#### Geodynamics of Earth's Deep Mantle

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Geology is the study of pressure and time. That's all it takes really, pressure, and time. That, and a big goddamn poster.

 $--Ellis \ Boyd \ `Red' \ Redding, \ The \ Shawshank \ Redemption$ 

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### Abstract

Seismic tomography and waveform modeling reveal several prominent structures in the Earth's lower mantle: (1) the D" discontinuity, defined by a seismic velocity increase of 1–3% about 250 km above the core-mantle boundary (CMB), (2) Ultralowvelocity zones (ULVZs), which are thin, isolated patches with anomalously low seismic wavespeed at the CMB, and (3) two large, low-shear velocity provinces (LLSVPs) beneath Africa and the Pacific Ocean. The geodynamics of these structures are investigated using numerical convection models that include new discoveries in mineral physics and recent insight from seismology. In addition, I assess the influence of an iron spin transition in a major lower mantle mineral (ferropericlase) on the style and vigor of mantle convection.

A phase change model for the D" discontinuity produces significant thermal and phase heterogeneity over small distances due to the interaction of slabs, plumes, and a phase transition. Perturbations to seismic arrivals are linked to the evolutionary stage of slabs and plumes and can be used to determine phase boundary properties, volumetric wavespeed anomaly beneath the discontinuity, and possibly the lengthscale of slab folding near the CMB.

I simulate convection within D" to deduce the stability and morphology of a

chemically distinct iron-enriched ULVZ. The chemical density anomaly largely dictates ULVZ shape, and the prescribed initial thickness (proxy for volume) of the chemically distinct layer controls its size. I synthesize the dynamic results with a Voigt-Reuss-Hill mixing model to provide insight into the inherent seismic trade-off between ULVZ thickness and wavespeed reduction.

The dynamics of the LLSVPs are investigated using global 3-D models of thermochemical structures that incorporate paleogeographic constraints from 250 Ma to present day. The structures deform and migrate along the CMB, either by coupling to plate motions or in response to slab stresses. Slabs from Paleo-Tethys and Tethys Ocean subduction push the African structure further to the southwest than inferred from tomography. Dense and viscous slabs can severely compromise the stability of thermochemical structures with a high bulk modulus at the CMB.

Finally, I explore the consequences of the intrinsic density change caused by the  $Fe^{2+}$  spin transition in ferropericlase on the style and vigor of mantle convection. The transition generates a net driving density difference for both upwellings and downwellings that dominantly enhances the positive thermal buoyancy of plumes in 2-D cylindrical geometry. Although the additional buoyancy does not fundamentally alter large-scale dynamics, the Nusselt number increases by 5–10%, and vertical velocities increase by 10–40% in the lower mantle. Advective heat transport is more effective and temperatures in the CMB region are reduced by up to 12%.

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# Chapter 1 Introduction

Unveiling the nature of the deep Earth demands a multidisciplinary approach and there are exciting new research directions at the intersection of mineral physics, seismology, and geodynamics. Seismic methods provide the most comprehensive sampling of the mantle and constrain wavespeeds, the sharpness of features, and the geographical distribution of heterogeneity. The dominant lower mantle minerals are aluminous ferromagnesian silicate perovskite, (Mg,Fe,Al)(Si,Al)O<sub>3</sub>, and magnesium iron oxide, (Mg,Fe)O, which occupy about 75 and 15 volume percent of the lower mantle, respectively (*Ringwood*, 1991). Recent advancements in mineral physics, notably diamond anvil cell technology, are enabling experimentalists to determine the wavespeeds and material properties of these phases to compare with seismic and dynamic inferences. New discoveries in the behavior of (Mg,Fe)SiO<sub>3</sub> and (Mg,Fe)O at extreme conditions motivate the research presented in three chapters of this thesis. Convection calculations elucidate how mass and heat transfer influence the morphology, stability, and longevity of structures in the mantle.

The core-mantle boundary (CMB) (3300–4400 K) separates the liquid iron-rich outer core from the solid silicate mantle at  $\sim 2890$  km depth (e.g., *Lay et al.*, 2008).

