Implications of grain-size evolution on the seismic structure of the oceanic upper mantle

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Abstract: We construct a 1-D steady-state channel flow model for grain size evolution in the oceanic upper mantle using a composite diffusion-dislocation creep rheology. Grain size evolution is calculated assuming that grain size is controlled by a competition between dynamic recrystallization and grain growth. Applying this grain size evolution model to the oceanic upper mantle we calculate grain size as a function of depth, seafloor age, and mantle water content. The resulting grain size structure is used to predict shear wave velocity (V_S) and seismic quality factor (Q). For a plate age of 60 Myr and an olivine water content of 1000 H/10^6Si, we find that grain size reaches a minimum of ~15 mm at ~150 km depth and then increases to ~20–30 mm at a depth of 400 km. This grain size structure produces a good fit to the low seismic shear wave velocity zone (LVZ) in oceanic upper mantle observed by surface wave studies assuming that the influence of hydrogen on anelastic behavior is similar to that observed for steady state creep. Further it predicts a viscosity of ~10^{19} Pa s at 150 km depth and dislocation creep to be the dominant deformation mechanism throughout the oceanic upper mantle, consistent with geophysical observations. We predict larger grain sizes than proposed in recent studies, in which the LVZ was explained by a dry mantle and a minimum grain size of 1 mm. However, we show that for a 1 mm grain size, diffusion creep is the dominant deformation mechanism above 100–200 km depth, inconsistent with abundant observations of seismic anisotropy from surface wave studies. We therefore conclude that a combination of grain size evolution and a hydrated upper mantle is the most likely explanation for both the isotropic and anisotropic seismic structure of the oceanic upper mantle. Our results also suggest that melt extraction from the mantle will be significantly more efficient than predicted in previous modeling studies that assumed grain sizes of ~1 mm.

Key Words: asthenosphere, grain size, oceanic upper mantle, seismic low velocity zone.

1. Introduction

Grain size is a key microstructural property of the Earth's mantle, because it influences rheology, deformation mode (e.g., diffusion vs. dislocation creep), seismic attenuation and wave-speeds, electrical conductivity, and melt permeability. However, due to the lack of direct constraints, and because grain size evolves in response to the surrounding flow field, little is known about the distribution of grain size in the upper mantle. While grain size is often estimated using a piezometric relationship, in which grain size is directly related to stress (e.g., *Twiss*, 1977; *Karato et al.*, 1980; *van der Wal*, 1993), more recent studies have proposed models in which grain size evolution is also sensitive to temperature and strain rate (*de Bresser et al.*, 2001; *Hall & Parmentier*, 2003; *Montési & Hirth*, 2003; *Austin & Evans*, 2007). However, to date these evolutions laws have not been incorporated in large-scale models of mantle flow, despite the potential importance of feedbacks between grain-size, rheology, and deformation.

Accurate estimates of grain size are important for interpreting upper mantle seismic structure. Laboratory data show that in addition to the well-known temperature-dependence of shear-wave speed (V_S) and attenuation (Q) (*Minster & Anderson*, 1981), V_S and Q are also sensitive to grain size (*Tan et al.*, 2001; *Cooper*, 2002; *Jackson et al.*, 2002). By extrapolating these data to upper mantle conditions the commonly observed low shear wave velocity zone (LVZ) beneath the ocean basins (e.g., *Gutenberg*, 1948) (Figure 1) can be explained by variations in grain size without requiring the presence of melt, H_2O, and/or compositional variations (*Faul & Jackson*, 2005). The origin of the LVZ is important for understanding global mantle convection, because this zone is thought to represent a region of low viscosity, which accommodates plate motions and promotes plate tectonics (*Richards et al.*, 2001). However, it is not clear whether the variation in grain size from 1 to 50 mm between 150 and 300 km depth required by *Faul & Jackson* (2005) is consistent with the deformation field in the upper oceanic mantle, and thus whether other factors such as water and/or melt are required to explain the LVZ.

