Seismic and Mineral Physics Constraints on the D" Layer
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ABSTRACT
We present a synthesis of results from seismic and mineral physics studies of the D" layer to improve constraints on Earth’s lowermost mantle. We focus on structures of two length scales, the seismic reflector at the top of this region and the structures of smaller scale known as ultralow velocity zones (ULVZs). A review of seismic observations for the D" layer and their interpretation is followed by a case study, where we combine new data with published results for the D" region beneath the Bering Sea and Alaska. Our evaluation of plausible interpretations includes features related to subducted slab debris that trade-off with petrology (mineral phase assemblage) and post-perovskite crystal chemistry. For the smaller-scale structures that exhibit lower than average seismic wave-speeds, the ULVZs, we consider hypotheses involving either iron-rich (Mg,Fe)O magnesiowüstite or iron-rich (Mg,Fe)SiO₃ post-perovskite. We use mineral physics data and previously published seismic reduction ratios of S- and P-wavespeeds with their respective uncertainties for a best-fit optimization approach with parameter correlations. Seismic wave reduction ratios ranging from 2 to 3 are well explained by phase assemblages containing elastically anisotropic iron-rich (Mg,Fe)O. Observations outside this range require different explanations than those considered here, thus suggesting diverse origins for ULVZs.

8.1. INTRODUCTION
The boundary between the core and mantle is a primary interface within the deep interior of Earth and has a fundamental influence on the cooling of the planet. Thus, this region may provide essential clues in revealing the planet’s thermo-chemical evolution. The lowermost mantle is characterized by anomalous seismic gradients that were first noted by Gutenberg (1914). This particular region of the mantle, referred to as the D" layer (Bullen, 1950) hosts a myriad of seismic features. These features range from abrupt velocity increases to regions characterized by a decrease in the velocity gradients, and have been the focus of several reviews (e.g., Cobden et al., 2015; Garnero, 2000; Garnero et al., 2016; Kendall and Silver, 1998; Lay, 2015; Nowacki et al., 2011; Romanowicz and Wenk, 2017; Weber et al., 1996; Wysession et al., 1998; Yu and Garnero, 2018). The various anomalous features have been associated with structures of different length scales, ranging from large-scale seismic velocity anomalies and seismic anisotropy to small-scale scatterers and ultralow velocity zones. Thermal and chemical heterogeneity, solid-solid phase transitions, lattice or shape preferred orientation, complex rheology, and melting are probably all necessary to explain the observed structures. Understanding the origin of these multi-scale structures requires, in part, advances in mineral physics, tightly coupled with seismological observations, geodynamic modeling, and geochemical analysis (e.g.,

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Bower et al., 2013a, 2011; Cobden et al., 2015; Deschamps and Tackley, 2008; Deschamps and Trampert, 2003; McNamara et al., 2010; Nowacki et al., 2011; Pisconti et al., 2019; Sun et al., 2019, 2016), while taking into account mutual uncertainties (e.g., Dobrosavlevic et al., 2019).

The D" layer is situated just above the largest radial density jump within the planet. Despite the relatively small volume of D", it may be the site of long-term differentiation and is often made a significant component of global mass balance problems; for example, the observed small-scale heterogeneity within D" may reveal long-term storage sites of heat-producing elements and/or volatiles (e.g., Albarède, 2005; Becker et al., 1999; Corgne and Wood, 2005; Helffrich and Wood, 2001; Hirose et al., 2004; Trompse et al., 2019; Turcotte et al., 2001). The nature of this layer in multicomponent chemical systems, how this layer’s character and location change with mantle composition, the influence of texture on observed seismic anisotropy, and the implications for mantle processes are important for understanding the dynamic evolution of the mantle and represent ongoing pursuits (e.g., Auzende et al., 2008; Bower et al., 2013b; Grocholski et al., 2012; Hernlund et al., 2005; Hirose, 2006; Hirose et al., 2008, 2005; Lay et al., 2008; Lay and Garnero, 2007; Lay and Helmberger, 1983a; Merkel et al., 2002; Miyagi et al., 2010; Murakami et al., 2005; Ono and Oganov, 2005; Pisconti et al., 2019; Ricolleau et al., 2008; Sakai et al., 2010; Shim, 2008; Sun and Helmberger, 2008; van der Hilst et al., 2007; Vinnik et al., 1989; Williams and Garnero, 1996).

The D" region is often marked by a reflector at its top that can provide information on the layer. The size of the velocity contrast across the layer and the depth of the reflector have been used to constrain the mineralogy. Other observables such as topography, velocity, and density contrasts across the reflector also help to infer the nature of the material within D" (see reviews by Cobden et al., 2015; Lay, 2015). The first part of this chapter will focus on the D" seismic reflector, including the range of seismic observations and plausible mineral physics interpretations with their associated trade-offs.

Small-scale structures within the D" layer that exhibit slower-than-average seismic wave speeds are typically termed ultralow velocity zones (ULVZs). In a recent review, Yu and Garnero (2018) present several key findings of ULVZs. In particular, modeling of seismic arrivals indicates the following with respect to the Preliminary Reference Earth Model, PREM (Dziewonski and Anderson, 1981) at the core-mantle boundary: a 3–25% decrease in \( V_P \) and 6–50% decrease in \( V_S \), thus indicating \( \delta V_S/\delta V_P \) could range from 1:1 to 6:1, and that ULVZ density contrast ranges from 0 to 22% higher than PREM. Nevertheless, it remains unclear whether these structures could harbor primordial material, are correlated with hotspot locations on Earth’s surface, or share a common origin with larger structures in the lower mantle, such as large low seismic velocity provinces. Many of these interpretations rely on understanding the composition of ULVZs. The second part of this chapter will discuss the range of ULVZ seismic observations, the distribution of these features, and present new results from best-fit minimizations of mineral phase assemblages.

### 8.2. THE D" REFLECTOR(S)

#### 8.2.1. Visibility of the Reflection

Lateral variations of seismic velocities in the lower mantle have been described in the past. For example, in the early 1970s, Wright and Cleary (1972) and Wright (1973), analyzing \( P \) waves, concluded that lateral velocity variations in the lowermost mantle exist. They suggest that these structures display features that vary depending on the region, from a reduced (or increased) velocity gradient, to abrupt changes in seismic velocity, and may be due to phase-changes in the mantle.

About a decade later, small seismic arrivals that appear between the S and ScS wave and the \( P \) and PcP wave, respectively, were observed and reveal a move-out (slowness) different from the main phases S and ScP (or \( P \) and PcP). These small additional arrivals have been interpreted as reflections off (triplications due to) a high-velocity layer near the core-mantle boundary (e.g., Lay and Helmberger, 1983b; Weber and Davis, 1990; Young and Lay, 1990). In the following we will call these arrivals \( SdS \) and \( PdP \) and include the reflected and refracted waves in this name (i.e., \( SdS \) and \( SDS \), or \( Sbc \) and \( Scd \), same for \( P \) waves) (Figure 8.1).

There have been many different studies on the D" reflection, and this review cannot cover all of the previous studies for every region. Therefore, the reader is also referred to several previous reviews on this topic (e.g., Cobden et al., 2015; Lay, 2015, 2007; Wysession et al., 1998). A summary of regions imaged with D" reflected waves is shown in Figure 8.2, which is based on the maps shown in Wysession et al. (1998) and Cobden et al. (2015) with the addition of a few more studies (Durand et al., 2019; Pisconti et al., 2019; Thomas and Laske, 2015; Whittaker et al., 2016; Yao et al., 2015).

The first observations of \( SdS \) arrivals (Lay and Helmberger, 1983b) were from regions where we expect paleo-subduction (Lithgow-Bertelloni and Richards, 1998), and tomographic inversions display fast seismic velocities (e.g., French and Romanowicz, 2014; Grand, 2002; Li et al., 2008; Ritsema et al., 2011). Due to the different move-out of these \( SdS \) phases compared with the \( S \) and ScS wave, the arrival could not be due to depth phases or other structures near the surface. Modeling confirmed
that a distinct layer with thickness of approximately 300 km at the CMB and an increase in impedance (i.e., the product of velocity and density) could produce arrivals that can explain the observations (Houard and Nataf, 1993; Lay and Helmbberger, 1983b; Weber, 1993; Young and Lay, 1990). Using array measurements, Weber and Davis (1990) used the travel time and the slowness of the new arrival compared with \( P \) and \( PcP \) values (Figure 8.1) and confirmed that the phase \( PdP \) had to be reflected off an approximately 300 km thick layer at the CMB (model PWDK: Weber and Davis, 1990; Weber et al., 1996).

The reflections off the \( D^\prime \) discontinuity are generally small and often not easily distinguishable in single records and in noisy data (e.g., Figure 8.3). Therefore, either distance dependent record sections aligned on either the direct wave (\( P \) or \( S \)) or the core reflected wave (\( PcP \) or \( ScS \)) or stacks of record sections help to distinguish between noise, Moho multiples, or \( D^\prime \) reflected arrivals, since the move-out (slowness) of the \( D^\prime \) reflection differs from that of the main phases. Vespagrams (i.e., velocity spectral analysis) (e.g., Davies et al., 1971; Rost and Thomas, 2002; Schweitzer et al., 2009) are constructed using recordings of a seismic array and, after shifting for different slowness values (related to the angle of incidence of the wave at the surface), the traces are stacked, either linearly or after some weighting with, for example the instantaneous phase (Schimmel and Paulssen, 1997), or after taking the \( N \)th root (e.g., Muirhead and Datt, 1976) before stacking. The vespagram process amplifies coherent waves, reduces the amplitude of the (incoherent) noise, and allows to identify the different seismic arrivals by their slowness (Figure 8.3). Often, the frequency-wavenumber (fk-analysis) (e.g., Capon, 1973; Rost and Thomas, 2009) or slowness backazimuth analysis are used to confirm that the wave, interpreted as a \( D^\prime \) reflection, travels with the slowness and backazimuth of such a reflected \( D^\prime \) wave. For a review on seismic array techniques, the reader is referred to Schweitzer et al. (2009) and Rost and Thomas (2002, 2009).

Since the early observations of \( SdS \) and \( PdP \) that were detected mostly from high-velocity regions in the lowermost mantle as seen in tomographic inversions, the interpretation as a reflection off the top of subducted lithosphere was a preferred explanation (e.g., Lay and Garnero, 2004; Scherbaum et al., 1997; Thomas et al., 2004b; Weber, 1993), while other possible scenarios are solid-solid phase transitions (Sidorin et al., 1999, 1998) and accumulation of mid-ocean ridge basalt (MORB) or other chemically different layers, possibly including partial melting (e.g., Garnero, 2000; Lay et al., 2004b; Lay and Garnero, 2004). In 2004, experimental and theoretical mineral physics observed that the major lower mantle phase MgSiO\(_3\) bridgmanite undergoes a structural phase transition to post-perovskite at \( D^\prime \) conditions (Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004). More detailed discussion on the range of interpretations for the reflected \( D^\prime \) wave can be found in section 8.2.4.

