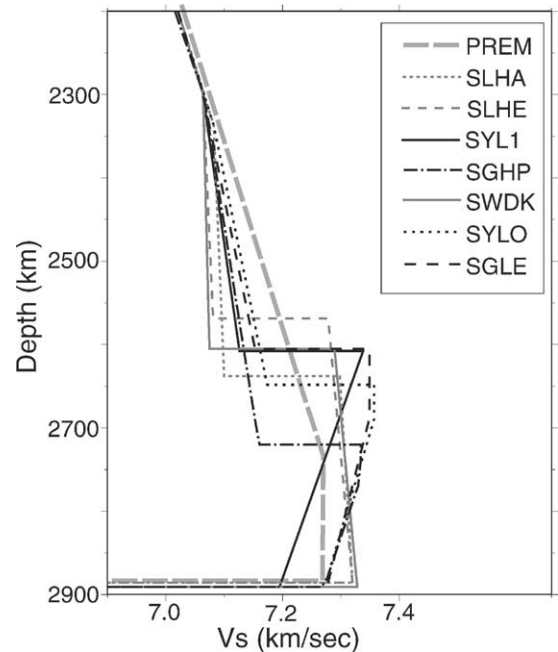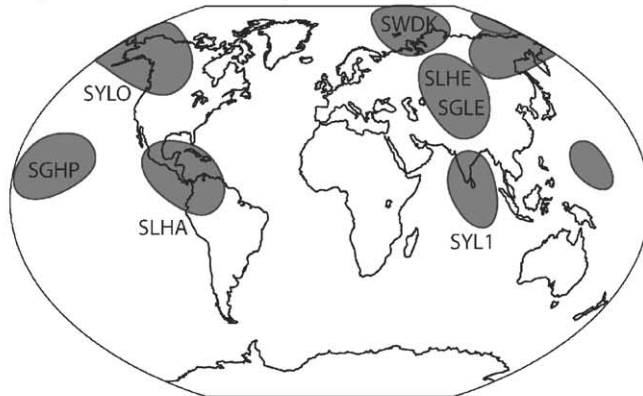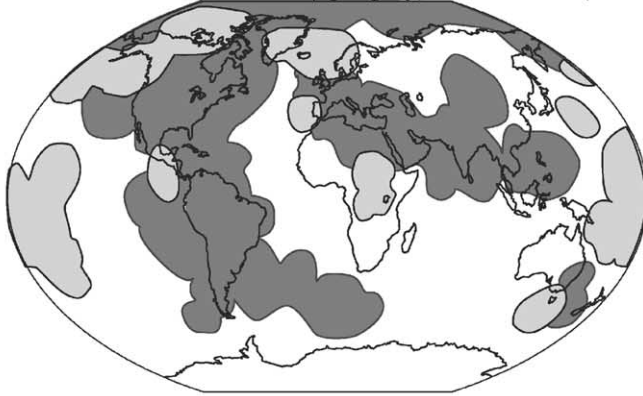

Fig. 3. Radial profiles of shear velocity in the lowermost mantle: PREM (Dziewonski and Anderson, 1981), SLHE, SLHA (Lay and Helmberger, 1983a), SYL1 (Young and Lay, 1987b), SGHP (Garnero et al., 1988), SWDK (Weber and Davis, 1990), SYLO (Young and Lay, 1990), and SGLE (Gaherty and Lay, 1992). The discontinuity models represent localized structures, determined for spatially limited regions of the D″ layer, the locations of which are indicated in Fig. 4. Shear velocity increases of 2.5–3.0% are found in regions under Eurasia (SWDK, SGLE), Alaska (SYLO), Central America (SLHA), the Indian Ocean (SYL1), and the central Pacific (SGHP). The velocity increase is typically modeled as a sharp discontinuity, but it may be distributed over up to 50 km in depth. Decreased velocity gradients above the discontinuity may exist, but are artifacts of the modeling in most cases. The reduction of velocity below the discontinuity in more recent models (orange), may be real, but may be an artifact of modeling a heterogeneous region with a one-dimensional model. The variations in depth of the discontinuity are uncertain due to the lack of constraint on velocity above and below the discontinuity, but some variation appears to exist.

Abrupt shear velocity decreases at depths a few hundred kilometers above the core–mantle boundary have also been detected, and can be characterized as discontinuities. This is found in regions where D″ velocities are very low, and abrupt decreases of 1–3% have been incorporated into models based on waveform modeling (e.g., Wen et al., 2001; Ni and Helmberger, 2003a). This is discussed in detail below.
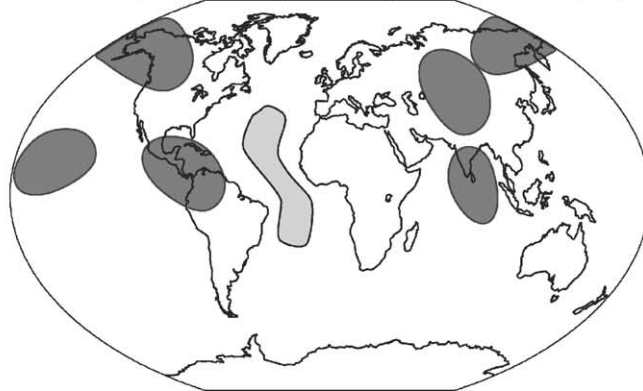
Fig. 4. Maps summarizing spatial variations of seismic wave characteristics of D″. (a) Regions where regional shear velocity discontinuities have been observed in large numbers of data, typically with 2–3% increases in velocity at depths from 200 to 300 km above the CMB (see labeled models in Fig. 3). Details of the data sampling and extensive references to work on both compressional and shear velocity discontinuity detections are given by Wysession et al. (1998). (b) Regions where ULVZ structures at the CMB have been detected or not, primarily based on SPdiffKS observations and assuming a Fresnel zone appropriate for a horizontal layer. Details of many studies and full references are given by Garnero et al. (1998). (c) Regions where regional studies of D″ shear wave splitting have been conducted. Most areas exhibiting splitting have waveforms compatible with vertical transverse isotropy, with decoupling (or only weak coupling) of the transverse and longitudinal components of the S wavefield, with 1–2% faster transverse components. Details of observations and data sampling are given by Lay et al. (1998b).

2.3. D″ ultra low velocities

Fig. 4b summarizes another important aspect of D″ that has been inferred from seismic waveform investigations; the widespread existence of a basal layer from 5 to 40 km thick with very strong V_p and V_s reductions of up to −10 and −30%, respectively. The observations of this ultra-low velocity zone (ULVZ) are summarized by Garnero et al. (1998), and include seismic wave reflections, conversions, and diffractions from an abrupt onset of the strong velocity reductions (e.g., Garnero et al., 1993a; Revenaugh and Meyer, 1997; Wen, 2000; Wen and Helmberger, 1998; Vidale and Hedlin, 1998). Extensive regions of ULVZ appear to exist, although the lateral extent may be exaggerated in Fig. 4b due to plotting of Fresnel zones for a layered model, since it has been shown that localized three-dimensional domes and blobs may also explain the data (Helmberger et al., 1998, 2000). Similarly, the absence of detectable ULVZ indicated in Fig. 4b explicitly emphasizes "detectability"; in many cases a layer less than 5 km thick simply cannot be ruled out by the observations. Nonetheless, there are regions where there is no evidence of complexity in structure right at the CMB in high quality short-period data (e.g., Castle and van der Hilst, 2000; Persch et al., 2001) or evidence for rapid small-scale variations in ULVZ structure (e.g., Havens and Revenaugh, 2001; Rost and Revenaugh, 2003). The ULVZ structures appear to be an end-member of regions of −3 to −5% low average V_s in the boundary layer beneath the central Pacific and southern Atlantic/Africa that may sometimes be much thicker, on the order of 300 km and more, as discussed below.