Fig. 1

Grain size also modulates the anisotropic structure of the upper mantle by affecting the relative rates of diffusion and dislocation creep. Deformation by diffusion creep occurs via diffusion of atoms along grain boundaries and produces a randomly aligned crystallographic fabric that is seismically isotropic. In contrast, dislocation creep occurs via slip along crystallographic planes, creating a preferred alignment of mineral grains, referred to as lattice preferred orientation (LPO). Olivine, the dominant phase in the Earth's upper mantle, is highly anisotropic, with a fast P-wave velocity (and shear wave polarization) direction oriented parallel to the crystallographic [100] axis (*Birch*, 1960, 1961; *Verma*, 1960). Thus, the crystallographic alignment of olivine crystals by dislocation creep produces an anisotropic fabric that can be measured using a variety of seismic techniques.

The relationship between seismic anisotropy and mantle flow is seen most clearly in the ocean basins, where observations of azimuthal anisotropy near the East Pacific Rise (*Wolfe & Solomon*, 1998; *Harmon et al*., 2004) and in young Pacific upper mantle (*Nishimura & Forsyth*, 1989; *Montagner & Tanimoto*, 1991; *Becker et al*., 2003; *Gaboret et al*., 2003; *Conrad et al*., 2007) are consistent with mantle flow in the direction of plate motion. Moreover, surface wave models indicate that the depth of strongest radial anisotropy increases with age beneath the ocean basins and corresponds to the center of the asthenosphere where shear flow is focused (*Nishimura & Forsyth*, 1989; *Gaherty et al*., 1996; *Nettles & Dziewonski*, 2008). Using a composite diffusion-dislocation creep rheology to model deformation in the oceanic upper mantle, *Podolefsky et al*. (2004) showed that the observed anisotropic structure is consistent with the depth range over which deformation is dominated by dislocation creep. However, this model assumed a constant grain size and thus did not account for grain size evolution associated with mantle flow.

The goal of this study is to quantify grain size evolution in the oceanic upper mantle and determine the influence of the resulting grain size distribution on seismic structure. We model deformation in the upper mantle using a 1-D channel flow model that incorporates a composite diffusion-dislocation creep rheology. Grain size evolution is calculated as a function of depth, seafloor age, and mantle water content using the scaling relations of *Austin & Evans* (2007). The resulting grain size profile is then used to predict the isotropic and anisotropic seismic structure of the oceanic upper mantle as a function of seafloor age. For a plate age of 60 Myr and a dry mantle (50 H/10^6Si in olivine), we find that grain size reaches a minimum of ~5 mm at ~150 km depth and increasing to only ~8 mm at a depth of 400 km. The magnitude of this variation in grain size with depth is significantly smaller than that required in the end-member model used by *Faul & Jackson* (2005) to explain the oceanic LVZ without the presence of water and/or melt.

However, if the mantle contains 1000 H/10^{6}Si in olivine the predicted seismic structure is consistent with both the LVZ and the presence of radial anisotropy in the oceanic upper mantle.

2. 1-D Channel Flow Model for Grain Size Evolution

2.1 Model Setup

We simulate deformation in the oceanic upper mantle using a 1-D channel flow model following the approach of *Podolefsky et al.* (2004). Flow within the channel is driven by an imposed plate velocity, U_p, at the surface and zero velocity at a depth, $z = z_o$ (Figure 2). Assuming no horizontal pressure and viscosity gradients, shear stress within the channel is constant and a function of only the viscosity structure and the vertical gradient of horizontal velocity,

Fig. 2

$$\tau = \eta \frac{\partial u}{\partial z} \qquad (1)$$

where τ is the shear stress, η is viscosity, and u is the horizontal velocity. Integrating Eq. (1) over the height of the channel allows us to write stress in terms of the plate velocity,

$$\tau = U_p \left(\int_{z_o}^{0} \frac{1}{\eta} dz \right)^{-1}. \qquad (2)$$

Experimental and theoretical studies show that the rheology of an olivine aggregate follows a power-law relationship between stress and strain-rate (*Karato & Wu*, 1993; *Hirth & Kohlstedt*, 2003),

$$\dot{\varepsilon}_i = A_i d^{-p_i} C_{OH}^{r_i} \tau^{n_i} \exp(-\frac{E_i + PV_i}{RT}) \qquad (3)$$

where $\dot{\varepsilon}_i$ is strain-rate, A_i is a material constant, p_i is the grain-size exponent, r_i is the water content exponent, n_i is the power-law exponent, E_i is the activation energy, V_i is the activation volume, R is the gas constant, d is the grain size, C_{OH} is the olivine water concentration (in H/10^{6}Si), P is pressure, and T is temperature. The subscript i denotes the parameters that depend on the deformation mechanism (e.g., diffusion or dislocation creep). Flow law parameters are taken from *Hirth & Kohlstedt* (2003) and are given in Supplemental Table S1. We note that the pre-exponential constants for both diffusion and dislocation creep have been reduced by a factor of 3 relative to the values in *Hirth & Kohlstedt* (2003) based on the calibration for water content in olivine (*Bell et al.*, 2003).