This interface defines the largest contrast in material and dynamic properties in the Earth. The high viscosity subsolidus lower mantle deforms by slow, creeping flow ( $\sim 1 \text{ cm/yr}$ ) (e.g., *Davies*, 1999), whereas the inviscid outer core is rapidly convecting ( $\sim 1 \text{ mm/s}$ ) (e.g., *Glatzmaier and Roberts*, 1995). Heat transfer across the CMB occurs predominantly by conduction and mass exchange is negligible. Total heat flow from the core to the mantle controls the power available to drive the geodynamo, the cooling rate of the core, and the growth rate of the inner core. The outer core boundary behaves as an isothermal free-slip surface to mantle convection because of the vastly different timescales associated with core and mantle dynamics.

Seismic waveform modeling elucidates the fine-scale features of the CMB region through the analyses of wavetrains that arrive before or after well-identified reference phases on seismograms. These wavetrains are sometimes visible on individual seismograms or may require data stacking to increase the signal-to-noise ratio. Arrivals with neighboring raypaths can be analyzed together to eliminate source dependency and constrain mantle heterogeneity along a particular segment of a propagation path. Waveform modeling can often distinguish between volumetric heterogeneity and sharp seismic gradients and has proven instrumental in shaping our view of the CMB region.

Lay and Helmberger (1983) discovered the D" discontinuity, a seismic interface characterized by a shear velocity increase of 1–3% approximately 250 km above the CMB. The boundary is inferred from an extra phase, known as SdS, that arrives between the direct S-wave, S, and the core-reflected S-wave, ScS, at post-critical distances. SdS turns in the higher velocity layer below the discontinuity, which produces a triplication in seismic data. Seismologists identify the triplication beneath regions of inferred paleosubduction including Alaska, the Caribbean, Central America, India, and Siberia. Detections beneath the seismically slow central Pacific are contrary to this trend and may suggest that the discontinuity height above the CMB or velocity increase are modulated by composition.

There are three probable explanations for the discontinuity, which are not necessarily mutually exclusive: phase change, thermal heterogeneity, or a chemical boundary. A phase change best explains the seismic data (*Sidorin et al.*, 1998). Contary to observations, thermal heterogeneity alone does not produce a strong SdS arrival, and a pre-existing chemical layer is pushed away from downwelling regions. Subsequent experimental and theoretical verification of a phase transition in MgSiO<sub>3</sub> from silicate perovskite, the major phase of the lower mantle, to a new phase, termed "post-perovskite", supports the phase change interpretation (*Murakami et al.*, 2004; *Oganov and Ono*, 2004). Furthermore, a "double crossing" of the phase boundary may explain neighboring seismic discontinuities (*Hernlund et al.*, 2005).

In Chapter 2 I investigate the fine-scale interaction of a slab as it descends through the phase transition and perturbs the thermal boundary layer at the CMB. The temperature anomalies of slabs and plumes elevate and suppress the phase boundary, respectively. I elucidate the expected perturbations to temperature and phase that map to variations in seismic structure and produce waveform complexity in synthetic seismograms. Modern three-component broadband seismic arrays such as USArray will provide data to compare with the predictions. Ultralow-velocity zones (ULVZs) are thin (< 100 km), isolated patches with anomalously low seismic wavespeed (reductions of  $\sim 10-30\%$ ) at the CMB originally detected beneath the western Pacific but since discovered in other regions. They were identified by the late arrival of the seismic phase SPdKS relative to SKS for distances between 105 and 120 degrees. SKS travels through the mantle and outer core and SPdKS follows a similar path except for a short diffracted segment (Pd) along the CMB. Waveform modeling using differential travel time and amplitude therefore constrains the P-wave velocity for this segment. Additionally, precursors and postcursors to core-reflected phases (PcP, ScP, ScS) can potentially constrain the P and S wavespeed, thickness, and density of ULVZs, although data stacking is required to enhance the signal-to-noise ratio.