2.4. D″ anisotropy

Another important property of the D″ region that has been established is the presence of anisotropic structure that causes shear wave splitting. The observations and models associated with anisotropy in D″ have been summarized by Lay et al. (1998b), Kendall and Silver (1998), and Kendall (2000). The large majority of observations involve horizontally polarized shear wave components traveling faster through D″ than vertically polarized shear waves for grazing incidence or wide-angle reflections, with relatively large-scale regions of D″ displaying 0.5–1.5%

anisotropy (e.g., Garnero and Lay, 2003; Thomas et al., 2002; Fouch et al., 2001; Vinnik et al., 1998; Kendall and Silver, 1996). Shear wave splitting appears to be linked to the onset of the velocity increase at the top of D″ in high velocity regions (e.g., Matzel et al., 1996; Garnero and Lay, 1997), but resolution of the depth extent of the anisotropy in the boundary layer remains very limited (Moore et al., 2004). Vertical transverse isotropy (VTI) compatible with the primary observations could be the result of lattice-preferred orientation (LPO) for a D″ mineral component, or the result of shape-preferred orientation (SPO) of chemical or partial melt components in a sheared boundary layer. A candidate major component of the lower mantle that may develop VTI in a horizontally sheared boundary layer is MgO (e.g., Karato, 1998; Stixrude, 1998; Karki et al., 1999; Kendall, 2000; Mainprice et al., 2000; Yamazaki and Karato, 2002), whereas low velocity lamellae comprised of partially melted crust or other chemical heterogeneities are also possible causes of VTI (e.g., Kendall and Silver, 1998; Wysession et al., 1999; Fouch et al., 2001; Moore et al., 2004). Localized observations of shear wave splitting in D″ incompatible with VTI have been reported, with localized upwelling in the boundary layer being invoked to modify the symmetry axis for SPO or LPO (e.g., Pulliam and Sen, 1998; Russell et al., 1998, 1999). McNamara et al. (2001, 2002, 2003) use thermal convection models to compute variations in temperature and stress regime that might result in localization of dislocation creep that favor LPO in some areas and diffusion dominated deformation in others that would require SPO to account for any anisotropy. These dynamic calculations indicate that conditions favorable for mid-mantle anisotropy may exist in downwellings, but as yet there is no clear evidence for anisotropy in the bulk of the mid-mantle (e.g., Kaneshima and Silver, 1995; Meade et al., 1995).

2.5. D″ scatterers

The final attribute of D″ velocity heterogeneity that needs to be noted is the clear evidence for small-scale heterogeneity which gives rise to scattering of short-wavelength seismic waves. Scattering of short-period P waves from CMB topography and/or D″ heterogeneity has been extensively observed for

decades, and continues to be studied using diffracted coda waves (e.g., Bataille and Lund, 1996), PKP precursors (e.g., Cormier, 1999; Hedlin and Shearer, 2000), PKKP reflections (e.g., Earle and Shearer, 1997), triplications (e.g., Kohler et al., 1997), and scatterer migrations (e.g., Thomas et al., 1999). While there is some debate as to whether small-scale scattering structure is concentrated near the CMB or is uniform across the lower mantle (Hedlin and Shearer, 2000), it is clear that at least some regions have very strong small-scale heterogeneity close to the CMB, possibly in ULVZ structure (e.g., Niu and Wen, 2001; Vidale and Hedlin, 1998; Wen and Helmberger, 1998). Some studies purport to show evidence of thin layers of anomalous properties, or lamellae in the boundary layer (e.g., Lay and Helmberger, 1983b; Weber, 1994; Thomas et al., 1998). The structural heterogeneities involve scale-lengths of a few to tens of kilometers, with various estimates of velocity fluctuations of a few to 10%. Cormier (2000) has developed the perspective of D″ involving a transition in the heterogeneity spectrum of the lowermost mantle, with D″ having a relatively 'red' spectrum for length scales longer than 50–100 km but comparable strength at short wavelengths relative to the overlying lower mantle. It is plausible that small scale structure also exists on the core side of the CMB, concentrated in topographic highs (e.g., Buffett et al., 2000; Garnero and Jeanloz, 2000; Rost and Revenaugh, 2001).

3. Evidence for chemical heterogeneity

The foregoing synthesis of key concepts and observations about the D″ region indicates that the perspective of a simple thermal boundary layer in a homogeneous lower mantle is inadequate, and greater complexity must be involved. The list of evidence that most strongly points in the direction of chemical heterogeneity in the lower mantle boundary layer is: (1) rapid P and S velocity increases are found at the top of D″ in high and moderately slow velocity regions; (2) abrupt S velocity decreases at the top of D″ are observed to overlie very low velocity regions; (3) acute lateral gradients in structure are observed; (4) ULVZ's are extensively observed at the CMB; (5) strong scattering of short wavelength waves is observed in the boundary layer; (6) S wave velocity vari-

ations disproportionate to P wave velocity variations are observed; (7) the boundary layer has substantial topography at short- to intermediate-scale lengths.

Efforts to explain the D″ discontinuity feature as a relic of cold slab material fail because the thermal structure is expected to be too smoothed (e.g., Sidorin et al., 1999a). A phase change explanation for the discontinuity fails because the feature sometimes involves both increases and decreases in velocity. Explaining the discontinuity as an onset of boundary layer anisotropy is hard to reconcile with the variations in short-wavelength topography and polarity of the discontinuity. Strong lateral gradients in D″ structure are likely to be incompatible with thermal structures alone, and thermally induced subsolidus fluctuations in the properties of a hot boundary layer probably cannot produce the small-scale scattering properties of the boundary layer. If slabs can reach D″ in relatively short descent times, strong gradients could perhaps result (e.g., Tan et al., 2002); however, there is no consensus on whether this occurs.

Thermally induced rigidity variations can produce large shear velocity fluctuations relative to compressional velocites ($R = \mathrm{d}(\ln V_s)/\mathrm{d}(\ln V_p) = 2.7$), but even this cannot match observed decoupling of V_s and V_p. Fig. 5a shows the bulk sound velocity anomaly model obtained by Masters et al. (2000), which represents the unaccounted-for variation of V_p after rigidity and density fluctuations are removed. Note the general anti-correlation with the shear velocity model shown in Fig. 2a; the central Pacific appears to have bulk modulus increases that at least partially offset the reduction in V_p expected from V_s behavior.