Assuming that the total strain-rate can be expressed as the summation of the diffusion and dislocation components (e.g., *Parmentier et al.*, 1976),

$$\dot{\varepsilon} = \dot{\varepsilon}_{diff} + \dot{\varepsilon}_{disl} \qquad (4)$$

we define an effective viscosity, η_{eff}, as

$$\eta_{eff} = \left(\frac{1}{\eta_{diff}} + \frac{1}{\eta_{disl}} \right)^{-1} \qquad (5)$$

which is controlled by the lower of the two viscosities. The conditions under which the dominant deformation mechanism switches between diffusion and dislocation creep are quantified through a transition stress, τ_T, defined as the stress for which $\dot{\varepsilon}_{diff} = \dot{\varepsilon}_{disl}$ (*Hall & Parmentier*, 2003; *Podolefsky et al.*, 2004).

2.2 Implementation of Grain Size Evolution Laws

Grain size in the Earth's mantle is controlled by the competition between dynamic recrystallization and static grain growth (*Karato*, 1984). During dynamic recrystallization, elastic strain energy is reduced by subgrain rotation and grain boundary bulging, producing smaller grains (*Twiss*, 1977; *Karato et al.*, 1980; *Poirier*, 1985; *van der Wal et al.*, 1993; *de Bresser et al.*, 1998). Grain size reduction can also occur via brittle processes (*Goodwin & Wenk*, 1995; *Bos & Spiers*, 2001; *de Bresser et al.*, 2001), however, for the high temperatures associated with asthenospheric flow these effects can be ignored. Grain growth occurs to reduce the interfacial energy of grain boundaries (*Urai et al.*, 1986, *Karato*, 1989; *Evans et al.*, 2001). Unlike dynamic recrystallization, which is only active in the dislocation creep regime, grain growth occurs in both the diffusion and dislocation regimes (*Karato & Wu*, 1993).

Grain size is frequently estimated using a piezometric relationship, in which grain size is related to only stress (e.g., *Karato et al.*, 1980; *Van der Wal et al.*, 1993). However, some experimental data suggests that grain size evolution is also sensitive to temperature and strain rate (e.g., *Poirier & Guillopé*, 1979; *de Bresser et al.*, 1998, 2001; *Drury*, 2005). Here we consider two models for grain size evolution: 1) the synchronous model of *Hall & Parmentier*

(2003), and 2) the paleowattmeter model of *Austin & Evans* (2007). Both of these models are based on the premise that grain size is controlled by the competition between grain growth and dynamic recrystallization:

$$\dot{d} = \dot{d}_{gg} - \dot{d}_{dr} \tag{6}$$

where, $\dot{d}$, is the change in grain size with time, $\dot{d}_{gg}$ is the rate of grain growth, and $\dot{d}_{dr}$ is the rate of dynamic recrystallization.

Hall & Parmentier (2003) parameterized the change in grain size with time as

$$\dot{d} = p_g^{-1} d^{1-p_g} G_o \exp\left(-\frac{E_g + PV_g}{RT}\right) - \lambda \dot{\varepsilon}_{disl} d \tag{7}$$

where the two terms on the right hand side of the equation represent grain growth and recrystallization, respectively, G_o is the grain growth rate constant, E_g and V_g are the activation enthalpy and volume for grain growth, p_g is an experimentally determined grain growth constant, and λ provides an estimate of the strain necessary to achieve a new grain size. Eq. (6) can be solved for a steady state grain size, d_{ss}, which results when the rates of recrystallization and grain growth are balanced

$$d_{ss} = \left(\frac{G_o}{p_g \lambda A_{disl}}\right)^{1/p_g} \left(\frac{\mu}{2\tau}\right)^{n_{disl}/p_g} \exp\left(\frac{\left(E_{disl} + PV_{disl}\right) - \left(E_g + PV_g\right)}{p_g RT}\right). \tag{8}$$

Here μ, is the shear modulus, and A_{disl}, n_{disl}, E_{disl} are the pre-factor, stress exponent, and activation energy for dislocation creep; the factor of 2 in front of the shear stress is necessary to convert to from shear to differential stress.