In the years following these early observations, many studies found evidence for \( D^\prime \) reflections in other high-velocity regions (see reviews by Cobden et al., 2015; Lay 2007, 2015; Wysession et al., 1998; see also Figure 8.2), and further details arose during those studies: the reflector, which was initially modeled as a one-dimensional structure, showed evidence for topography in that the differential travel time of the reflected phase with respect to the main phases (\( P, S \) or \( PcP, ScS \)) varied between different events or locations (e.g., Hutko et al., 2006; Kendall and Nangini, 1996; Kendall and Shearer, 1994; Thomas et al., 2004a, 2004b). For example, the reflector beneath the Caribbean showed a strong variation in depth, estimated from the arrival time of the reflection, dropping from around 400 km above the CMB to around 200 km above the CMB (e.g., Hutko et al., 2006; Kendall and Nangini, 1996; Kito et al., 2007; Lay et al., 2004a; Thomas et al., 2004a; Thorne et al., 2007; van der Hilst et al., 2007). Other places also seemed to exhibit strong topography, for example beneath Siberia (e.g., Gaherty and Lay, 1992; Houard and Nataf, 1993; Thomas et al.,

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**Figure 8.1** Ray paths of seismic phases, \( PdP \) and \( SdS \), sampling \( D^\prime \) that are discussed in this Chapter. The inset shows the reflected and diving wave \( PdP \) (or \( SdS \)) and \( PDP \) (or \( SDS \)). \( SdS \) is also called \( Sbc \), \( SDS \) is also called \( Scd \), same for \( P \) waves.
In addition to reflections found in fast-velocity regions, regions that exhibit low seismic velocities in tomographic inversions have been investigated and D'' reflections from these areas are visible (e.g., Yamada and Nakanishi 1996, 1998; Kito and Krüger 2001; Lay et al. 2006; Ohta et al. 2008; Kawai and Geller 2010; Takeuchi and Obara 2010; Cobden and Thomas 2013). Areas that transition between fast and slow seismic velocities in tomographic models also seem to generate arrivals that arrive between P and PcP or S and ScS. These areas include but are not limited to the Atlantic and the western Pacific (e.g., Durand et al., 2019; Pisconti et al., 2019; Thomas and Laske, 2015; Whittaker et al., 2016; Yao et al., 2015). In many cases, array methods were used for these reflections to confirm that they have the appropriate travel time, slowness, and the back azimuth that classify them as D'' reflections. The amplitude of reflections at a discontinuity with a velocity decrease would be smaller than for a reflector with a positive velocity contrast, and the influence of the diving wave (SdS or PdP) would be decreased for a low-velocity layer compared with high-velocity layer. This could be a reason for fewer detections in low-velocity regions.

It should be noted that sampling of the D'' region with reflected waves is limited due to source-receiver combinations that can be used to test the CMB region. The best epicentral distance to search for the reflector is 60–85 degrees distance (e.g., Cobden et al., 2015; Weber, 1993; Wysession et al., 1998), but smaller epicentral distances have been used as well (e.g., Rost and Thomas, 2010; Schimmel and Paulssen, 1996). Those smaller epicentral distances corresponding to a small angle of incidence at the reflector suffer from a small reflection coefficient and hence generally produce weaker reflections (Figure 8.4).

There seem to be very few places where no reflected wave from D'' is unequivocally visible when using stacking of seismic data, i.e., array methods (gray stars in Figure 8.2). Neuberg and Wahr (1991) reported an absence of the D'' arrival east of Australia, however, the epicentral distance for this study was 35 degrees where the reflection coefficient for PdP and SdS is very small (see Figure 8.4). Another region where no arrival is detected between P and PdP is the area beneath the Pacific Ocean (Thomas and Laske, 2015); however, this

Figure 8.2 Places with D'' detections in different studies following the maps in Wysession et al. (1998) and Cobden et al. (2015). Green areas indicate S wave studies, blue areas are P wave studies. Grey stars show places where no D'' reflection was detected (e.g., Neuberg and Wahr, 1991; Thomas and Laske, 2015; Chambers and Woodhouse, 2006) and yellow stars indicate the place of the D'' case study from both Sun et al. (2016) and this work. The ULVZ regions discussed in the text are shown as red areas. Sources: From D'' studies summarized in this figure are given in Wysession et al. (1998) and Cobden et al. (2015). In addition, locations from Thomas and Laske (2015), Yao et al. (2015), Whittaker et al. (2016), Durand et al. (2019), Pisconti et al. (2019), and Pisconti (pers. comm.) are shown. For more information, see text.
Figure 8.3 Examples of $PdP$ observations in different regions showing amplitude differences and polarity variations. Event dates and arrays are given for each event, see also Appendix Table 8.A2. GRSN - German Regional Seismic Network; NWT- Polaris array, Northwest Territories, Canada. On the left are the seismic traces, aligned on $P$ and $S$, respectively, and on the right the corresponding vespagrams. For the 12 November 2003 event, the predicted arrival time of $PdP$ for a 300 km thick $D^*$ layer is indicated. In the other cases, the dashed lines indicate the arrivals of $PdP$/$SdS$ and $PcP$/$ScS$. In the seismogram of 30 May 2007 the Moho arrival is also marked. The amplification is 100 for all $P$ wave vespagrams after normalizing the traces and stacking them with a nonlinear stacking technique (4th root).
Figure 8.4 Examples of the reflection coefficients for \( P \) waves \((R_{PP})\) and \( S \) waves \((R_{SS})\) for select \( D^\prime \) scenarios. Blue line: for velocity contrast of \( V_P \) and \( V_S \) of +3%, based on model PWDK, black line for \( V_P \) and \( V_S \) of -3% and red line for \( V_P \) of -1% and \( V_S \) of +3%. The density contrast is always set to a 3% increase but it does not affect the reflection coefficient in distance ranges between 60 degrees and above. The red curve for \( R_{SS} \) is underneath the blue curve. The critical incidence angle for the blue curve (i.e., from which total reflection happens) is 76.09 deg for \( P \) waves and 76.12 deg for \( S \) waves, which corresponds to a distance of 70 and 71 degrees, respectively. The epicentral distance that corresponds to the incidence angle is given above the graph for \( P \) and \( S \) waves and is calculated for a reflector 300 km above the CMB and a \( P \) and \( S \) velocity for the \( D^\prime \) region consistent with PWDK.

is also an example where the epicentral distances are short and the amplitude of \( PdP \) is predicted to be very small. Beneath the Aleutians it seems that areas without a \( D^\prime \) reflector exist in two different regions (Figure 8.3 and 8.5; Sun et al., 2006, 2016), but they are close to regions where a reflector is found. Scherbaum et al. (1997) suggested that localized inhomogeneity (scatterers) could be a reason for intermittent observation of \( D^\prime \) reflections. It has also been suggested that strong topography can create record sections without a \( D^\prime \) reflection or with two arrivals, due to focusing and defocusing effects (e.g., Thomas and Weber, 1997; Whittacker et al., 2016), while Sun et al. (2016, 2006) indicate an interrupted reflector due to an upwelling plume, i.e., a more dynamically inspired cause. A similar scenario as the one observed by Sun et al. (2016) has been reported by Chambers and Woodhouse (2006) beneath North-central Asia. Taking all reports of the presence or absence of \( D^\prime \) reflections together suggests that in almost all tested regions, where data quality is good and the epicentral distances ensure a large reflection coefficient, arrivals have been detected in the datasets with a move-out (slowness) and timing that agree with a \( D^\prime \) reflected \( PdP \) or \( SdS \) (e.g., Cobden et al., 2015; Lay, 2015; Wysession et al., 1998). The cases where data quality is good but no \( D^\prime \) reflection has been consistently observed in one region seem to be the exception rather than the rule. In this latter case, it is still possible that a reflector is present but cannot be imaged with currently available source-receiver combinations, that there is topography, and hot upwelling (e.g., Sun et al., 2016), or that the impedance contrast is too small to allow detections (Thomas and Weber, 1997; Whittacker et al., 2016).

In many cases a clear distinction of the \( D^\prime \) reflection from other interfering phases is difficult: Moho multiples and depth phases make observations of the weaker \( D^\prime \) reflections difficult, and even though the move-out, i.e., the slowness, would help to distinguish these waves, the often-high amplitude depth phases or Moho multiples may interfere with the \( D^\prime \) reflection and may render it invisible (Lessing et al., 2015).

In several regions, a second arrival between \( P \) and \( PcP \) or \( S \) and \( ScS \), in addition to \( PdP/SdS \), has been reported: beneath the Caribbean (Hutko et al., 2009; Kawai et al., 2007; Kito et al., 2007; Thomas et al., 2004a), Southeast Asia (Chaloner et al., 2009), Siberia (Thomas et al., 2004b), and the Pacific (Kawai and Geller, 2010). Lay et al. (2006) and Ohta et al. (2008) report up to three arrivals between \( S \) and \( ScS \) in the Pacific. These additional arrivals point to a second and possibly third reflector beneath the top of the \( D^\prime \) layer that is visible beneath at least parts of the examined regions. Beneath the Caribbean, for example, the second reflector seems to be absent where the upper \( D^\prime \) reflector is found closer to the CMB (e.g., Hutko et al., 2006; Kito...
et al., 2007; Thomas et al., 2004a). Using an extensive dataset, van der Hilst et al. (2007) show an anti-correlation in depth of the lower reflector with the top reflector.

8.2.2. Travel Times of the Reflection(s)

The travel time between the main phase \(P, S, \text{ and } PcP, ScS\) and the \(D''\) reflection \(PdP, SdS\) is an important observable to establish whether the arrival is indeed a \(D''\) reflection, and it also helps to measure the depth of the reflector assuming a horizontal (i.e., 1D) reflector. For a reflector 300 km above the CMB and an epicentral distance of around 65–75 degrees, the \(D''\) reflection is expected with a travel time between \(P\) and \(PcP\) (or \(S\) and \(ScS\)), as can be seen in Figure 8.3 (see also Weber, 1993). For deeper reflectors, the \(D''\) reflection arrival appears closer to the core-mantle boundary reflection, whereas for shallower reflectors one expects the reflected wave closer to the direct wave (Weber et al., 1996). For large distances, the diving wave \(PDP\) or \(SDS\) may arrive before the \(P\) or \(S\) wave (e.g., Wysession et al., 1998; Young and Lay, 1990).

The differential travel time to either the \(P\) (\(S\)) wave or the \(PcP\) (\(ScS\)) wave can be used to constrain the depth of the reflector (e.g., Chaloner, et al., 2009). Often, the differential travel time between \(PcP\) and \(PdP\) (same for \(S\) waves) is used because the two waves travel along a
similar path through the mantle and it is assumed that the influence from mantle structure on the travel time is negligible. The calculation of the depth of the reflector for this case, however, then depends on the velocity inside D" since a seismically fast layer would speed up the PcP reflection and lower the differential travel time between PcP and PdP and therefore place the D" reflector at deeper depths. This trade-off between thickness of the D" layer and the velocity contrast within the D" layer should be kept in mind when interpreting reflector depths. On the other hand, using the differential travel time between P and PdP would allow constraints on the depth of the reflector, and PcP could then be used to constrain the velocity in D". However, the P and PdP waves travel through different parts of the mantle and could be influenced by different velocity structures in the mantle. Hence, the travel time difference could in part be due to different structures encountered by either P or PdP on the path and may therefore lead to an estimated reflector depth either too shallow or too deep. Travel time corrections for mantle structure are often applied, based on tomographic models (e.g., Hutko et al., 2006; Kito et al., 2007; Thomas et al., 2004b) and for large-scale velocity variations this helps to reduce the influence from mantle structure, but these corrections depend strongly on the tomographic model used. A good knowledge of seismic velocities along the path is important for the depth estimation of the reflector. Since the PdP or SdS wave can arrive before the P or S wave for large distances (e.g., Lay and Young, 1991), this wave could potentially be used to constrain the velocity within D", thus reducing or eliminating some of the uncertainty.

Many studies find the D" reflection at travel times that correspond to a structure near 2650–2600 km depth, i.e. 250–300 km above the CMB (e.g., Lay and Helmberger, 1983b; Weber, 1993); see also reviews by Wyssession et al. (1998), Cobden et al. (2015), and Lay (2015). In some regions strong topography has been detected, for example beneath the Caribbean (e.g., Hutko et al., 2006; Kendall and Nangini, 1996; Kendall and Shearer, 1994; Kito et al., 2007; Lay et al., 2004a; Thomas et al., 2004a, 2004b), Siberia (Houard and Natel, 1993; Scherbaum et al., 1997; Thomas and Weber, 1997; Weber, 1993), and the Eastern Pacific (Takeuchi and Obara, 2010; Yamada and Nakanishi, 1998, 1996). The variation in depth is usually around ±100–150 km from a reflector with an average height of 250 km above the CMB. The Central and Western Pacific region shows strong topography of the reflector toward the western edge of the large low seismic velocity anomaly (Lay et al., 2006; Ohta et al., 2008), and the region beneath the Bering Sea indicates topography up to 300 km (see Figure 8.5 and Kendall and Shearer 1994; Sun et al., 2016).