This requirement of the existence of bulk sound velocity anomalies is also found in regional studies. We discuss results from one particularly well-characterized region in some detail, as it provides an illustrative example of phenomena that may be regionally common within D″. Fig. 5b indicates the central Pacific SPAC and PPAC models obtained by waveform stacking (Russell et al., 2001), relative to a reference model (PREM-H) for which mid-mantle velocity gradients in PREM are extrapolated through D″ to the CMB. The V_s jump at a depth of 2661 km is +1.7% and the V_p increase is +0.75%. These structures were obtained under the reasonable constraint that the discontinuities in V_s and V_p must be at the same depth. The depth estimate of the discontinuity

(a) Bulk sound velocity, model Sb10l18
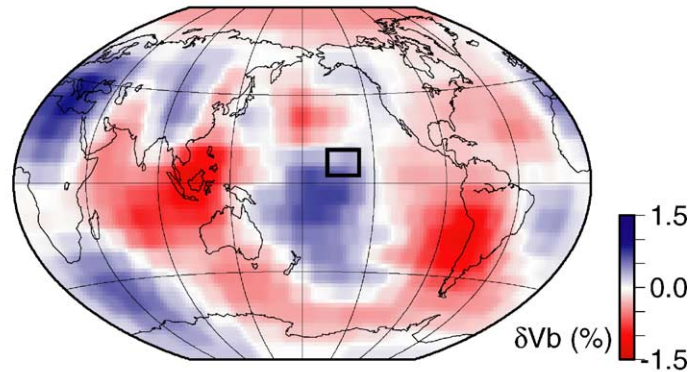
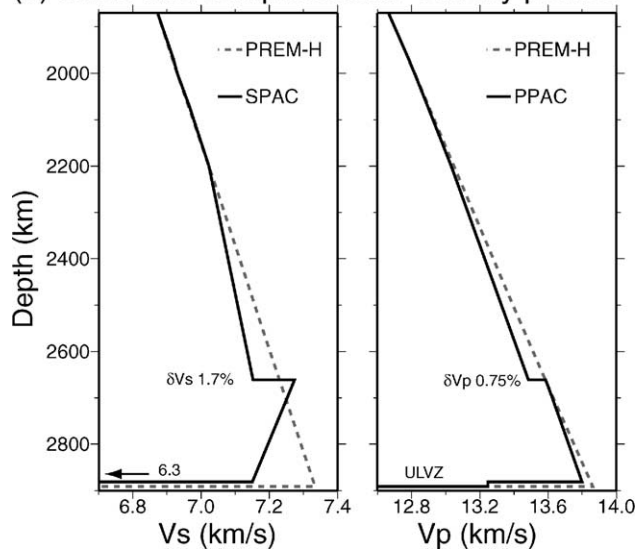## (b) Shear and compressional velocity profiles

Fig. 5. (a) Map of bulk sound velocity (V_b) variations in the D″ region from the tomographic inversion model Sb10l18 of Masters et al. (2000). This model can be compared with the shear and compressional velocity models in Fig. 2 to see that there is an anticorrelation of bulk sound velocity and shear velocity in D″ in the central Pacific associated with the greater reductions in shear velocity relative to those in compressional velocity. The small box indicates the region of a detailed analysis of S and P wave triplication observations by Russell et al. (2001). (b) Models SPAC and PPAC obtained by Russell et al. (2001) for the central Pacific, along with a reference structure (PREM-H) involving a modification of the PREM model of Dziewonski and Anderson (1981) with D″ having the same velocity gradients as in the overlying lower mantle rather than reduced gradients as in PREM. This is viewed as an empirical homogeneous, adiabatic reference model relative to which effects of thermal and chemical heterogeneity in the boundary layer should be assessed. The size of the velocity discontinuities at 2661 km depth are indicated, along with the presence of a 10 km thick ULVZ for models SPAC and PPAC.

trades-off with velocity gradients above and below the discontinuity; placing the discontinuity shallower in the mantle requires V_p to increase within D″ to values above PREM-H, while placing it deeper reduces the V_s gradient to below the critical gradient, which was constrained in this general region by the M1 model

of Ritsema et al. (1997). The V_s jump is significantly weaker than found in models for high velocity regions (Fig. 3). The central Pacific models have a 10 km thick ULVZ, with $V_s = 6.3$ km/s and $V_p = 13.3$ km/s (-14 and -4.4% relative to PREM-H, respectively, with a $+1\%$ bulk velocity anomaly relative to PREM-H). Just

above the ULVZ, $V_s = 7.15$ km/s and $V_p = 13.8$ km/s (-2.5 and -0.4% relative to PREM-H, with a $+1\%$ bulk sound velocity anomaly relative to PREM-H). Assuming the PREM-H density is correct, the rigidity reduction required for the shear velocity just above the ULVZ is -5%, and -26% in the ULVZ. The bulk modulus anomaly in this case is about $+2\%$ at the same depths. The value of R is 6.9 just above the ULVZ, and R is 3.2 within the ULVZ, in both cases exceeding the value for thermally-induced rigidity variations alone. The bulk velocity anomaly is consistent with that inferred from global tomography, about $+1\%$ in this region (small box in Fig. 5a). While there is non-uniqueness in the models, the strong V_s reductions and negative gradient in the boundary layer are supported by several studies (e.g., Bréger et al., 2001; Ritsema et al., 1997) while P diffraction modeling supports the positive V_p gradient in this region (Young and Lay, 1989). Chemical heterogeneity appears to be the only viable way to account for the strong relative variations of V_s and V_p in this region, even if partial melting is allowed, as discussed below. Wysession et al. (1999) provide similar evidence for anomalous V_p/V_s behavior in the north Pacific based on diffracted wave studies.

Topographic variations in the boundary layer, mapped as variable depth of D″ reflectors from velocity increases or decreases are also difficult to account for by any model other than a CBL. Large horizontal scale variations in shear wave discontinuity depths of from 130 to 450 km have been reported (e.g., Kendall and Shearer, 1994; Wysession et al., 1998), and 100 km variations of topography on shorter-scales of 200–300 km (Fig. 6a) are present (e.g., Lay et al., 1997, 2004; Avants et al., 2004; Thomas et al., 2004). Such large topography is unlikely to be explained by a phase change, or by the notion of a transition in anisotropic fabric within D″.

Fig. 6b is a schematic of the thick, low shear velocity region under the southern Atlantic and Africa, which has a horizontal scale of several thousand kilometers. This feature has an abrupt shear velocity decrease of -1 to -3% near 250–300 km above the CMB, with average V_s anomalies across the D″ layer being on the order of -3 to -5% relative to PREM (about -1% more than this relative to PREM-H) (Wen et al., 2001; Wen, 2001; Ni and Helmberger, 2003a,b). These average velocities are significantly lower than for the cen-
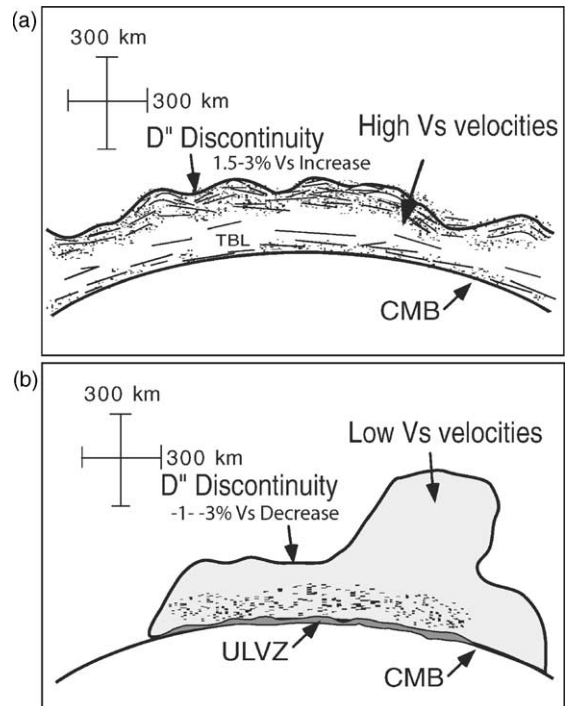