Austin & Evans (2007) proposed a similar model for grain size evolution based on the balance of mechanical work required for grain growth and dynamic grain size reduction. In practical terms, the primary difference between the *Austin & Evans* (2007) model and that proposed by *Hall & Parmentier* (2003), is that *Austin & Evans* (2007) assume changes in the internal energy of the system are proportional to grain boundary area and thus the time-scale for dynamic recrystallization scales as $\sim \tau \dot{\varepsilon} d^2$ rather than $\sim \dot{\varepsilon} d$ as in Eq. (7). The steady state grain size for the *Austin & Evans* (2007) model can then be approximated as

$$d_{ss} = \left(\frac{G_o \exp\left(-\frac{E_g + PV_g}{RT} \right) p_g^{-1} c\gamma}{2\tau\chi\dot{\varepsilon}_{disl}} \right)^{\frac{1}{1+p_g}} \tag{9}$$

where γ is the average specific grain boundary energy, χ is the fraction of the work done by dislocation creep associated with changing grain boundary area, and c is a geometrical constant. Grain growth parameters for both models are given in Supplemental Table S2.

We calculate the steady state grain size with depth in our 1-D channel flow model assuming a fixed plate velocity, U_p, and mantle temperature structure. Temperature is calculated based on a half-space cooling model with a mantle potential temperature T_m and an adiabatic gradient of 0.3ºC/km. To solve for grain size with depth we initially assume a uniform value of 1 mm throughout the model space and iterate to calculate stress following the approach of *Podolefsky et al.* (2004). We then use the resulting stress value to calculate a new grain size profile with depth using either Eq. (8) or (9). The new grain size profile is used to recalculate stress and the procedure is repeated until subsequent iterations change grain size by < 1%.

2.3 Calibration of Grain Size Evolution Models to Laboratory Data

Before applying the *Hall & Parmentier* (2003) and *Austin & Evans* (2007) grain size evolution models to the upper mantle, we assessed their ability to reproduce laboratory data on grain size evolution during deformation experiments. Remarkably, the kinetics of grain growth remain poorly quantified. For example, analyzed grain boundary mobilities vary by > 3 orders of magnitude under laboratory conditions owing to differences in sample composition and the presence of residual porosity and/or melt (*Evans et al*., 2001; *Faul & Scott*, 2006). Furthermore the activation enthalpy for grain growth has yet to be determined for dry, high-pressure conditions (*Karato*, 1989). However, grain size evolution models can still be tested using laboratory data on recrystallized grain size produced over a temperature range of 1100ºC to 1650ºC (*Karato et al*., 1980; *Van der Wal et al*., 1993). Thus, our first test before applying the grain size evolution models to the Earth is to duplicate these laboratory results and in so doing generate a grain growth law that is consistent with the available data (c.f., *Austin & Evans*, 2007).

We compare the *Hall & Parmentier* (2003) and *Austin & Evans* (2007) models to experimental data on wet (600 H/10^{6}Si) and dry (50 H/10^{6}Si) olivine (*Karato et al.*, 1980; *Van der Wal et al.*, 1993). To do this we modified the 1-D channel flow model described above to simulate laboratory conditions (e.g., constant pressure and temperature) and adjust strain-rate to evaluate the relationship between grain size and stress over a range of stresses. Flow laws for wet olivine aggregates (*Hirth & Kohlstedt*, 2003) and dry $[101]_c$ olivine single crystals (*Bai et al.*, 1991) were used to simulate the experimental data of *Van der Wal et al.* (1993) and *Karato et al.* (1980), respectively. In all calculations we used the high-pressure grain growth data of *Karato* (1989).