It should be noted that the topography of the reflector is usually estimated using arrival times for single events and bins of stations and is calculated using 1D models. This might lead to wrong estimates of reflector depths: topography will change the wave path, and a reflection at an inclined surface will likely be in a different position and depth compared with the one calculated for a 1D model. Migration of PdP and SdS waves could reduce errors (e.g., Hutko et al., 2006; Thomas et al., 2004b, 2004a), but a large amount of source-receiver combinations is needed to gain a complete picture of the reflector topography (e.g., van der Hilst et al., 2007). Thorne et al. (2007) and Wittaker et al. (2016) analyze the effects of topography on D" reflected waves and find that topography may generate double reflections that might lead to misinterpretation. A thorough investigation of the influence of 2D or 3D structures on the travel times, and hence on the estimated reflector depth, would be beneficial for future studies.

8.2.3. Amplitude and Polarity of the Reflection(s)

The early reported SdS arrivals as well as some PdP arrivals show large amplitudes (Figure 8.3) and are clearly visible in single seismograms (e.g., Kendall and Shearer, 1995, 1994; Lay and Helmberger, 1983b; Thomas and Weber, 1997). Migration of SdS waves caused reduction in error (e.g., Hutko et al., 2006; Thomas et al., 2004b, 2004a), which led to seismic velocity models that exhibit a large velocity jump of 2–3% for P and S waves at the top of the D" reflector: e.g., SYL0 (Young and Lay, 1990) and PWDK (Weber and Davis, 1990). Wysession et al. (1998) provide a compilation of velocity jumps across D". Many observed SdS and especially PdP arrivals, however, have smaller amplitude and point to a smaller velocity jump in S- and particularly in P-wave velocity (see also the examples in Figure 8.3). Calculations of synthetic data using full waveform modeling showed an agreement for PdP amplitudes with a 1% velocity jump at a first-order discontinuity (e.g., Chaloner et al., 2009). In most cases the arrivals, especially for P waves, are not visible for single seismograms or distance-dependent seismogram sections, but can be detected using array seismic methods (e.g., Rost and Thomas, 2002; Schweitzer et al., 2009).

One way to explain the large amplitude of PdP and SdS waves seen in some cases (e.g., Figure 8.3, 17 Dec 1991) compared with P and S amplitudes could be topography of the reflector. Focusing and defocusing effects will change the amplitude of the wave considerably, and in some cases render the reflection invisible (e.g., Thomas and Weber, 1997). Such strong topography is detected in several regions as detailed above (for example, beneath the Caribbean and Siberia), as well as in those regions where events with large amplitude reflections and events without a discernible D" reflection have been reported.
side by side (e.g., Chambers and Woodhouse, 2006; Hutko et al., 2006; Kito et al., 2007; Sun et al., 2016, 2006; Thomas and Weber, 1997).

On the other hand, it is also possible that large lateral velocity variations exist in D" and those could cause regions with stronger reflections due to larger velocity contrasts across the boundary (e.g., Kendall and Nangini, 1996; Lay et al., 2004a). It is, however, difficult to explain such strong velocity variations over such short distances (e.g., Thomas and Weber, 1997) unless scattering is invoked as a cause (e.g., Scherbaum et al., 1997). The reflection points of events with and without D"-reflected waves are essentially within the 1D Fresnel zone (e.g., Thomas and Weber, 1997; Weber, 1993) for the region beneath Siberia; however, beneath the Aleutians and Bering Sea (Figure 8.5), the region where no reflections are found is distinct from the region exhibiting D" reflections and separated by approximately 8–10 degrees (which is larger than one Fresnel zone for the dominant periods of the waves of 1 to 3 s used here).

A third possibility for the variation in amplitude could be changes in the velocity gradient across the D" reflector, i.e., the sharpness of the reflector. A gradient would likely reduce the amplitude of the reflected wave (Lay, 2008; Weber, 1993), but the detailed shape of the gradient zone will also influence the amplitude of the reflection (Hernlund, 2008) and possibly lead to different depth-estimates of the reflector. A region where the gradient changes from steep to shallow within the gradient zone may be interpreted as a lower reflector, and vice versa. This, however, would overlook the fact that if the gradient is due to a mineral phase transition, then this transition may occur at shallower depths than seismically imaged, and this could lead to discrepancies between seismic observations and mineral physics results.

The amplitudes of waves reflected at additional structures beneath the top of D" as seen by several investigations (e.g., Hutko et al., 2006; Lay et al., 2006; Thomas et al., 2004a, 2004b; van der Hilst et al., 2007) are much smaller compared with the top reflections. This makes them difficult to observe and in some cases, their existence has been cast into doubt, as discussed by Flores and Lay (2005). The modeling attempt of Whittaker et al. (2016) also shows that topography could create a secondary reflector, and it would be important to test the lateral variation of this phenomenon (i.e., anti-correlation, lateral extent of second reflector) to distinguish between this scenario and a true deeper reflector. The additional arrival’s appearance in vespagrams and slowness–back azimuth analyses, however, indicates that they are coherent arrivals that agree with a reflection from a deeper structure rather than a processing artifact, and modeling confirms that the negative velocity contrasts needed for these reflections can indeed generate small reflected arrivals (e.g., Hernlund et al., 2005). It should be noted that the size of the velocity contrast for the lower reflector is not well constrained yet.

While amplitude measurements can be influenced by many different factors such as attenuation (e.g., Durand et al., 2013), energy partitioning, as well as anisotropy in D" (Pisconti et al., 2019; Thomas et al., 2011), the polarity of the seismic wave (i.e. the waveform) is another observable that can be used to analyze the D" reflectors. If the radiation pattern of an event is such that PcP and P (or ScS and S) have the same polarity, the reflection off of D" should have the same polarity as the main phases for a positive velocity jump across the D" reflector, because the D"-reflected wave has a take-off angle between P and PcP (or S and ScS) for distances between 60 and 80 degrees. This means that if the P-PD wavelet has an up-swing first, the PdP wave will also have an upsing first (e.g. Figure 8.3, S wave example). Conversely, a negative velocity jump should create a polarity opposite to P and PcP (or S and ScS), as shown in Figure 8.4.

Opposite polarity observations have been found in several studies for PdP waves (Chaloner et al., 2009; Cobden and Thomas, 2013; Hutko et al., 2008; Pisconti et al., 2019; Thomas et al., 2004a, 2004b). This would point to a negative velocity jump for P waves. One explanation for these opposite polarity PdP waves could be the negative P velocity jump associated with the phase transition from bridgmanite (“Br”) to post-perovskite (“PPv”), a result of the large drop in bulk modulus for PPv compared with Br (Wookey et al., 2005), although a recent theoretical study predicts an increase in both P and S waves across the Br-PPv transition (Zhang et al., 2016). Interestingly, to our knowledge, no opposite SdS-wave polarities compared with S and ScS have been reported in regions with either lower or higher than average velocity in tomographic models. This leads to velocity models including a D" layer with a positive S wave jump and either a negative gradient or positive gradient below the top of D" (e.g., SYLO: Lay and Young (1991), SWDK: Weber and Davis, 1990)). Regions where PdP waves exhibit opposite polarities compared with P and PcP, SdS waves have the same polarity as S and ScS (e.g., Cobden and Thomas, 2013), ruling out a simple thermal origin, thus pointing to the Br to PPv transition or a chemically different D" region. For these scenarios it is important to verify that the polarities are the same in all travel directions to rule out anisotropy in D" (e.g., Pisconti et al., 2019; Thomas et al., 2011).

It should be noted that the reflection coefficient of P and S waves depends on the impedance contrast (velocity times density) across the D" reflector and the incidence angle of the reflected wave. An example using model PWDK is shown in Figure 8.4. Here, if the wave arrives with an incidence angle of 60 degrees, the reflection
The phase transition in pure MgSiO$_3$ occurs at pressures (Wentzcovitch et al., 2007), although uncertainties remain. and velocity contrasts (e.g., Murakami et al., 2004; many other structures in the D” region due to its density Ono, 2004), has been used to explain the reflections and (Murakami et al., 2004; Tsuchiya et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004).

The phase transition from Br to PPv, discovered in 2004 (Murakami et al., 2004; Tsuchiya et al., 2004; Oganov and Ono, 2004), has been used to explain the reflections and many other structures in the D” region due to its density and velocity contrasts (e.g., Murakami et al., 2004; Wentzcovitch et al., 2007), although uncertainties remain. The phase transition in pure MgSiO$_3$ occurs at pressures and temperatures associated with the D” reflec-
tor depth in cold and average-temperature regions. Topography of the reflector could thus be explained by temperature variations (Hernlund et al., 2005) and predicted temperature estimates for the Br to PPv transition using a Clapeyron slope (γ) of 9 MPa/K produce a distribution of heights of the D” reflector, ranging from zero to a few 100 km above the CMB (Sun et al., 2009), in agreement with many observations. However, strong changes in topography, e.g., beneath the Bering Sea (Figure 8.5 and Sun et al., 2016) would need a large temperature contrast over fairly small distances, which is difficult to explain with most geodynamic scenarios, unless a hot upwelling intersects the D” region (Sun et al., 2016).

Short-period seismic waves with dominant periods of 1 s detect the reflector (e.g., Weber 1993), thus the velocity gradient needs to be sharp, on the order of a few 10 s of km (e.g., Cobden and Thomas, 2013; Lay, 2008; Thomas and Weber, 1997). However, the Br-PPv phase transition poses some problems to explain the sharpness: when using a more likely situation in the deep mantle, that is bridgmanite in solid solution with Fe and Al (i.e., other than pure MgSiO$_3$), a relatively wide Br-PPv coexistence phase-loop

is observed (Akber-Knutson et al., 2005; Caracas and Cohen, 2007; Catalli et al., 2009; Grocholski et al., 2012; Sun et al., 2018), as opposed to a sharp transition for the MgSiO$_3$ end-member. Depending on the Al and Fe concentration of PPv, the onset depth of the phase transition also changes (e.g., Grocholski et al., 2012; Mao et al., 2004; Sun et al., 2018). To detect this larger transition with seismic data, long-period seismic waves, likely with dominant periods larger than 5s, are needed, and this may be the reason that the SdS wave is more readily observed due to its longer periods compared with PdP.

As mentioned above, the shape of the gradient is also important (Hernlund, 2008); thus far, it seems difficult to simultaneously constrain the size and shape of the gradient across D” with reflected waves.

Another challenge that the PPv phase transition presents is that experiments at room-temperature on the magnesium end-member suggest a shear wave velocity increase (e.g. Murakami et al., 2007) that is much smaller than the shear wave contrast found in the D” models (e.g., SYLO, PWDK). There is likely an even smaller contrast in P-wave velocity (Wookey et al., 2005) as discussed above, both of which contradict the large PdP and SdS observations as seen in some studies (e.g., Lay and Helmberger, 1983b; Weber, 1993; Young and Lay, 1990) (see also Figure 8.3). Where PdP and SdS have strong amplitudes would therefore likely represent regions where there is either very little Fe and Al in PPv (a narrow Br-PPv phase-loop) (e.g., Murakami et al., 2004; Sun et al., 2018), focusing or defocusing effects, or a chemistry distinct enough, such as an isolated pile of primordial mantle (Hansen and Yuen, 1988). Variations in amplitude could also be due to changes in velocity inside a thermo-chemical boundary layer, possibly with internal convection (e.g., Lay and Garnero, 2004). On the other hand, a recent study by Langrand et al. (2019) shows that it is possible that kinetics of the phase transition from Br to PPv could influence the reflection amplitude and generate large reflections for large gradient zones, although more work on this subject is needed.