Fig. 6. Schematic attributes of seismic models for D″ supporting the notion of chemical heterogeneity in the region. (a) Both large-scale and small-scale topography is observed on the shear wave discontinuity at the top of the boundary layer in high velocity regions. These areas also show an increase in shear wave splitting associated with wave energy that penetrates into the layer. Undulations of 50–100 km over lateral length scales of 250–300 km are reported by Lay et al. (1987), Thomas et al. (2004) and Avants et al. (2004). This is very hard to reconcile with a phase change or with fabric gradients into the boundary layer (stippling suggests the development of anisotropic structure). (b) Large scale low-velocity regions found at the base of 'superplumes' beneath the south Pacific and the south Atlantic/Africa regions have abrupt velocity reductions about 250 km above the CMB (the same depth as the velocity increase in fast areas like in (a)). The lateral boundaries of these regions appears to be quite abrupt, on the order of tens of kilometers, which is very difficult to reconcile with simple thermal variations. Portions of the slowest boundary layer under Africa appear to extend upward into the mid-mantle perhaps as much as 800–1000 km above the CMB (e.g., Ni and Helmberger, 2003a,b).

tral Pacific sampled in Fig. 5, but are comparable to estimates of shear velocity reductions under the core of the south Pacific 'superplume' region (e.g., Tanaka, 2002). The models of Wen et al. (2001) and Wen (2001) favor strong negative shear velocity gradients within the D″ layer, with velocities decreasing from

−1 to −9 to −12% across the boundary layer, with no pronounced ULVZ at the base of the layer across most of the region. Ni and Helmberger (2003a,b) favor a uniform −3% drop of shear velocity throughout the layer with more extensive regions of ULVZ, so the precise velocity structure is still being determined. It seems remarkable that the depth range around 250 km above the CMB exhibits 2–3% increases in high shear velocity regions, 1–1.5% increases in moderately slow velocity regions, and −1 to −3% decreases in the slowest velocity regions. There are certainly strong lateral gradients on the margins of these thick low velocity regions that again seem incompatible with thermal variations alone, without a superimposed chemical or melting effect (e.g., Ni et al., 2002; Wen et al., 2001). The localized upward extent of these low velocity regions to as much as 1000 km above the CMB may be viewed as dramatic topography on the boundary layer, although continuity of the structures is not uniquely demonstrated. Even in the mid-mantle the lateral gradients remain strong: once again, a first-order observation that is difficult, if not impossible, to explain by simple thermal gradients (e.g., Ni et al., 2002).

There is some indication that density heterogeneity exists at the base of the mantle based on analysis of normal modes, and that it may be anticorrelated with shear velocity (and hence, possibly correlated with bulk velocity models like in Fig. 6), favoring chemical heterogeneity (Ishii and Tromp, 1999), but this remains a topic of much uncertainty (e.g., Romanowicz, 2001; Kuo and Romanowicz, 2002). Resolving this is critical for assessing whether low velocity features in 'superplume' regions are buoyant or not. Testing for the presence of a global high density layer at the base of the mantle using normal modes is possible, but requires linear perturbation theory which may be invalidated by the very strong variations in material properties in the ULVZ.

Recent experiments on the spin-state of Fe at lower mantle pressures (Badro et al., 2003) provides support for a long standing idea (e.g., Gaffney and Anderson, 1973) that the presence of low-spin Fe^{2+} in the lower mantle could dramatically affect composition of the deep mantle. A pressure-induced transition from high-spin to low-spin Fe is observed for ferropericlase $(Mg_{0.83}Fe_{0.17})O$ at pressures in the 60–70 GPa pressure range, corresponding to depths near 2000 km in the lower mantle. The lack of such a transition in silicate perovskite suggests that Fe will concentrate into the ferropericlase structure, leaving the perovskite almost iron-free. This has possible implications for viscosity, electric conductivity, and thermal conductivity of the lowermost mantle (Badro et al., 2003). While this transition may occur above D″, leading to multiple layering of the lower mantle, it is also possible that it occurs deeper and is directly coupled to anomalous chemistry and properties of D″.

It seems clear that chemical heterogeneity must be present in the D″ boundary layer, just as it is in the surface boundary layer. The variable nature of the seismic observations (Table 1) appears to preclude end-member versions of the CBL model (Fig. 1c), chemical dregs model (Fig. 1d), slab graveyard model (Fig. 1e) or phase change model (Fig. 1f). The need to account for the seismic observations discussed above prompts the hybrid model of Fig. 1g, with slabs graveyards, mounds of low velocity heterogeneities under upwellings, and possibly including a superimposed phase change to reconcile all observations. But an added dimension needs to be considered prior to embracing such hybrid models: the possibly dominant effect of partial melting of the boundary layer.

4. Partial melting in D″ and its effects

The identification of the ULVZ with partial melting of the lowermost mantle appears to be quite robust, as both the estimated magnitudes and ratios of the shear to compressional velocity decrements within this layer are entirely consistent with the ~3 to 3.5:1 V_s-to-V_p reduction ratio expected for partial melting (e.g., Williams and Garnero, 1996; Berryman, 2000). The frequently observed ~10% V_p decrement associated with the ULVZ and more poorly constrained ~30% V_s velocity decrease (see Garnero et al., 1998, for discussion) imply melt fractions of between ~6%, for 1:100 aspect ratio films of melt and ~30% for spherical melt inclusions (Williams and Garnero, 1996; Berryman, 2000). While velocity decrements are smaller within the thicker D″ layer, the V_s-to-V_p fluctuations can be very large, sometimes exceeding those expected for melting effects alone as discussed above. The presence of chemical heterogeneity accompanying (and being accentuated by) the melting makes it challenging to estimate melt fractions within