Iron enrichment of solid phases, specifically the increase in Fe/(Fe+Mg) ratio, can simultaneously increase density and reduce compressional and shear velocity (e.g., *Karato and Karki*, 2001). This partly inspired the notion of solid, iron-rich ULVZs, such as a metal-bearing layer (*Knittle and Jeanloz*, 1991; *Manga and Jeanloz*, 1996), subducted banded iron formations (*Dobson and Brodholt*, 2005), or iron-enriched post-perovskite (*Mao et al.*, 2006; *Stackhouse and Brodholt*, 2008). Iron-rich systems are typically denser than the surrounding mantle, which is required to explain the locations of ULVZs at the base of the mantle.

Recent high-pressure experiments have uncovered very low sound velocities in ironrich (Mg,Fe)O that could explain the origin of some ULVZs (*Wicks et al.*, 2010). I explore this hypothesis in Chapter 3 by developing a thermochemical convection model of a solid-state ULVZ that contains a small volume fraction of iron-rich (Mg,Fe)O. A mineral physics mixing model combines the material properties for the oxide phase and ambient material using select chemical partitioning models to determine the thermoelastic parameters of the assemblage. The model satisfies current seismic modeling constraints.

The behavior of (Mg,Fe)O at high pressure and temperature conditions also motivates the study presented in Chapter 4. A high-spin (four unpaired d electrons) to low-spin (no unpaired d electrons) electronic transition of ferrous iron in an octahedral local environment increases the density of (Mg,Fe)O ferropericlase by 2–4% at mid-lower mantle pressure around 50 GPa (*Sturhahn et al.*, 2005; *Badro et al.*, 2003). This transformation occurs over a pressure range that is small at ambient temperature (~ 300 K) and broad at high temperature (~ 3000 K). The spin transition is continuous along a lower mantle geotherm (*Sturhahn et al.*, 2005; *Tsuchiya et al.*, 2006). However, downwellings and upwellings may generate substantial temperature anomalies in the mantle, so that convective flow may be modified by buoyancy forces arising through the spin-state of the material.

I investigate how the spin transition in (Mg,Fe)O impacts the large-scale style and vigor of mantle convection in Chapter 4. The body-force due to the spin-state of the material is included in the momentum equation. To determine the influence of the spin transition I observe the pattern of convection, time average heat flux, and time average depth profiles for the horizontally averaged temperature and RMS vertical velocity. Seismic tomography reveals two antipodal large, low-shear velocity provinces (LLSVPs) at the base of the mantle beneath the Pacific Ocean and Africa. The circum-Pacific belt of fast material is attributed to relic slabs from paleosubduction (*Richards and Engebretson*, 1992). The LLSVPs occupy approximately 20% of the surface area of the CMB and contain about 1.6 vol. % and 1.9 mass % of the mantle (e.g., *Burke et al.*, 2008). *Ni and Helmberger* (2003a) model the 3-D geometry of the African LLSVP as a ridge-like structure approximately 1200 km high and 1000 km wide that extends 7000 km from central Africa to the Indian Ocean. The Pacific LLSVP may be divided into a western province that is 1000 km wide and rises 740 km above the CMB and an eastern section that is 1800 km wide and 340–650 km high (*He and Wen*, 2009).

A thermochemical origin is necessary to explain anti-correlated shear wave and bulk sound velocity anomalies (*Su and Dziewonski*, 1997; *Masters et al.*, 2000), putative anti-correlated shear wave and density anomalies (*Ishii and Tromp*, 1999, 2004), multipathing for waves sampling its steep edges (*Ni et al.*, 2002), and geological inferences of stability over 200–300 Myr (*Burke and Torsvik*, 2004). These observations are suggestive of a material with a higher bulk modulus and higher zero-pressure density than ambient mantle (*Tan and Gurnis*, 2005). Furthermore, surface plate history influences the morphology and location of the LLSVPs (*McNamara and Zhong*, 2005).

In Chapter 5 I investigate the response of high bulk modulus structures in the lower mantle to evolving surface tectonics from 250 Ma to present day. A novel time-dependent thermal and kinematic boundary condition is derived from a highresolution plate history model that encodes global plate motions and paleosubduction locations. These paleogeographic constraints are incorporated into 3-D spherical convection models with a high bulk modulus material with a higher zero-pressure density than ambient mantle.