D” anisotropy (e.g., Kendall, 2000; Kendall and Silver, 1998; Lay et al., 1998; Nowacki et al., 2011; Wookey and Kendall, 2007) has been explained by aligned minerals inside slabs or sheared melt pockets (e.g., Kendall and Silver, 1998, 2000, Lay et al., 1998). Provided that PPv is weak (Amman et al., 2010), partial alignment of PPv could sharpen the reflector (Ammann et al., 2010; Thomas et al., 2011) and cause seismic anisotropy. The link between seismic anisotropy and the PPv phase in the D” region has been evaluated in many previous studies (e.g., Ford et al., 2015; Merkel et al., 2007, 2006; Nowacki et al., 2011; Thomas et al., 2011; Wookey and Kendall, 2007; Wu et al., 2017) and we refer the reader to several of these reviews. Here, we simply point out that seismic
anisotropy caused by alignment of PPv could also generate variations in reflection polarities (Thomas et al., 2011; Pisconti et al., 2019) due to variations of the velocity contrast with azimuth across the discontinuity. Therefore, the observation of variable polarities of PdP waves with distance or travel direction together with polarity observations of SdS waves (and splitting measurements, if possible) can be a powerful approach to constrain the style of deformation in D" (e.g., Creasy et al., 2019; Pisconti et al., 2019; Thomas et al., 2011).

The deeper reflector that has been observed in several studies beneath the top of D" has been explained with a range of causes. Hernlund et al. (2005) show that it can be due to the buck-transformation from PPv to Br closer to the CMB due to high temperatures in the thermal boundary layer near the core. Other studies explain additional reflectors as being due to phase-changes in minerals (e.g., Ohta et al., 2008), folding of lithosphere (e.g., Hutko et al., 2006), ultralow velocity zones (Ohta et al., 2008, Lay et al., 2006), heating up and partially melting of material beneath a subducted slab (Tan et al., 2002), or a combination of these (e.g., Lay et al., 2006).

In order to explain the wide range of observables, variations in mineralogy, temperature, topography and deformation are likely required, each connected to a range of processes. However, it is important to emphasize that the various mechanisms described here affect not just one observable but other observables as well (i.e., there are trade-offs). For example, variations in Fe- and Al-concentrations in bridgmanite undergoing the transition to PPv affects the sharpness, depth, and the velocity contrast of the reflected wave. Topography of a reflector would affect the depth estimation of the reflector, since slanted sides of a reflector would change the wavepath and hence the travel time would no longer reflect the 1D interpretation of reflector depth. Lastly, to explain reflectors in areas identified as low-velocity regions in tomography studies, strong compositional boundaries may be needed. In the next section, we consider the above interpretations and trade-offs in a case study underneath the northern Pacific region.

8.2.5. Case Study: Observations and Interpretations of D" Underneath the Northern Pacific Region

The lowermost mantle underneath the northern Pacific region, spanning the Bering Sea to Alaska, has been sampled by several investigators (Castle and van der Hilst, 2000; Kendall and Shearer, 1994; Nowacki et al., 2011; Persh et al., 2001; Revenaugh and Meyer, 1997; Rost and Thomas, 2010; Sun et al., 2016; Vidale and Benz, 1992), many of which sampled the eastern part of the Aleutians and Alaska. The region lies to the north of the large low-velocity anomaly beneath the Pacific and is likely characterized by past subduction (Lithgow-Bertelloni and Richards, 1998). The seismic observations of the D" region have been strongly variable, with reflector depths ranging from an absence of a reflector to deep reflections of around 100 km above the CMB (e.g., Kendall and Shearer, 1994; Rost and Thomas, 2010), to observations of up to 400 km above the CMB (e.g., Kendall and Shearer, 1994; Sun et al., 2016; Young and Lay, 1990). In this study, we include new observations underneath the Bering Sea using P waves (Figure 8.5) and combine them with previous S wave observations underneath the Alaska region (Sun et al., 2016) to gain a better understanding of the dynamics and mineralogy in this area.

Our P-wave data cover a region that had previously been explored by Young and Lay (1990) with S-wave data, and it lies next to the region imaged by Kendall and Shearer (1994). We use events from the Western Pacific (Appendix Table 8.A2) and stations in Canada, specifically the POLARIS array Northwest Territories (NWT) and British Columbia (BC) deployments (Eaton et al., 2005). We use array methods to detect arrivals between P and PcP, that have a slowness and travel time indicative for a D" reflection. We confirm these reflections with slowness–back azimuth analyses, to ensure that they also have the correct back azimuth and are coherent arrivals. The amplitudes of the detected PdP arrivals are small and agree better with a 1% P-wave contrast than a 3% P-wave contrast, in agreement with other P-wave studies (e.g., Chaloner et al., 2009; Kito et al., 2007). We find several events that show no additional reflection between P and PcP with the appropriate slowness and travel time, and these nonobservations all cluster in one area (see Figures 8.3, 8.5, and 8.6). We also find differential travel times between the reflected waves and the P-wave that suggest strong topography of the reflector, in that in some cases the D" reflection arrives close to PcP and can be interpreted as a deeper reflector (Figure 8.5). Combining our new observations with previous work, we find a range of complex features in the D" layer, which are summarized in Figure 8.6 from west to east (regions A to F) and described below. Again, it should be kept in mind that the depth of the reflector is estimated using a 1D model.

The western area underneath the Bering Sea (region B) shows evidence for a D" reflector at depths around 300–400 km above the CMB, in agreement with Kendall and Shearer (1994) and the observations of Young and Lay (1990). Both studies used S-wave reflections, in contrast to the P-wave observations used here (Figure 8.5 and 8.6). The superposition of the D" reflection points and their respective depth are superimposed on the S-wave tomography model S40RTS (Ritsema et al., 2011), taken at 2700 km depth (Figure 8.6). Figure 8.6 indicates that we image a structure with low velocity that is surrounded by
an area of relatively high velocities. Our analysis using $P$-waves indicates that the structure appears to have steep sides and falls off northwestward to CMB level (region A), over a distance of approximately 300 km. Although several tomography models, including the one shown in Figure 8.6, display a slow velocity region at 2700 km depth, other models such as the PRI-S05 and PRI-P05 models (Montelli et al., 2006) indicate fast velocities at this depth. At shallower depths (2500–2600 km depth), many tomography models display relatively fast velocities.
and others show changes between slow and fast velocities (for a range of models see Hosseini et al., 2018). The westernmost region (region A) displays no obvious $PdP$ (Figure 8.5), which could point to the wide and incomplete Br-PPv phase transition loop (~450 km) recently reported for average (or pyrolitic) mantle material (Sun et al., 2018). Toward the East, the reported $D^\prime$ reflector from Kendall and Shearer (1994) is imaged at heights between 150 and 350 km above the CMB.

In region C of our investigation region, north of the observations made by Kendall and Shearer (1994), a relatively sharp $D^\prime$ reflector is observed based on clear and strong $D^\prime$ reflections: Sun et al. (2016) reported strong $SdS$ waves, requiring a sharp $\delta V_S = 2.5\%$ increase at 270 km above the CMB, also in agreement with models SYLO (Young and Lay, 1990); this region resides directly adjacent to region B, where we find $PdP$ reflections from a structure around 300 km above the CMB. Collectively, these observations suggest a continuous structure in regions B and C of Figure 8.6. The regions where $PdP$ and $SdS$ are strong could represent a mantle with relatively depleted Fe and Al in PPv (e.g., Murakami et al., 2004; Sun et al., 2018), in order to explain the sharp increase in reflected $S$ and $P$ velocities. One could explain this depletion in Fe by the nearby nascent plume (region D, discussed below); that is, Fe could be partitioned into the (partially molten?) plume root. However, an Fe-depleted Br-PPv transition would not explain the low velocities proximal to the CMB in the tomography studies in region B; thus, we consider another possibility.

One scenario that could produce reflections in regions of slow velocities inferred from tomography (regions B and C) is if subducted mid-ocean ridge basalt (MORB) could reach the bottom of the mantle (e.g., Komabayashi et al., 2009; Nakagawa and Tackley, 2008; Tan et al., 2002). MORB is denser than the surrounding mantle material at lower mantle conditions (Hirose et al., 2005) and therefore could be present at the base of the mantle, representing a chemical boundary (e.g., Lay and Garnero, 2004). At these depths, the PPv phase is stabilized in subducted MORB, as the Br-PPv transition occurs about 550 km above the CMB (Sun et al., 2018). Based on recent experiments, the bulk sound velocity contrast between Br in pyrolitic mantle and PPv in MORB (Fe- and Al-rich PPv) would likely be positive with respect to PREM (Sun et al., 2018), and capable of producing $PdP$ and $SdS$ reflections. Although our data are not clear enough to confirm this, the velocity contrast for $PdP$ appears to be positive. Waveform modeling of $S$-waves in region C is consistent with a relatively sharp velocity increase that creates strong $SdS$ waves, followed by a small positive velocity contrast down to about 2800 km depth, and a further significant drop in velocity down the CMB, similar to model SYLO.

To the east of the region with strong $PdP$ (region B) and $SdS$ phases (region C) lies a region where no clear $SdS$ phases are found (region D) (Lay and Garnero, 1997; Sun et al., 2016). Kendall and Shearer (1994) find deep $SdS$ reflections (200–250 km above the CMB), whereas Rost and Thomas (2010) find low-amplitude $PdP$ reflections deeper than that (~110 km above the CMB). Sun et al. (2016) used detailed modeling to show that the distinct pattern of $S$-wave travel time delays, waveform distortions, and amplitude patterns in region D reveals a circular anomaly about 100 km wide and about 400 km high (based on measurements of $S$-wave turning points) with a reduction in shear velocity of 5%. By considering dynamic modeling of relic slabs at the CMB that reveal plumes preferentially develop at the edge of slabs (e.g., Bower et al., 2013b; Heron et al., 2015; Nakagawa and Tackley, 2008; Tan et al., 2002), Sun et al. (2016) interpret their observations as a plume-like structure. A hot plume would produce a gap in the continuity of a $D^\prime$ reflector due to the temperature-dependent Br-PPv boundary (Bower et al., 2013b; Sun et al., 2009). This high, but relatively narrow, plume-like structure could be a feature that tomography models average over, thus explaining why several tomography models display low velocities near the CMB in this region.

The easternmost region (regions E and F) displays more complexity, such that the strong $SdS$ phase from a structure 270 km above the CMB requires a gradient increase in $V_S$ down to a depth of 2800 km, followed by a decrease in $V_S$ down to the CMB (Sun et al., 2016). This region F is also likely influenced by relic subducted slab debris that has reached the lowermost mantle (e.g., Bower et al., 2013a; Davies and Gurnis, 1986; Tackley, 2002). In their recent experimental investigations of the Br-PPv phase transition, Sun et al. (2018) showed that a pyrolite-like composition, (Mg$_{0.9}$Fe$_{0.1}$Al$_{0.1}$Si$_{0.9}$O$_{3}$) (Catalli et al., 2009), and a more Fe-rich composition (Mg$_{0.735}$Fe$_{0.21}$Al$_{0.07}$Si$_{0.965}$O$_{3}$) are characterized by Br-PPv phase transition widths of about 25 GPa and 450 km, respectively, with the more Fe- and Al-rich composition transitioning about 8 GPa lower (150 km shallower) than the pyrolite-like Br, a result that is in qualitative agreement with earlier experiments (Mao et al., 2004) and theoretical studies (e.g., Caracas and Cohen, 2008, 2007, 2005; Stackhouse et al., 2006). Both transitions are essentially incomplete at the CMB, thus unlikely to produce a sharp seismic reflector. As discussed above, anisotropy and/or focusing effects associated with the presence of relic slab debris could act to sharpen such an otherwise diffuse reflector. Nevertheless, the results presented in Sun et al. (2018) show that the bulk sound velocity gradient associated with a (Mg$_{0.735}$Fe$_{0.21}$Al$_{0.07}$Si$_{0.965}$O$_{3}$)-Br to PPv transition is positive, which is consistent with the seismic observation of a gradient increase in $V_S$ (region F, lower panel) (Sun et al., 2016). Some of the variability in seismic observations can also be explained by successive
Figure 8.6. The presence of phases such as δ-(Al,Fe)OOH (Ohira et al., 2019) and/or the NAL phase (Wu et al., 2016) could contribute to the observed seismic anomalies. For example, if a hydrated phase similar to that of δ-(Al,Fe)OOH is present (Ohira et al., 2019) and dehydrates as it heats up in the thermal boundary layer, then dehydration of this phase could partially melt the surrounding material, explaining the LVZ above the speculated slab-like feature. More petrology-inspired experiments under CMB conditions are certainly required to test these hypotheses.