Table 1
Seismological characteristics of the lower mantle boundary layer

Feature	Characteristics	Common interpretation(s)	Issues
Large-scale V_s and V_p heterogeneity	±3–4% V_s, ±1% V_p, degree 2 dominance ±1% bulk sound velocity circum-Pacific high velocity C. Pacific/S. Atlantic low velocity strongest in lowermost 300–400 km	Thermal origin in large-scale flow regime, slabs cause high velocity, chemical heterogeneity in slow regions, superplumes	Shallow connectivity, control from above or below, R values larger than 2.7
D″ discontinuities	+1.5 to +3% in V_s, +0.5 to +3% in V_p 0–30 km thick transition zone in high velocity regions, intermittent, -1.0 to -3% in shear velocity in low velocity regions, depth varies from 130 to 300+ km above CMB	Slab related, phase change, chemical boundary, gradient in fabric, gradient in heterogeneity, scattered feature	Small-scale topography sharpness hard to explain thermally, no candidate phase change, anisotropy relationship
D″ anisotropy	Large scale 1–2% in boundary layer, primarily with VTI symmetry in high velocity regions, variable strength, symmetry in low velocity regions. Absent from average regions	LPO in MgO, SPO in chemical/melt, lamellae from sheared chemical anomalies	Vertical distribution, relationship to large-scale structure, relationship to discontinuities
D″ scattering	1–10% rms heterogeneity in boundary layer, 10–100 km scalelengths related to ULVZ, change in spectrum relative to mid-mantle	CMB topography, chemical/melt variations, thermal explanation not likely without melt	Spectrum, relationship to large-scale structure, relationship to anisotropy
ULVZ	5–10% V_p reductions, 10–30% V_s reductions, 5–40 km thickness sometimes sharp onset (<few km) best developed in low velocity regions, but present in high velocity regions widespread	Partial melt in basal boundary layer, piles of chemical heterogeneities, melting implies chemical heterogeneity	Relationship to large-scale structure, geometry: piles or layers, melting implies chemical heterogeneity

D″, but it is presumably bounded by the levels found in ULVZs.

Perhaps, the most peculiar aspect of partial melt in the basal layer of the mantle is its apparent coexistence with abundant solids at this depth, as demonstrated by the depressed, but still robust, shear wave velocity observed within the ULVZ. In short, melt and solid appear to coexist with one another at spatial dimensions far less than those of seismic waves, without the melt (if denser than the coexisting solids) simply percolating to depth and forming a pure melt layer overlying the core. Alternatively, if the melt is buoyant, it would be expected to either rise to its depth of neutral buoyancy, or to resolidify during adiabatic ascent. This juxtaposition of solids and liquids thus implies that one of several possible effects occur within the ULVZ: (1) the melt is not interconnected, and thus is physically

unable to efficiently drain from the surrounding solids; (2) the melt density closely matches that of the surrounding solids, so the buoyancy forces on the melt are insufficient to allow the melt to efficiently percolate; and/or (3) the average vertical convective velocity within the ULVZ is substantially greater than the velocity of melt percolation. We view the first alternative as unlikely: the results of Bulau et al. (1979) show that even for dihedral angles of 180°, the critical melt fraction needed to produce an interconnected network is near 30%. Thus, although essentially no textural data exist on melts at deep mantle conditions, we would anticipate from the melt fraction inferred to be present in the UVLZ that if spherical inclusions of melt are present, the liquid is likely to be interconnected, and melt segregation is expected. This need not be the case throughout the boundary layer in general.

There are two (non-exclusive) alternatives: melts that are essentially neutrally buoyant and/or a region that is dynamically sufficiently active that it can advect partially molten material upward (or downward) faster than melt can drain out of the material. In either instance, *there is no a priori reason that melt within D″ should be confined to the ULVZ*. Naturally, the location of the solidus relative to the laterally varying geotherm is the most critical parameter with respect to the presence of melt within D″: we simply note that both abundant impurities/chemical heterogeneities (whether core-derived or otherwise) and laterally varying temperatures are expected within D″. Each of these effects would be expected to favor the generation of melts (probably at low melt fractions) at depths substantially shallower than the ULVZ. Indeed, the geophysical parameter that is perhaps most demonstrative of the presence of melt, Poisson's ratio, shows essentially a monotonic increase in depth within the region of D″ underneath the Central Pacific (Russell et al., 2001), producing a trajectory through D″ that ultimately coincides with the markedly high value of Poisson's ratio observed within the ULVZ (Fig. 7b). Fig. 7a shows the change in Poisson's ratio for 2 somewhat extreme melt geometries (e.g., Williams and Garnero, 1996): spherical melt inclusions and 1:100 aspect ratio films. Clearly, for the film, amounts of melt of less than 0.5% are required to generate the elevation of Poisson's ratio observed in the bulk of D″ in this likely relatively hot zone. This does not preclude the existence of strong gradients in melt fraction that could give rise to the sharpness of the ULVZ onset at the base of D″ in this region.

Would such melt be neutrally buoyant within D″, or would its presence require that it be either descending or ascending, and/or that it be dynamically advected? There is ample evidence that the density contrast between isochemical silicate liquids and solids at very high pressure conditions is small: shock studies have indicated that $(Mg,Fe)_2SiO_4$ melts under shock-loading with less than a 1% volume change (Brown et al., 1987). Similarly, both static sink–float experiments and shock experiments on silicate liquids indicate that small density changes on melting (order 0.5% or less) are expected (Rigden et al., 1989; Ohtani and Maeda, 2001). Thus, chemical effects (such as iron partitioning) and even, prospectively, differences in thermal expansions between solids and liquids
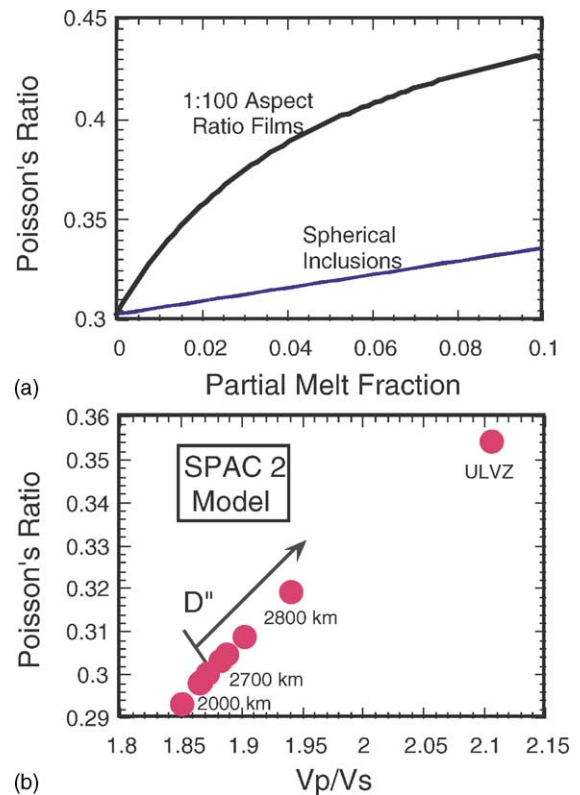

Fig. 7. (a) Variation in Poisson's ratio as a function of partial melt fraction for melt distributed in thin films, with aspect ratio 1:100 and in spherical inclusions within D″ material. Melt and solid elastic parameters used are described in Williams and Garnero (1996). (b) Observed Poisson ratio variations associated with the shear and compressional models in Fig. 5b plotted as functions of the V_p/V_s ratio. The increase in Poisson's ratio across the boundary layer indicated by the velocity models implies an increase in partial melt fraction with depth. Depending on the melt geometry, maximum melt fractions may be as large as 15% in the ULVZ or as small as 2%.