The region beneath Alaska and the Bering Sea has also been shown to exhibit seismic anisotropy, such that observations of $V_{SH} > V_{SV}$ are interpreted as horizontally emplaced relic slabs (e.g., Cottaar et al., 2014; Fouch et al., 2001; Garnero and Lay, 1997; Lay and Young, 1991; Long, 2013; Matzel et al., 1996; Wyssession et al., 1999); see also Nowacki et al. (2011) for a review. Similar observations of seismic complexity in D" have been reported in other regions thought to be influenced by slab-like features. More petrology-inspired experiments under CMB conditions are certainly required to test these hypotheses.

In summary, the structure beneath the Aleutians, from the Bering Sea to Alaska, is complex. Considering that many tomographic models show an area of low velocities near the CMB beneath the Aleutians and fast velocities at ~2400 km depth, together with the regional waveform studies presented here, a consistent interpretation involves relatively large variations in temperature and composition, associated with the dynamics of relic slab debris. Recent experimental results on the complex characteristics of the bridgmanite to post-perovskite phase transition in a multicomponent system underscore these interpretations.

8.3. ULTRALOW VELOCITY ZONES

8.3.1. Seismic Observations

Within the D" layer, near the base of the mantle, lies a distribution of low and ultralow velocity zones (ULVZs) that are generally characterized by dimensions ranging from a few to tens of km thick, with lateral dimensions ranging from tens of km to ~800 km (e.g., Garnero and Helmberger, 1995; Hutko et al., 2009; Mori and Helmberger, 1995; Revenaugh and Meyer, 1997; Rost et al., 2006; Thorne et al., 2013). Several studies provide locations of ULVZs at the base of the mantle, which were summarized in McNamara et al. (2010) and more recently in Yu and Garnero (2018). The locations of select ULVZs near the borders of the large low seismic velocity (LLSV) anomalies beneath the Pacific and Africa led to the hypothesis that ULVZs may be connected to mantle upwellings and hotspots near the surface of the Earth (e.g., Burke et al., 2008; Torsvik et al., 2006; Williams et al., 1998; Yuan and Romanowicz, 2017).

ULVZs have been observed with a variety of seismic waves (see Figure 8.7). Figure 8.8 provides examples of detections of ULVZ in seismic data together with model ak135 (Kennett et al., 1995). Most often, the observations of SpKS and SKPds waves are used (e.g., Garnero and Helmberger, 1998, 1996; Thorne et al., 2020, 2013; Thorne and Garnero, 2004) and the modeling of travel times, amplitudes, and waveform of these waves yields velocity differences with respect to the average velocity at the CMB (e.g., Figure 8.8). SpKS and SKPds are waves that diffract for a short distance around the core (Pd) and travel as an SKS wave for the rest of the path with their amplitudes and travel times influenced by strong low-velocity regions near the CMB (e.g., Garnero and Helmberger, 1998; Thorne et al., 2020). Enhanced PKPdiff waves, i.e., waves that are diffracted around the core for a short distance, but traveling as PKP waves otherwise, can also be explained by trapping the diffracted energy near the CMB due to an ULVZ (Thomas et al., 2009; Wen and Helmberger, 1998a).

Another approach to image ULVZs is detailed modeling of pre- and postcursor amplitudes of PcP and ScP waves (Figures 8.7 and 8.8); the travel times and polarities of these waves surrounding PcP or ScP can be used to extract the velocity contrast, while also allowing the determination of the density contrast (e.g., Gassner et al., 2015; Hansen et al., 2020; Rost et al., 2010, 2006). Trade-offs in density and velocity were discussed in Zhang et al. (2018) for the small amplitude PcP waves at near nodal distances (0–12 degrees) and also by Braña and Helffrich (2004) for larger epicentral distances. In addition, as discussed in the section on the D" reflector, there is often a trade-off between velocity contrast and the modeled thickness of the patch. The 3D character of an ULVZ may also influence the results. Modeling studies by Wen and Helmberger (1998b), Thorne et al. (2013) and Vanacore et al. (2016) showed that some amplitude and timing differences of the waves used to detect ULVZs can result from the modeling method used (1D versus 2D, 2.5D modeling), a subject for more detailed studies in the future.

Coherent scattered waves (Figures 8.7 and 8.8) that arrive as precursors to PKPdiff have been explained by Ma et al. (2019) and Ma and Thomas (2020) as a result
of PKP waves with an ULVZ at the core-mantle boundary. Scattering observations as precursors to the PKP wave were reported in the 1930s (Gutenberg and Richter, 1934) and explored in more detail in the 1970s (e.g., Doorbos and Vlaar, 1973; Haddon and Cleary, 1974; King et al., 1974). Since these scattered waves travel a different path compared with PKP (e.g., Cleary and Haddon, 1972; Thomas et al., 1999; Vidale and Hedlin, 1998), they have shorter travel times and arrive up to 30 s before the PKP wave (Figure 8.7) and appear to display variations in amplitude and travel time with respect to a standard Earth model used for ULVZ detection.

PKP precursors, enhanced amplitudes of PKPbdiff, as well as PuP (reflection off the top of a ULVZ) together with PcP, ScS, and ScP. SPdKS and SKPdS differ by having the P-diffracted wave either on the source or on the receiver side. PKPbdiff and SPdKS/SPdS are also standard phases and their changes in amplitude and travel time with respect to a standard Earth model are used for ULVZ detection.

Figure 8.7 Ray paths of seismic phases for detection of ULVZs referred to in this chapter: SPdKS and SKPdS, PKPdf, and (coherent) PKP precursors, enhanced amplitudes of PKPbdiff, as well as PuP (reflection off the top of a ULVZ) together with PcP, ScS, and ScP. SPdKS and SKPdS differ by having the P-diffracted wave either on the source or on the receiver side. PKPbdiff and SPdKS/SPdS are also standard phases and their changes in amplitude and travel time with respect to a standard Earth model are used for ULVZ detection.

velocity anomalies at the CMB, providing an additional possibility to map new regions of ULVZs. Detailed analyses of density variations related to PKP precursors are, to our knowledge, not provided in the literature.

In a comprehensive global assessment of ULVZ studies, Yu and Garnero (2018) present several key findings: (i) modeling of seismic arrivals indicates a 3–25% drop in $V_p$, 6–50% drop in $V_S$, and that $8F_S:6V_P$ range from 1:1 to 6:1 (noting that many studies fix this ratio a priori at integer levels), (ii) ULVZ density contrast ranges from 0 to 22% higher than PREM following seismic waveform modeling, (iii) there is no statistically significant correlation of ULVZs detected using core-reflected phases and the location of hotspots on Earth’s surface, and (iv) there is no simple mapping of ULVZ locations and lowermost mantle reduced tomographic velocities, showing that a significant fraction of ULVZs are located outside these provinces. At the time of the Yu and Garnero (2018) global assessment, only 17.1% of the CMB had been sampled by ULVZ studies, with 10.3% of the total CMB amounting to positive ULVZ detection. In a new collection of 58,155 broadband recordings of the seismic phase SPdKS, roughly half of the CMB has now been sampled in a search for anomalous SPdKS waveforms (Thorne et al., 2020). Using a Bayesian approach, Thorne et al. (2020) determine the regions that have the highest probability of containing ULVZs. In their work they find several regions with ULVZ presence that were not previously detected. They also confirm other regions that were known to have ULVZs, but they find no obvious correlation with hotspots or LLSVP edges, as inferred from $S$-wave tomography. The source-receiver ambiguity (e.g., Thorne et al., 2020) creates some uncertainty, in that it is difficult to determine whether the wave was altered by structures at the entry into or exit from the core. A recent study using core-reflected ScP waves recorded by the Transantarctic Mountains Northern Network in Antarctica concluded that ULVZs may be ubiquitous along the CMB, thus not particularly associated with hotspot locations on Earth’s surface (Hansen et al., 2020).

Other characteristics of ULVZs include structures with a diffusive top or a vertical velocity gradient within, whereas others have been interpreted as multilayered structures (e.g., Yu and Garnero, 2018). However, it is likely premature to draw firm conclusions in this respect due to the effects of finite frequency on the sensitivity of different probes to the range of structures (e.g., Yu and Garnero, 2018). It is important to add to this summary that there have been few studies investigating the presence of seismic anisotropy within ULVZ structures. In a recent study using differential SKS-SKKS shear-wave splitting underneath Central Africa, Reiss et al. (2019) identify strongly discrepant splitting for those two waves in an area previously mapped as an ULVZ. Reiss et al.
suggest that this anomalous structure could be a ULVZ that contains certain alignments of partial melt or iron-rich (Mg,Fe)O (Finkelstein et al., 2018).

8.3.2. Plausible Explanations

Considering the wide range of anomalous wave speed reductions, two scenarios have been the primary focus for explaining the origin of ULVZs, namely partial melting and/or extreme chemical and phase heterogeneity. A third scenario, anisotropy of a low-velocity and low-viscosity solid phase, like iron-rich (Mg,Fe)O magnesiowüstite (Finkelstein et al., 2018; Reali et al., 2019a), will be explored here as well. We briefly summarize these three scenarios below.

**Partial Melt.** A partial melt origin for ULVZs presents a model suggesting that the $S$ to $P$ wavespeed reduction would be about 3:1 (e.g., Berryman, 2000; Hier-Majumder, 2014; Williams and Garnero, 1996), in which the velocities of the average assemblage are decreased by melt formed due to partial melting of the mantle and/or by fluid reaction products of the Fe-rich liquid outer core with silicate-rich mantle (e.g., Andraut et al., 2014; Jackson et al., 1987; Liu et al., 2016; Nomura et al., 2014; Ohtani and Maeda, 2001; Pradhan et al., 2015). The

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**Figure 8.8** (a–c) Examples of waves used for the detection of a ULVZ (black lines) with model ak135 (red lines). (a) Stronger amplitudes of PKP diffracted waves than predicted by standard Earth models. Event 4. Oct 2002 recorded at EAGLE stations. (b) SPdKS waves with higher amplitudes and shifted travel times compared with ak135. Event 25. May 1997 recorded at TWIST array (Kendall et al., 2002). (c) Coherent precursors to the wave PKPdf (event 9). April 2009 recorded at TA stations. Model ak135 is not shown here. (d) $PuP$ waves as precursors and postcursors to the wave $PcP$. Note that this example shows synthetic data for ak135 (red) and a model with a 7 km thick ULVZ (black).
hypothesis of melt origin has been drawn based in part on suggestions of a correlation between ULVZs and plume generation zones or hotspots (Torsvik et al., 2014; Williams et al., 1998). However, the assessment provided in Yu and Garnero (2018) showed that there is no statistically significant correlation of ULVZs and the location of hotspots on Earth’s surface. The recent studies of Thorne et al. (2020) and Hansen et al. (2020) also cast this correlation into doubt.

Although early dynamical calculations questioned the possibility to produce a dense and nonpercolating melt phase in the deep Earth (Hernlund and Tackley, 2007), a later study showed that the stirring of ULVZs by the larger-scale convective motions of the mantle can potentially maintain a partially molten region (Hernlund and Jellinek, 2010; McNamara et al., 2010). However, not only does the range of S to P wave speed reductions of partial melt assemblages depend on the melt distribution, but the actual reductions are not constrained experimentally or theoretically at CMB conditions. Shock wave measurements that constrained the densities of Fe-bearing silicate liquids suggest that for a range of plausible mantle compositions, candidate partial melts such as those similar to mid-ocean ridge basalt, would not be dense enough to remain at the CMB over reasonable timescales to be seismically observable at the base of the mantle today (Thomas and Asimow, 2013). The explanation of partial melt also requires a relatively special circumstance, that is the mantle geotherm needs to intersect the mantle solidus (neither of which are tightly constrained) just a few kilometers above the core-mantle boundary.