could play nearly as significant roles in determining the buoyancy of silicate melts at CMB conditions as the volume of fusion. Fig. 8 shows an illustrative example from calculations (Moore et al., 2004) that incorporate available constraints on liquid–solid partitioning of iron in silicates at high pressure (see Knittle, 1998, for a review), and assumes that (1) silicate perovskite is the solidus phase at CMB conditions (e.g., Williams, 1990; Ito and Katsura, 1992), (2) the volume change on fusion is 0.5%, (3) the thermal expansion of the liquid exceeds that of coexisting solids by $8 \times 10^{-6} \, K^{-1}$ at CMB pressures and
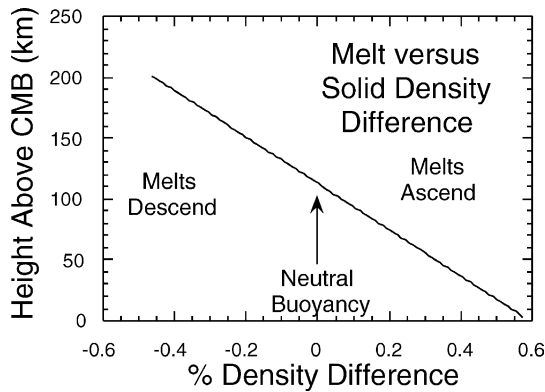
Fig. 8. Representative calculation of the possible density contrast between silicate melt and coexisting solids within a superadiabatic thermal gradient across the D″ layer. Specific parameters for the calculation are given in the text. In the presence of a strong, superadiabatic thermal gradient across D″, partial melting involving a small density change on melting may be close to neutrally buoyant, and hence distributed within the boundary layer rather than ponded at the base of the mantle.

temperatures, and (4) the superadiabatic temperature change across D″ is 1500 K, distributed linearly over a 300 km depth range. Our intent here is to simply illustrate that parameter sets exist that can readily produce melts that are neutrally buoyant within D″, as well as positively (or negatively) buoyant at other depths. The crucial point is that there are quite delicate trade-offs between volume changes on fusion, iron partitioning, and thermal effects for melts at these depths in the planet. We thus anticipate that, depending upon their precise chemistries, melts within D″ could be either negatively, positively or neutrally buoyant. Thus, at any given time, a suite of melts of varying chemistry and dynamics could exist within or throughout this layer, with complex mixing, contamination, crystallization, and zone refining effects. To go beyond this level of understanding, such as developing a melt percolation or compaction model, requires knowledge of so many poorly constrained parameters that we have not attempted calculation of melt percolation velocities at this time.

The evolution of D″ as a whole may be modulated by magmatic processes, with small quantities of partial melt in the upper few hundred kilometers of this layer, and large quantities at its base. The effect of such partial melting on the rheology of D″ is likely profound: under upper mantle conditions, even small quantities of partial melt depress viscosity substantially (Hirth and Kohlstedt, 1995; Mei et al., 2002). The magnitude of this melt-associated viscosity decrement is difficult to assess, as it is sensitive to melt geometry and grain size effects, and particularly whether flow of the solids occurs in the diffusional or dislocation creep regimes (Mei et al., 2002). The first-order observation is, however, that melt would be expected to weaken the aggregate material within D″ relative to the viscosity inferred for purely solid-state boundary layer material, and we would expect advective velocities in this layer to be greater than those within completely solid mantle material. Improved understanding of melt densities, melt distributions, and viscosity of the matrix are all critical areas for further research.

Apart from its dynamical effects, the presence of this melt is likely to have both enhanced chemical interactions with the core through time, and may be indicative of an enrichment of this zone in elements that are incompatible in mantle minerals near CMB pressures and temperatures. Thus, iron-enrichment of D″ may have occurred through both (perhaps) melt descent from above (e.g., Knittle, 1998), and through core interactions from below. Moreover, enrichment of radiogenic elements in D″ (and perhaps particularly at its base) is generally consistent with a magmatic evolution for this boundary layer. Such radiogenic element enrichments within the boundary layer have been suggested as a mechanism to reduce the heat flux out of the outer core (Buffett, 2003), although thermal stratification of the mantle is an alternative. Our association of negative velocity gradients and increased Poisson's ratio with partial melting (Fig. 7) implies that D″ is a layer whose chemistry and dynamics are governed by magmatic processes: processes that have in turn given rise to a chemically distinct layer through time.

5. A TCBL with partial melting

The profound effects of partial melting on seismic velocities noted above and the logical appeal of invoking partial melting in the mantle's lowermost boundary layer where the temperatures exceed those anywhere else in the mantle, prompts an attempt to 'simplify' our conceptual notions of processes occurring in the D″ region. While our knowledge of the near-surface boundary layer indicates that there is no

particular reason to expect a simple explanation for D″, the potential effects of partial melting may enable this. Given the evidence summarized above for existence of chemical heterogeneity and partial melting in the boundary layer, we invoke a very plausible notion for an irreversibly chemically differentiated planet like Earth: there is a globally extensive chemically distinct layer at the base of the mantle (Fig. 9). This results in a thermo-chemical boundary layer throughout D″, which behaves as a separate mantle layer dynamically. The intrinsic (above solidus) bulk material properties of the layer are slightly higher density (1–2%), shear velocity (2–3%), and P velocity (1–2%) than the overlying mantle, but these properties are strongly modulated by lateral variations in partial melt, temperature, and composition. The mid-mantle is undoubtedly undergoing large-scale convection, with broad regions of downwelling that appear to correspond to areas of recent lithospheric subduction, and return flow involving upwellings with comparably large scale lengths. Embracing a top-down tectonics notion (e.g., Anderson, 2001), the high viscosity, sluggish mid-mantle controls the D″ thermo-chemical boundary layer thermally; slab-cooled downwelling regions in the mid-mantle will induce high heat flow out of the boundary layer, lowering its average temperature, whereas warm areas of upwelling return flow will have lower heat flow out of the boundary layer, allowing its internal temperature structure to be warmer. Essentially, the upper mantle history of plate subduction (e.g., Lithgow-Bertelloni and Richards, 1998) induces (or is controlled by) large scale-patterns in mid-mantle flow that in-turn induce and control large-scale patterns in D″ thermal structure. The high viscosity of the lower mantle sustains the long-term patterns affecting D″, which may thus decouple from surface tectonic processes. Large-scale dynamic topography on the boundary layer is expected, with downwelling regions in the mid-mantle thinning the boundary layer and upwellings thickening it. Observed variations of discontinuity depth of several hundred kilometers on large scale are at least qualitatively consistent with this; the thickest regions of D″ are in low velocity areas with overlying mid-mantle low velocities that likely involve upwellings. Small-scale convection is expected within the TCBL, which should impart small-scale topography on the boundary layer and on the CMB. An alternate scenario of bottom-up control of the system, with variable thermal structure in D″ as a result of varying heat production and upwelling can also be considered, but it is more difficult to imagine a low viscosity, hot boundary layer sustaining very large scale structure over long periods of time unless there is strong internal chemical heterogeneity in the layer (in which case, the notion of a layer becomes more problematic than viable).