**Extreme Chemical or Phase Heterogeneity.** 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; Muir and Brodholt, 2015). This hypothesis partly inspired the notion of solid, iron-rich ULVZs, such as a metal-bearing layer (Knittle and Jeanloz, 1991), subducted banded iron formations (Dobson and Brodholt, 2005), hydrous iron peroxide (Liu et al., 2017), iron-rich post-perovskite (e.g., Mao et al., 2004; Stackhouse et al., 2006), and iron-rich (Mg,Fe)O (Chen et al., 2012; Dobrosavljevic et al., 2019; Labrosse et al., 2007; Solomatova et al., 2016; Wicks et al., 2017, 2010). The enhanced density of iron-rich systems compared to the surrounding mantle is also helpful in explaining the locations of ULVZs at the base of the mantle (e.g., Li et al., 2017). The preferential alignment of post-perovskite crystals has been implicated as the primary source for explaining such anisotropy near the base of the mantle (e.g., Ford et al., 2015; Oganov et al., 2005; Pisconti et al., 2019; Tommasi et al., 2018; Wu et al., 2017). However, these are relatively large regions compared with most ULVZs, and in regions characterized by high temperatures, such as at the base of upwellings or edges of slabs, the post-perovskite phase is not stable (e.g., Hernlund et al., 2005; Hirose, 2006; Shim, 2008) and other mechanisms are then required to explain the anisotropy, in particular, for regions of very low velocities.

Finkelstein et al. (2018) conducted high-resolution inelastic scattering measurements up to 41 GPa on a single crystal of (Mg,Fe)O magnesiowüstite with 76 mol% FeO and constrained the pressure dependence of the elastic tensor. They show that the cubic form of magnesiowüstite develops extreme elastic anisotropy at high pressures. Using the following definition of anisotropy:

\[
\text{anisotropy (\%)} = 100 \times \left( \frac{V_{\text{max}} - V_{\text{min}}}{(V_{\text{max}} + V_{\text{min}})/2} \right),
\]

the compressional and shear wave anisotropies of iron-rich (Mg,Fe)O rise up to 18 ± 3% and 58 ± 2%, respectively, at 31 GPa. Note that the shear anisotropy of PPs and iron-poor (Mg,Fe)O ferropericlase only reach values of about 30% and 40%, respectively, at lower mantle conditions, as summarized in Finkelstein et al. (2018). We compute the velocity ratios for magnesiowüstite along specific crystallographic directions from the elastic tensor measured at 31 GPa (see Table S3a in Finkelstein et al. 2018) and they are: [100] \( V_P/V_S = 3.15 \pm 0.16 \) and for [110] \( V_P/V_S \) ranges from 1.52 ± 0.08 \( (V_{SD}) \) to 2.76 ± 0.08 \( (V_{SI}) \). Provided the temperatures are below magnesiowüstite’s solidus, a 3:1 reduction ratio of S to P wave speeds could be explained with a preferred alignment of iron-rich magnesiowüstite, thus not requiring partial melt. We will quantitatively explore this hypothesis in the next section.

Provided the range and geographic diversity of ULVZ seismic observations to date (e.g., Thorne et al., 2020; Yu and Garnero, 2018), it is reasonable to consider that the chemical and physical characterizations of these structures vary from one ULVZ to another.

**8.3.3. Inversion of Iron-Rich Phase Assemblages with Seismic Observations**

Studies have indicated preferential iron partitioning into (Mg,Fe)O coexisting with bridgmanite or post-perovskite under the pressure-temperature conditions of Earth’s lower and lowermost mantle (e.g., Sinmyo et al., 2008; Tange et al., 2009). Further interest in the role of iron-rich (Mg,Fe)O at Earth’s core-mantle boundary has been drawn based on the very low sound speeds of this
material at pressures up to 120 GPa (Wicks et al., 2017, 2010) and the ability of silicate mixtures containing this material to reproduce the topography of some ULVZs (Bower et al., 2011). To broaden the scope of this hypothesis, we have developed a forward modeling approach through misfit minimization to solve for the concentration of a range of iron-rich (Mg,Fe)O compositions coexisting with bridgmanite (Dobrosavljevic et al., 2019; Sturhahn, 2020) that could match two different ULVZ seismic observations, underneath the S. Atlantic (Simmons and Grand, 2002) and Coral Sea (Rost et al., 2006).

In this chapter, we expand this approach by looking at several ULVZ case studies, while considering two iron-rich systems, (Mg,Fe)O and (Mg,Fe)SiO₃ PPv, as well as preferred alignments of iron-rich (Mg,Fe)O magnesiowüstite. Our approach consists of several phases with various material properties to match a set of target seismically observable ULVZ properties (VP, VS, and density) given in the literature. The seismically observable properties and estimated uncertainties are then converted to bulk and shear moduli in the mixing model. Specifically, the forward model is the set of minerals with elastic properties mixed together using the Voigt and Reuss mixing bounds (Watt et al., 1976), and the approach optimizes the concentrations of each mineral phase to minimize the misfit with the seismic observables. The variances (or uncertainties) of mineral properties and seismic targets (observations) are included in the inversion strategy, and best-fit properties of the inversion are evaluated with parameter correlations.

For the iron-rich (Mg,Fe)O assemblage, the description and selection of elastic properties are given in Dobrosavljevic et al. (2019) and briefly summarized here. The composition of bridgmanite coexisting with (Mg₀.०६Fe₀.८४)O was calculated using KD (8.2). This is relatively iron-poor and thus in the low-spin state at 130 GPa and 3000 K. The elastic properties for low-spin ferropericlase are taken from a theoretical study of the thermoelastic properties of (Mg₀.८०Fe₀.२०)O through the spin crossover up to 130 GPa and 4000 K (Wu and Wentzcovitch, 2014). The elastic properties of these three phases used in the Fe-rich PPv inversions are listed in Appendix Table 8.A1.

In the case where we explore the anisotropy of magnesiowüstite (Case 5), we use recent high-energy resolution inelastic X-ray scattering results on single-crystal B1-structured (Mg,Fe)O containing 76 mol% FeO, measured at 31 GPa (Finkelstein et al., 2018). This particular compression point displays the largest measured elastic anisotropy in the measured dataset. As an estimate of the properties of an assemblage containing preferred alignments of anisotropic magnesiowüstite, we start from the isotropic velocities and density of (Mg₀.०६Fe₀.८४)O at 135.8 GPa and 3800 K, as given in Dobrosavljevic et al. (2019) and used in our assemblages of randomly oriented crystals. We then apply the VP:VS ratios computed at 31 GPa from the elastic tensor (see section on Anisotropy above) and obtain the following values for preferred alignments along [110]: VP = 9.07 ± 0.14 km/s, VS = 3.29 ± 0.09 km/s and along [100]: VP = 9.07 ± 0.14 km/s, VS = 2.88 ± 0.08 km/s. From these values, we then calculate the bulk and shear moduli for the mixing model.

With these inversions, we aim to quantify the phase proportions within the proposed assemblages that can generate ULVZ seismic signatures within their respective uncertainties. We constrain the concentrations of two of the phases, such as Br14 and Mw84, which allows the determination of the CaPv concentration. We analyze five different ULVZ case studies, which are described below and summarized in Table 8.1. The locations of these case studies are shown as red areas in Figure 8.2. Select results are plotted in Figures 8.9 and 8.10. In this study, we focus on the Reuss bound results. For ULVZ case studies that include Voigt bound results, see Dobrosavljevic et al. (2019).

ULVZ Case 1: Europe and Western Asia. Gassner et al. (2015) studied the CMB under the Volga River region of Europe and western Asia. Their study searched for and analyzed precursors to PcP to assess characteristics of the CMB in this region. Modeling of the amplitudes and travel times of the precursors showed that a range of VP and VS reductions were needed to explain the PcP precursors (δVP: ~5% to ~10%, δVS: ~15% to ~30%), as well as a gradient in density (δρ: ~5% to δρ: ~15%, including up to ~30%) for a ~13 km thick ULVZ. The ULVZ properties are estimated with respect to PREM velocities and density at 135.8 GPa. We use the following seismic observables in our inversion: ~5% δVP, ~15% δVS, and ~15% δρ, with respect to PREM,
Table 8.1 | Seismic observations and best fitting Reuss–bound results for the five ULVZ case studies. (a) Mineral phase properties for Cases 1–4 are (Mg0.86Fe0.14)SiO3–bröggenite, (Mg0.16Fe0.84)O, and CaSiO3 perovskite (Dobrosavljevic et al. 2019). For Case 5, we use the elastic properties of Mw84 computed for the two crystallographic directions in magnesiowüstite representing the highest levels of elastic anisotropy. Given are vol% of Br14, Mw84 and CaPv. (b) Mineral phases are (Mg0.60Fe0.40)SiO3 post–perovskite, low–spin (Mg0.80Fe0.20)O ferropericlase and CaSiO3 perovskite (Appendix Table 8.A1). Given are vol% of PPv40, Fp20 and CaPv. Results for all cases of percent reductions (δVP and δVS) and elevations (δρ) are with respect to PREM at the CMB. For Central America and the Coral Sea, a few different seismic studies are used. See text for details on the individual case studies and Dobrosavljevic et al. (2019) for a description of the inversion approach.

<table>
<thead>
<tr>
<th>Table 8.1</th>
<th>Input seismic values for inversion [Values or range from seismic studies]</th>
<th>Best fit mineral proportions</th>
<th>Best fit seismic properties [Deviation from PREM at the CMB]</th>
</tr>
</thead>
<tbody>
<tr>
<td>δVP, δVS, δρ (%)</td>
<td>δVP/δVP</td>
<td>Br14* (vol%)</td>
<td>Mw84 (vol%)</td>
</tr>
<tr>
<td>Case 1. Europe and W Asia</td>
<td>(Volga River Region)</td>
<td>–5(3), –15(3), 15(10)</td>
<td>[–5 to 10, –15 to 30, 5 to 30]</td>
</tr>
<tr>
<td>Case 2. NW America</td>
<td></td>
<td>–5(3), –8(2), 0(3)</td>
<td>[–2 to 6, 10 to 10, 1]</td>
</tr>
<tr>
<td>Case 3. Central America</td>
<td></td>
<td>(a) –10(2), –20(2), 14(5)</td>
<td>[–10, –20, 14]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(b) –10(2), –30(2), 1(1)</td>
<td>[–10, –30, 1]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>–10, –30, 1</td>
<td>(no uncertainties)</td>
</tr>
<tr>
<td>Case 4. Coral Sea</td>
<td></td>
<td>(a)</td>
<td>–10(2), –10(2), 6(3)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(b)</td>
<td>–10(2), –30(2), 10(5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(c)</td>
<td>–10(2), –35(2), 20(5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(d)</td>
<td>–10(2), –50(2), 15(5)</td>
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<tr>
<td></td>
<td></td>
<td>(e)</td>
<td>–8(3), –35(15), 5(5)</td>
</tr>
<tr>
<td></td>
<td>(continued overleaf)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(100) alignment</td>
<td></td>
</tr>
<tr>
<td>Case 5. Anisotropic magnesiowüstite</td>
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<td>NW America</td>
<td>–5(3), –8(2), 0(3)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Europe and W Asia</td>
<td>–5(2), –15(2), 5(5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Central America</td>
<td>–10(2), –30(2), 1(1)</td>
</tr>
</tbody>
</table>
Table 8.1 (continued)

<table>
<thead>
<tr>
<th>Table 8.1a</th>
<th>Input seismic values for inversion</th>
<th>Best fit mineral proportions</th>
<th>Best fit seismic properties</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[Values or range from seismic studies]</td>
<td></td>
<td>[Deviation from PREM at the CMB]</td>
</tr>
<tr>
<td>δVP, δVS, δρ (%)</td>
<td>δVP, δVS, δρ (%)</td>
<td>Br14* (vol%)</td>
<td>Mw84 (vol%)</td>
</tr>
<tr>
<td>case (d)</td>
<td>–10(2), –30(2), 10(5)</td>
<td>3</td>
<td>70(4)</td>
</tr>
<tr>
<td>[110] alignment</td>
<td>case (a)</td>
<td>NW America</td>
<td>[2 to 3]</td>
</tr>
<tr>
<td>case (b)</td>
<td>Central America</td>
<td>–10(2), –30(2), 11(1)</td>
<td>3</td>
</tr>
</tbody>
</table>

Target seismic input values and their estimated uncertainties (in parentheses) are provided. The 1σ (68%) uncertainties for the results are given in parentheses for the last reported significant digit(s) of the best fitting phase assemblage (mineral proportions and phase assemblage seismic wave speeds and density).  For Br14, a starting value of 0.70 with a prior window of 0.05 was used, because of the strong trade-off between Br and CaPv due to their similar elastic properties at the CMB.

Table 8.1b

<table>
<thead>
<tr>
<th>Input seismic values for inversion</th>
<th>Best fit mineral proportions</th>
<th>Best fit seismic properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Values or range from seismic studies]</td>
<td></td>
<td>[Deviation from PREM at the CMB]</td>
</tr>
<tr>
<td>δVP, δVS, δρ (%)</td>
<td>δVP, δVS, δρ (%)</td>
<td>PPv40a,b (vol%)</td>
</tr>
<tr>
<td>Case 1. Europe &amp; west Asia (Volga River Region)</td>
<td>–5(3), –15(3), +15(10)</td>
<td>8*</td>
</tr>
<tr>
<td>Case 2. NW America</td>
<td>–5(3), –8(2), 0(3)</td>
<td>6*</td>
</tr>
<tr>
<td>Case 3. Central America</td>
<td>–10(2), –30(2), +1(1)</td>
<td>47*</td>
</tr>
</tbody>
</table>

Target seismic input values and their estimated uncertainties (in parentheses) are provided. The 1σ uncertainties for the results are given in parentheses for the last reported significant digit(s) of the best fitting phase assemblage (mineral proportions and phase assemblage seismic wave speeds and density).  For CaPv, a starting value of 0.20 for CaPv with a prior window of 0.10 was used, because of the strong trade-off with Fp20 due to their similar elastic properties at the CMB.  These inversions use a starting value of 0.70 for PPv40b with a prior window of 0.10, because of the strong trade-offs with Fp20 and CaPv.
and assigned uncertainties of 3% for \( V_P \) and \( V_S \) and 10% for \( \rho \), to account for the range of seismic models presented in Gassner et al. (2015), and determine the best-fit mineral proportions. Our best-fitting model results in 71(5) vol\% Br14, 17(7) vol\% Mw84 and 12 vol\% CaPv, where the number in parentheses represents the 1σ error of the last significant digit from the inversion. This implies that within the uncertainties of both the mineral elastic properties and the estimated uncertainties in the seismic observations, \( \delta V_S = -13\% \), \( \delta V_P = -6\% \) and a density contrast of \( \delta \rho = +7\% \), with \( \delta V_S : \delta V_P \) of 2.1(1) provides a good fit for this region (see Figure 8.9a and Table 8.1a).

When testing whether the presence of iron-rich post-perovskite can fit these seismic observations, the results are not well-constrained, in part due to the wide range of elastic properties reported for iron-rich PPv (Caracas and Cohen, 2008; Mao et al., 2006) (Appendix Table 8.A1). Using these different sets of elastic properties, the results of the inversions show very large uncertainties and point to a mantle phase assemblage that requires either a very large fraction of (Mg,Fe)O ferropericlase and a negative density anomaly or no ferropericlase and a positive density anomaly: 8% PPv40 (Mao et al., 2006), 72(17)% Fp20, and 20(14)% CaPv (with \( \delta \rho = -1.4\% \)), for an assemblage with 69(16)% PPv40 (Caracas and Cohen, 2008), 31(16)% CaPv, and no ferropericlase, with \( \delta \rho = +4\% \) (Table 8.1b).

**ULVZ Case 2: NW America.** Sun et al. (2013) used SKPdS and SKKS to study the CMB region underneath Nevada and British Columbia in a region where high velocities were reported in most tomographic models and previously thought devoid of ULVZs (Rost et al., 2010). Their analysis of differential travel times for SKPdS and SKKS show regions with and without small-scale structures near the CMB, with heights ranging from 0 to 100 km and velocity variations for \( \delta V_P \) and \( \delta V_S \) centered on \( -5 \pm 3 \) and \( -8 \pm 2\% \), respectively, indicating large-topography lowvelocity regions that are not detected with tomographic inversions (Sun et al. 2013). Although their modeling of travel times does not provide constraints on density, their interpretation of the proportion of iron-rich oxides in this region suggested a density elevation of 1.5–2%. However, this density elevation was calculated using older equations of state and did not consider the presence of CaPv. We model concentrations of Br14, Mw84, and CaPv with the consideration that no constraints on density were reported (a value of 0% ± 3% for \( \delta \rho \) was used as an input). We find 69(7) vol\% of Br14, 12(5) vol\% of Mw84, and 20 vol\% CaPv, which leads to a best-fit density of 5.8(1) g/cm³ (\( \delta V_P, \delta V_S, \delta \rho = -3.2\%, -7.6\%, +4\% \) compared with PREM) (see Table 8.1a and Figure 8.9a). When testing whether an Fe-rich PPv assemblage can explain these observations, we find similar extreme ranges of phase assemblages as we found for Case 1 (Table 8.1b).

**ULVZ Case 3: Central America.** In their review of ULVZs, Yu and Garnero (2018) also assessed ULVZ location with respect to high-velocity regions in a range of tomographic models, finding 11% of the ULVZs are shaded.
located within seismically fast regions of tomography models, regions often associated with down-wellings (e.g., Frost and Rost, 2014; Koelmeijer et al., 2016; Ritsema et al., 2011; Simmons et al., 2010). One of these regions lies beneath Central America and has been extensively sampled by core-reflected phases (PeP and ScS, e.g., Kito et al., 2007). This is a region where strong lateral seismic velocity gradients exist (Thorne et al., 2004) and a transition from relatively slow wave speeds in the northeast Pacific LLSVP to relatively fast wave speeds eastward (Frost and Rost, 2014; Simmons et al., 2010).

Near this region, Havens and Revenaugh (2001) use PeP-waves and detect a 10–20 km thick ULVZ beneath Mexico. They find \( \delta V_S : \delta V_P = 2 \) with \( \delta \rho = 14\% \) relative to PREM for three of their four models/locations studied, which leads to a well-constrained presence of 26(2)\% iron-rich (Mg,Fe)O as Mw84, coexisting with 70(2)\% Br14 and 4\% CaPv, resulting in \( \delta V_S : \delta V_P = 1.94(9) \) with \( \delta \rho = 11.3\% \) (see Table 8.1a and Figure 8.9a).

In their fourth location underneath Central America, they report ~10\% in \( V_P \) and ~30\% in \( V_S \) (\( \delta V_S : \delta V_P = 3 \) with \( \delta \rho = 1\% \)). Using these values as inputs with a rough estimate of the uncertainties, the inversion results in a smaller \( \delta V_S \) (~12\%). If no uncertainties are placed on the seismic observation for the inversion, no solution is reached for the case of iron-rich (Mg,Fe)O. Thus, with such a negligible elevation in density and a large decrease in S-wave speed, iron-rich (Mg,Fe)O is an unlikely explanation (Table 8.1a). When testing whether the presence of Fe-rich PPv can fit these seismic observations, the results require a significant fraction of ferropericlase: 47\% PPv40 (Mao et al., 2006), 34(6)\% Fp20, and 19(6)\% CaPv (Table 8.1b). There is no solution within 1\( \sigma \) if the elastic properties of PPv40 from Caracas and Cohen (2008) are used. In this scenario, where the velocities are significantly reduced (~10\% in \( V_P \) and ~30\% in \( V_S \)) and the density contrast is close to zero, partial melt may provide an explanation. Indeed, as discussed in our case study in the D\( ^{\prime} \) section, dynamic simulations predict patches of very low seismic velocity beneath and at the edges of large-scale high-velocity structures (slabs) at the CMB (Tan et al., 2002), due to higher-than-average temperatures. This scenario could lead to partial melting. However, there remains a challenge of stabilizing partial melts such that they are seismically observable, and the range of \( S \) to \( P \) wave speed reductions of a partial melt assemblage, melt-pocket geometries and the relative thermal profiles of the solidus and geotherm are not well constrained at CMB conditions.

ULVZ Case 4: Coral Sea. The CMB region underneath the Coral Sea, located just off of the east coast of Australia, has been extensively studied using core-reflected phases (e.g., Brown et al., 2015; Koper and Pyle, 2004; Rost et al., 2010, 2006, 2005; Rost and Revenaugh, 2003), PKP (Koper and Pyle, 2004; Thomas et al., 2009) and SKS (Jensen et al., 2013). This region is within the southwest corner of the Pacific LLSVP (Frost and Rost, 2014; Simmons et al., 2010).

In many of these studies, both \( \delta V_S \) and \( \delta V_P \) have been reported (typically \( \delta V_P \) around ~10\%), but vary significantly in their relative \( \delta V_S \) decrements. In most of these studies, density elevations have also been reported. We consider the following observations that have been made: (Case 4a) \( \delta V_S : \delta V_P = 1 \) and \( \delta \rho = 6\% \) (Brown et al., 2015), (Case 4b) \( \delta V_S : \delta V_P = 3 \) (Jensen et al., 2013; Rost et al., 2010, 2006; Rost and Revenaugh, 2003) and \( \delta V_S : \delta V_P = 3.125 \) (Rost et al., 2005) with \( \delta \rho = 10\% \), (Case 4c) \( \delta V_S : \delta V_P = 3.5 \) and \( \delta \rho = 20\% \) (Koper and Pyle, 2004), (Case 4d) \( \delta V_S : \delta V_P = 5 \) and \( \delta \rho = 15\% \) (Rost and Revenaugh, 2003), and (Case 4e) \( \delta V_S : \delta V_P = 2.5–5 \) with no constraints on density elevation, using PKP diffracted waves (Thomas et al., 2009) (Table 8.1a).

We primarily focus on iron-rich (Mg,Fe)O assemblages, due to the challenges discussed above involving Fe-rich PPv assemblages. The best-fit concentrations of the minerals for the Coral Sea observations are provided in Table 8.1a. We find for Cases 4a and 4e that although the resulting best fit concentrations of Br14, Mw84, and CaPv are similar, the uncertainties for case 4e are significantly larger, mostly due to the loose seismic constraints provided in Case 4e (Figure 8.9a). The best fit value that considers the mutual uncertainties in mineral physics properties and seismic properties and seismic observations is for density elevations around 6–7\%, with a \( \delta V_S : \delta V_P \approx 2.2 \) for concentrations of around 70\% Br14, 15\% Mw84, and 15\% CaPv. Therefore, in the Coral Sea region, seismic observations that tightly constrain \( \delta V_S : \delta V_P \approx 2 \) can be explained by the presence of iron-rich (Mg,Fe)O. Whereas higher ratios of seismic reductions associated with large negative velocity contrasts and large positive density contrasts yield no solution for Fe-rich (Mg,Fe)O or Fe-rich PPv, within 1\( \sigma \), and likely require different explanations.

ULVZ Case 5: Anisotropy. The cases we have explored thus far have assumed isotropic wave velocities of the individual phases and randomly orientated aggregates. As discussed in the section on D\( ^{\prime} \), mantle dynamics could induce large-scale flow (McNamara et al., 2002, 2001), which could be seismically detected (e.g., Kendall and Silver, 1998, 2000, Nowacki et al., 2010). Crystals in this flow field could align to produce observable seismic anisotropy and this has been tested for the D\( ^{\prime} \) region using mineral physics results of iron-poor PPvs and iron-poor (Mg,Fe)O (e.g., Antonangeli et al., 2011; Crowhurst et al., 2008; Immoor et al., 2018; Jackson et al., 2006; Marquardt et al., 2009; Tommasi et al., 2006; Tommasi et al., 2018). The role of anisotropy for the detection and seismic properties of ULVZs, in particular the role
iron-rich (Mg,Fe)O magnesiowüstite, has only recently been explored (Finkelstein et al., 2018; Reiss et al., 2019).