The compositional anomaly in the boundary layer is unknown, but it may involve dense oxides concentrated there during accretion and core formation or early subduction, or iron-rich/reduced core–mantle reaction products accumulated over time. This chemistry of melt within the bulk of D″ will likely be that of a eutectic system, probably with a lower solidus curve than the overlying mid-mantle (under the assumption that adding chemical components leads to greater potential for a depressed eutectic). The key issues from the perspective of the phase equilibrium of the lowermost mantle are: (1) which additional, non-trace chemical components might serve to depress the solidus temperature within D″ and in the ULVZ from that of the overlying mantle; and (2) how much has the ULVZ depleted the overlying mantle in its most incompatible components? Each of these issues bears critically on the degree of chemical stratification with D″, the interplay between magmatic processes and the evolution of chemical stratification in this zone, and the level of variability of melt chemistry within D″. Just as the solidus in D″ may differ from that in the overlying mantle due to the presence of additional, abundant chemical components, the solidus within the ULVZ might differ from that in D″ if (for example) hydrogen has been sequestered through time within the ULVZ, and been depleted within the bulk of D″. The underlying uncertainty here lies in the degree to which D″ has been zone-refined through time by magmatic processes. The first-order observation of ULVZs at the base of the boundary layer suggests that partial melting takes place in the rapid temperature increase over the lowermost few tens of kilometers in hot regions: yet, the rapid temperature increase need not necessarily be a prerequisite for the presence of abundant melt at this depth. Chemical effects/heterogeneity might also be sufficient to produce abundant basal melt. Indeed, hot regions within D″ could also be those that have had their incompatible elements most efficiently extracted into a basal layer. The relative effects of chemistry
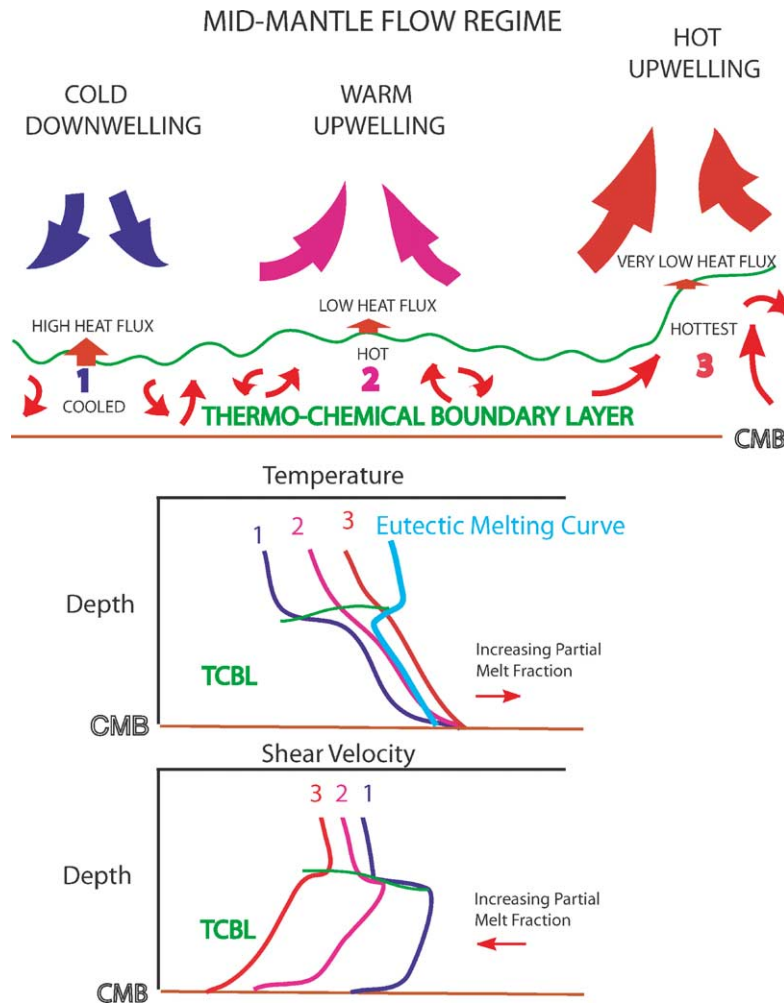
Fig. 9. Schematic illustration of the D″ model involving a thermo-chemical boundary layer (TCBL) comprised of a compositionally stratified, dense, hot layer at the base of the mantle. This region is overlain by a mid-mantle dynamic system involving downwellings and upwellings, largely driven from above by cooling of downwelling slab material beneath subduction zones. The relatively cool mid-mantle regions produce high heat flow out of the TCBL, cooling the layer locally (1). Warm upwelling regions in the mid-mantle lead to low heat flow out of the boundary layer, and it heats up (2), with the warmest areas of the TCBL possibly destabilizing somewhat and rising above the D″ region (3). Large-scale topography on the TCBL is induced by the mid-mantle flow, and small scale boundary layer convection within the TCBL induces small scale topography on the TCBL. The thermal profile in each of these regions is indicated in the middle panel, with a double thermal boundary layer developing at the top and bottom of the TCBL, under the constraint of uniform CMB temperature. The eutectic solidus decreases in the TCBL and is exceeded in the hottest regions (3) over the entire layer, partially exceeded in the warm regions (2) and only exceeded at the very base of the mantle in the cooler regions. The resulting partial melt causes strong shear velocity reductions, reducing the size of the shear discontinuity at the top of D″ (2), or even causing an abrupt decrease. Three to five percent melt fractions produce the 5–6% velocity reductions, with larger melt fractions in the basal thermal boundary layer of 10–30% causing pronounced ultra low velocity regions. Stability of the TCBL requires a density increase of 1% or more, while the existence of the shear and compressional velocity discontinuities requires increases in rigidity and bulk modulus of material in the TCBL. Partial melt in the TCBL must be neutrally or negatively buoyant.

and temperature in the generation of partial melting in the lowermost mantle remain uncertain, but the strong likelihood is that the two are critically linked; magmatic differentiation through partial melting is likely to be as important as we know it to be near the surface. Viscous shear heating may also contribute to melting in the ULVZ (e.g., Steinbach and Yuen, 1999), with melting in turn reducing the viscosity and affecting the strain localization.

We postulate that the hottest regions, thermally insolated under strong mid-mantle warm upwellings, exceed the solidus throughout the boundary layer, leading to significant partial melt fractions right up to the top of D″ (case 3 in Fig. 9). This is consistent with the ideas of Wen et al. (2001), but they invoke the notion of a localized chemical anomaly rather than a TCBL. Even modest melt fractions of order 0.5% can cause shear velocity decreases of −4 to −6% (assuming that the melt is distributed in films of 100:1 aspect ratio), reversing the sign of the shear velocity contrast at the top of the layer from +3% to −1 to −3%. The discontinuity is on-average around 300 km above the CMB in this region, but may shallow by hundreds of kilometers under the localized region of strongest mid-mantle upwelling. The strong lateral gradients in velocity on the margins of the low velocity regions (e.g., Wen et al., 2001; Wen, 2001) likely involve lateral intersections with the solidus comparable to the radial intersection, with this either being enhanced by lateral chemical variations within the layer or simply as a consequence of the non-linear affect of the onset of partial melting on the seismic velocity field. The strong radial gradients with depth found in the low velocity region models of Wen et al. (2001) and Wen (2001) are consistent with the notion of strong increase in degree of partial melting across the hot thermal boundary layer, and relative insignificance of ULVZ at the base of these thick very low velocity regions.

The central Pacific region shown in Fig. 5 corresponds to an intermediate region for which the D″ shear velocity discontinuity is still positive (albeit reduced due to presence of small melt fraction), and a strong negative gradient in shear velocity extends down to the ULVZ (case 2 in Fig. 9). The velocity discontinuity is on-average near 230 km depth above the CMB in this region, which is not very different from that in the circum-Pacific regions, but it has substantial small-scale variations. For P velocity in this region to remain relatively high with a positive velocity gradient, variation in chemical properties with depth across the boundary layer must be invoked chemical partitioning that accompanies the melt may modify the aggregate bulk modulus, accounting for the enhanced detectability of a bulk sound velocity anomaly in low velocity regions.

The lower panel of Fig. 9 summarizes the range of shear velocity structures predicted for this form of partial melt fraction varying TCBL, which matches the range of observations, at least qualitatively. The large-scale pattern on the thermal structure leads to the large-scale velocity heterogeneity observed at the base of the mantle as well as the large topography of seismic discontinuities at the top of D″. Attempting to quantify the thermal variations required to produce the observed velocity variations is fraught with many uncertainties about thermodynamic parameters at the base of the mantle (e.g., Trampert et al., 2001). This holds as well for quantification of the dynamical regime. For example, if thermal expansion coefficients are very small, as expected, the buoyancy effects of temperature variations may be directly offset by development of slightly dense melt distributions.

Survival of such a TCBL as a coherent layer is necessary to avoid invoking hybrid models that rely on slab continuity to the CMB, or a hypothetical phase change to yield the shear velocity increase in areas where TCBL is swept aside. Early geodynamical calculations suggest that the TCBL must have a density contrast of 3–6% or more to avoid disruption, and this has been the main reason for downweighting the notion of a uniform chemical layer (e.g., Sidorin and Gurnis, 1998). However, as discussed above, this argument is not particularly compelling and more recent calculations suggest that very little density anomaly may be required for a TCBL to survive in a layered convection system (Zhong and Hager, 2003), particularly if there is low viscosity in the deeper layer (Namiki, 2003). The inference of diffuse, large-scale mid-mantle velocity heterogeneities found in global tomography being slabs structures has many caveats (e.g., Scrivner and Anderson, 1992; Ray and Anderson, 1994; Wen and Anderson, 1997). Very few, if any, of such images are continuous down to the CMB, yet the numerical models in which downwellings sweep aside CBL often involve thousands of kilometers of slab material piled up in the deepest mantle,

for which there is no clear tomographic evidence. It is very unclear whether such models are steady state, with the variability between calculations suggesting the contrary. The possibility of mid-mantle stratification could greatly buffer topography on a dense D'' TCBL along with preventing significant penetration of high viscosity downwelling to the boundary layer. The many parameters entering into deep slab penetration models include uncertain amounts of deformational heating as slabs fold, buckle, and deform due to difficulties in penetrating through the transition zone phase changes and into the high viscosity lower mantle. While the existence of large-scale circulation is indeed an element of the TCBL model in Fig. 9, essential for imparting a large-scale pattern to the TCBL thermal structure (and hence on the seismic velocity structure), one needs to appeal to remarkable slab durability down to the CMB to have the flow displace and push aside a dense TCBL in D''. Certainly, induced topography (mid-mantle downwellings will thin the boundary layer whereas upwellings will thicken it; possibly involving hundreds of kilometers of topography) and some (perhaps significant) entrainment over time will take place, but we view the key impact of the mid-mantle regime as being the source of long-term thermal control on the boundary layer downwellings in the mid-mantle are very likely to impart stresses in the cooled regions of D'', which will favor the development of LPO, whereas regions with extensive partial melting presumably have strong shear flows that abet development of SPO (e.g., McNamara et al., 2002; Moore et al., 2004). It appears that the anomalous chemistry and state of the TCBL are more conducive to formation of LPO or SPO than in the overlying mantle.

A long-enduring TCBL at the base of the mantle provides many attractive avenues for accounting for geochemical heterogeneities in the mantle, depending on how the TCBL evolved. If it evolved over time by segregation of melts or recycled crust, it is of particular interest to geochemists, whereas an accumulation of core–mantle interactions is perhaps less important for geochemical models. Coupled to this question of the mechanism of TCBL formation is the temporal evolution of the system in a slowly cooling Earth. Is the current TCBL a thinned residue of a formerly thicker layer that has been eroded, or is it an actively growing layer with accumulating chemical

heterogeneity? Various evolutionary scenarios can be considered, but all are poorly constrained. No clear observational attribute yet resolves this issue, and perhaps the greatest promise will be in the imaging of downwelling and upwelling regions in the mid-mantle to much higher precision than currently provided by seismic tomography. Topography and thermal variations in the upper boundary layer of the TCBL may help to pin upwellings in the mid-mantle (Jellinek and Manga, 2002), along with providing sampling of trace element reservoirs, particularly for those with chemical signatures of core components (e.g., Brandon et al., 1998; Meibom et al., 2002; Meibom and Frei, 2002). Even though the most extensively heated and partially molten regions of D'' may be very thick, the boundary layer will not completely detach (if it is to survive over long periods of time), and thus, the presence of the TCBL will not necessarily augment heat transport to the surface as speculated for ideas about superplumes (e.g., Romanowicz and Gung, 2002). Indeed, the heat transfer across the double thermal boundary layer of the TCBL is not readily quantified, for viscosity reductions due to partial melting will compete with possible negative buoyancy of the melt in terms of how the small-scale boundary layer dynamics affect overall heat flow. The complexity of such systems is just beginning to be addressed (e.g., Namiki and Kurita, 2003). Consideration of the long-term evolution of a partially molten boundary TCBL at the base of the mantle is left for future work.

6. Conclusions

Our synthesis of observations and modeling studies of the boundary layer at the base of the mantle leads us to propose a conceptual model for the region that is simpler than emerging hybrid models. The D'' region may be a compositionally stratified layer, for which the solidus lies below the uniform CMB temperature. This gives rise to partial melting in the lowermost thermal boundary layer, with lateral variations in the melt fraction within the layer arising due to large-scale lateral variations in the temperature structure across the boundary layer. These variations are sustained by top-down mid-mantle thermal convection, with cooled regions of downwelling inducing high heat flux and

cooling of the boundary layer, leaving most of the material sub-solidus. Warm regions of mid-mantle upwelling cause increase of temperature in the boundary layer and more extensive partial melting, even to the top of layer. The strong effect of partial melt on seismic velocity modulates the intrinsic (subsolidus) velocity increase of the high bulk modulus, high rigidity, and somewhat higher density material in the boundary layer, leading to variations in the strength and sign of the velocity contrast across the top of the layer along with strong variations in velocity gradients across the boundary layer. Dynamic stresses from overlying flow and small-scale convection within the boundary layer impart fabrics to the structure that give rise to scattering and anisotropy of the boundary layer as well as small-scale topography on the upper velocity discontinuity. The most extensively partially melted regions of the boundary layer may develop sufficient thermal buoyancy to overcome the density increase of the layer, leading to substantial thickening of the boundary layer beneath warm mid-mantle upwellings. Neutral- or negative-buoyancy of melts in the boundary layer is implicit, along with a sufficient density anomaly to have the thermo-chemical boundary layer survive depleting entrainment over time. Future dynamical analyses of such a partially melted thermo-chemical boundary layer can establish whether this relatively simple model indeed provides an explanation for the panoply of seismological and geochemical observations. Extensive work on the material properties, phase equilibria and eutectic behavior of high pressure assemblages that may exist in D″ is also needed.

Acknowledgements

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