The northeast Pacific region is characterized by complex seismic anisotropy signatures (see Nowacki et al., 2011 for a review), where some studies suggest \( V_{SH} > V_{SV} \) (Fouch et al., 2001; Vinnik et al., 1998, 1995, 1989), \( V_{SH} < V_{SV} \) (Kawai and Geller, 2010; Ritsema et al., 1998) as well as both (Pulliam and Sen, 1998; Russell et al., 1999, 1998) and, further south, isotropy (Kendall and Silver, 1998). As described above, (Mg,Fe)O magnesiowüstite displays compressional and shear wave anisotropies approaching 20% and 60%, respectively. We now replace randomly oriented Mw84 with preferred alignments of magnesiowüstite in the [110] and [100] crystallographic directions \( (V_S:V_P \text{ of } 2.76 \text{ and } 3.15, \text{ respectively}) \) and explore a few of the ULVZ regions discussed above. We find that \( \delta V_S: \delta V_P = 3.3(1) \) and 2.64(8) can be achieved by aligning 8(2)% and 13.0(5)% of the magnesiowüstite crystals in the [100] crystallographic direction. For the ULVZ cases explored, \( \delta V_S: \delta V_P \approx 2 \text{ to } 3.3 \) can be achieved with preferred alignments of iron-rich (Mg,Fe)O (Table 8.1a). Thus, \( \delta V_S: \delta V_P \approx 3 \) is achieved without the need for partial melt to be present. In general, the cases of preferred alignment of magnesiowüstite lead to reduced \( 1\sigma \) uncertainties and less parameter correlations, compared with the assemblages involving randomly orientated crystallites. These conclusions are best illustrated in Figures 8.9 and 8.10.

Evidence from studies on iron-poor (Mg,Fe)O suggest that the magnitude of seismic anisotropy originating from (Mg,Fe)O would be determined by the active slip systems and deformation partitioning between all coexisting phases (e.g., Merkel et al., 2007; Miyagi et al., 2010; Girard et al., 2012; Yamazaki et al., 2014; Marquardt and Miyagi, 2015; Wu et al., 2017; Immoor et al., 2018; Thielmann, et al., 2020). Currently, the active slip systems in iron-rich (Mg,Fe)O and the effect of deformation partitioning between silicates (e.g., Reali et al., 2019b) and relatively low-viscosity magnesiowüstite (Reali et al., 2019a) are not well-understood at lower-mantle conditions, thus we refrain from speculating further on this topic. Future work is needed in order to precisely map alignment of magnesiowüstite from strain fields induced by mantle convection.

### 8.3.4. ULVZ Topography

The density of a magnesiowüstite-bearing ULVZ has been shown to affect ULVZ topography (Bower et al., 2011). Many of the ULVZ case studies examined here show that for seismic observations of \( \delta V_S: \delta V_P \approx 2 \text{ to } 3 \), an assemblage containing iron-rich (Mg,Fe)O provides a good explanation, corresponding to \( \delta \rho \) ranging from about +2 to +13%. The lower-density elevations would correspond to a buoyancy number of about 1, which would maintain topographic relief (20–70 km) (Bower et al., 2011; Sun et al., 2013). Density elevations of around 7% would lead to buoyancy values between 4 and 5, sustaining structures up to about 35 km thick. For density elevations greater than 7%, the buoyancy values would be > 5, normally leading to topographically “flat” structures at the CMB. However, there may be a possibility to produce a garden of assorted ULVZ structures (variable heights and topography) at the CMB (Wen and Helmberger, 1998b) with magnesiowüstite-bearing assemblages, considering the possibility of dynamic stirring of a low-viscosity phase such as iron-rich (Mg,Fe)O (Reali et al., 2019a). Similar mechanisms were explored with partially molten ULVZs, that is stirring or deformation of ULVZs by the larger-scale convective motions of the mantle (Hernlund and Jellinek, 2010; McNamara et al., 2010), suggesting the possibility of maintaining such a low-viscosity solid phase like iron-rich magnesiowüstite with relatively high topographic relief.

#### 8.3.5. Summary of ULVZ Case Studies

We explored four distinct geographic regions containing ULVZs and performed a best-fitting analysis with assemblages containing Fe-rich (Mg,Fe)O and PPv, and preferred alignments of Fe-rich (Mg,Fe)O. We see that the large discrepancy in elastic properties of Fe-rich PPv reported from ab initio calculations (Caracas and Cohen, 2008) compared with those from experiments (Mao et al., 2006) (Appendix Table 8.A1) lead to very different conclusions about the amount of PPv present and density contrasts (some are negative), while yielding relatively unconstrained proportions of phases (Table 8.1b).

The case studies explored here show that seismic observations providing \( \delta V_S: \delta V_P \approx 2 \text{ to } 3 \), with \( \delta \rho \) ranging from about +2 to +13%, can be explained by the presence of an aggregate containing randomly oriented or preferred alignments of iron-rich (Mg,Fe)O magnesiowüstite (Table 8.1a and Figure 8.9). In many cases, preferred alignments of magnesiowüstite significantly improve the fits to the seismic observations (Figure 8.10). For example, preferred alignment of 8% magnesiowüstite grains with [100] orientations provides a very good match to \( \delta V_S: \delta V_P = 3.3(1) \). These results are consistent with the recent seismic study of Reiss et al. (2019) that performed forward modeling of single-crystal elasticity data presented in Finkelstein et al. (2018) to suggest that the alignment of 12% magnesiowüstite crystals is a viable interpretation of SKS-SKKS splitting discrepancy beneath Central Africa. A full quantitative evaluation of the hypothesis that aligned iron-rich (Mg,Fe)O can explain ULVZ properties would require the inclusion of
a geodynamic model that predicts total strain development, as well as knowledge of the active slip systems of iron-rich (Mg,Fe)O and how strain partitions between lower mantle phases that are characterized by relatively large viscosity contrasts.

For cases of well-constrained velocity ratios (that is seismic uncertainties of less than 1%), the observations of $\delta V_S/\delta V_P \geq 3$ associated with larger velocity reductions ($\approx -10\%$ in $V_P$ and $\geq -30\%$ in $V_S$) and $\delta \rho \approx 1\%$ (some regions under Central America, for example) yield no solution for Fe-rich (Mg,Fe)O or Fe-rich PPv, within 1σ. Small density contrasts could be achieved by partial melts of the lowermost mantle (Thomas and Asimow, 2013), although the velocity reductions of these assemblages require more study. Observations reporting $\delta V_S/\delta V_P \geq 3$ associated with large velocity reductions and high density contrasts ($\delta \rho \approx 6$ to 13%) remain challenging to explain. Explaining these latter cases not only require having better experimental and theoretical constraints on the range of expected petrologies and their elastic properties at CMB.

Figure 8.10 Corner plot showing error correlation ellipses (1σ) from the best-fitting results of select ULVZ case studies (Table 8.1a and Figure 8.9). Solid ellipses correspond to the results with randomly oriented Br14, Mw84, and CaPv. Dotted ellipses are for the same regional ULVZ seismic observations, but for cases involving anisotropy; preferred orientations of Mw84 are indicated in the legend. For reference, $V_P = 13.72$ km/s, $V_S = 7.26$ km/s, and density = 5.57 g/cm$^3$ at the CMB (PREM).
conditions, but a better understanding of how melt would be distributed, and the trade-offs between shape, thickness, and velocity reduction of these structures.

### 8.4. SUMMARY AND CONCLUSIONS

We have shown a range of observations for the D" region, while exploring some of the complexity and causes for select seismically observed structures, such as reflectors and ultralow velocity zones (Figure 8.11).

While several observables such as travel time, amplitudes, polarities and waveforms constrain certain properties of the structures, there are trade-offs within these observables and with other factors. For example, travel times, which constrain the depth of a reflector are influenced not only by the reflection depth but by path deviations, attenuation, and anisotropy. Amplitudes are affected by attenuation, velocity, and density jumps and their gradients, as well as anisotropy. It is therefore not straightforward to interpret observables without taking all factors into consideration.

We present a case study of the D" reflector in a region beneath the Aleutians where our observations range from nondetection to complex waveforms, with most of the imaged region characterized by a positive velocity jump across D". Tomographic models of this region also show strong variations in their resolved velocities, both laterally and with depth, with some tomographic models indicating a low velocity region. Our interpretation of the complex seismicity in this region indicates that there is a need for changes in mineral phase assemblages, their compositions, and their temperature across relatively small distances, all of which requires changes in the dynamics over similarly small distances. A consistent interpretation involves the dynamics of subducted slab debris, corroborated with the complex mineral physics characteristics of the bridgmanite to post-perovskite phase transition in multicomponent systems.

On the shorter-scale end of observations, we concentrate on ultralow velocity zones: the travel times and amplitudes of waves imaging ultralow velocity zones lead to a large number of published velocity variations in $V_P$ and $V_S$, while a subset of these studies also provide constraints on density. The observables of these structures can be influenced by other factors as discussed above, thus requiring the need to consider their trade-offs and exercise caution when interpreting one observable alone. We use the published $V_P$ to $V_S$ decrements and density for a range of case studies to invert for compositionally distinct ULVZ phase assemblies. In this chapter, we also explore the effect of preferred alignments of elastically anisotropic magnesiowüstite for causing ultralow velocity regions.

While considering assemblages that contain either iron-rich (Mg,Fe)O or iron-rich post-perovskite, we discussed several challenges to explain ULVZs with iron-rich post-perovskite. Phase assemblages that include iron-rich (Mg,Fe)O magnesiowüstite provide the best matches to many of the ULVZ case studies examined here: (i) if the seismic observations have the uncertainties and trade-offs that we apply in our analysis, then a velocity reduction ratio of $\delta V_S/\delta V_P \approx 2$ for a wide-range of velocity decrements and density elevations can be explained by a mixture of randomly oriented magnesiowüstite, bridgmanite, and calcium silicate perovskite, and (ii) for cases with $\delta V_S/\delta V_P$ ranging from 2 to 3, preferred alignment of a small amount of iron-rich (Mg,Fe)O crystals could explain the observations. Reduction ratios below 2 or above 3, particularly with large density enhancements for the latter, require different explanations than those considered here. Our analysis therefore suggests a large diversity of ULVZs, rather than a single origin.

The mounting collection of seismic studies observing the D" region, in particular the increase in spatial coverage, will provide unprecedented constraints on the three-dimensional characteristics and distribution of these structures. In combination with geochemical analysis, mineral physics results, and geodynamical modeling, future studies will enhance our understanding of the causal links between the diversity and origin of structures at Earth’s core-mantle boundary and the changes in surface processes over geologic time.

**Figure 8.11** Schematic showing possible interactions between slabs, plumes, ultralow velocity zones (ULVZs) and large low seismic velocity provinces (LLSVP). Scatterers could be parcels of relic slab debris (faster wave velocities: blue dashes) or iron-rich parcels related to ULVZs (slower wave velocities: red dashes). Slabs can induce large-scale flow to push LLSVPs aside, while crystals such as iron-rich (Mg,Fe)O magnesiowüstite could align (black lines) within ULVZs, producing observable seismic anisotropy. Dynamics involving slabs and/or the presence of iron-rich (Mg,Fe)O may also feed or cause upwellings in the form of deep-seated plumes. Note that the D" reflector (black dashed thick and thin lines) could be located in regions that are imaged as faster or slower than average seismic wave speeds in tomography studies. Source: Modified from Sun et al. (2019).
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APPENDIX

Appendix Table 8.A1  Seismic properties and their uncertainties for (Mg0.60Fe0.40)SiO3 post-perovskite, (Mg0.80Fe0.20)O ferropericlase, CaSiO3 perovskite, calculated at 130 GPa and 3000 K from their bulk and shear elastic moduli.

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aMao et al., (2006)
bCaracas and Cohen (2008); Dorfman and Duffy (2014); Wentzcovitch et al. (2010)
cWu and Wentzcovitch (2014)
dGréaux et al. (2019)

Appendix Table 8.A2  Events used for examples in Figures 3, 5, and 8 (1–10) and events for the Bering Sea study (11–28). Earthquake parameters are from NEIC (National Earthquake Information Centre, United States Geological Survey). For events 11–28, reflector depths are calculated with the P wave as reference phase. A star (*) means no PdP reflection despite good signal to noise ratio. ‘-’ indicates events for which not enough traces were recorded for the event or where the epicentral distance was too large.

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