Fig. 3

For each model, we calculated the sensitivity of our results to the activation energy (E_g), activation volume (V_g) and grain growth exponent (p_g) (Figure 3). There is confusion in the literature regarding how to evaluate the sensitivity of kinetic laws to changes in the activation energy, volume, and/or stress exponent. Specifically, the co-variation of the pre-exponential terms with the other parameters is often ignored. Assuming a reference condition we can account for this co-variation in the grain growth laws by recalculating G_o after adjustment of E_g, V_g and p_g

$$G_o = \frac{\left(G'_o \left(\frac{C_{OH}}{C_{OH(gref)}} \right) \exp\left(-\frac{E_{gref} + V_{gref} P_{gref}}{RT_{gref}} \right) t_{gref} + d_{gref}^{p_{gref}} \right)^{\frac{p}{p_{gref}}} - d_{gref}^{p}}{\exp\left(-\frac{E_g + V_g P_{gref}}{RT_{gref}} \right) t_{gref}} \qquad (10)$$

where G'_o is the original value of the grain growth rate constant. Supplemental Table S2 gives the reference conditions and resulting values of E_g, V_g and p_g based on the grain growth parameters of *Karato* (1989) that we use in our models.

The grain sizes predicted by the *Austin & Evans* (2007) model using the high-pressure grain growth data (*Karato*, 1989) are systematically smaller than observed. As shown by *Austin and Evans* (2007), adequate fits to the data can be obtained by increasing G_o. This is justified by the presence of small amounts of porosity on the grain boundaries (resulting from fabrication of laboratory samples) that inhibit grain boundary mobility. By contrast, grain boundaries formed by dynamic recrystallization will not have pores. As stated above, no activation energy for grain growth (at high pressure, dry conditions) is given in *Karato* (1989), thus we examined a range of values between 200 and 500 kJ/mol (Figure 3D). With E_g = 350 kJ/mol, G_o must be increased by a factor of ~180 compared to that determined in the dry experiments of *Karato* (1989) (Figure 3D). A similar increase in G_o provides a good fit to the wet data (Figure 3B). Note that because a reference temperature of 1250ºC was used, variations in activation enthalpy do not affect the model predictions for the wet olivine data, but strongly affect the predictions based on the dry olivine data that were collected at 1650ºC.

Using the high-pressure grain growth parameters (G_o and E_g) of *Karato* (1989), we find that the *Hall & Parmentier* (2003) model systematically over-predicts grain size in the wet olivine data and under-predicts the dry olivine data (Figures 3A & 3C). In their original model, *Hall & Parmentier* (2003) used the grain growth parameters determined from the 1 atm experiments of *Karato* (1989). In these experiments grain growth was significantly inhibited due to the presence of residual porosity in the sample. Using the parameters derived from the 1 atm data would therefore further degrade the fit to the dry data, because the predicted grain size at a given stress would be smaller. This effect is even more pronounced at lower temperature. The fit to the dry data in Figure 3C could be improved by increasing G_o (similar to the approach of *Austin & Evans* (2007)). However, this would simultaneously degrade the fit to the wet data.

In summary, we find that the *Austin & Evans* (2007) model provides a better fit to the available data over a range of conditions than does the *Hall & Parmentier* (2003) model. Based on these results we use the *Austin & Evans* (2007) model for the remainder of this study, choosing values of p_g = 3 and E_g = 350 kJ/mol for both the wet and dry olivine data. While the laboratory data are equally well explained by p_g = 2 and E_g = 500 kJ/mol, a grain growth exponent of 3 is likely more relevant for mantle lithologies where grain boundary mobility is affected by grain boundary solutes (e.g., calcium and aluminum) [*Evans et al.*, 2001; *Hiraga et al.*, 2003]. Further, while E_g is not well constrained from laboratory data at high pressure, the limited data available indicate values less than 500 kJ/mol [*Karato*, 1989].

2.4 Application to the Oceanic Upper Mantle

Grain size evolution was calculated for the oceanic upper mantle assuming an age of 60 Myr, a plate velocity of 10 cm/yr, and an olivine water content of 1000 H/10^6Si (Figure 4). We examined 3 cases with an activation volume for grain growth, V_g, ranging from 4–12 × 10^{-6}

Fig. 4

m^3/mol. In all cases, grain size decreases rapidly from the surface to a depth ~100 km. This gradient is the result of the increase in strain-rate with depth beneath the thermal boundary layer. For the intermediate case of $V_g = 8 \times 10^{-6}$ m^3/mol, we find grain-size reaches a minimum of ~15 mm at ~150 km depth, below which it increases slowly to ~22 mm at 400 km (Figure 4A). The predicted grain size and the magnitude of the variations with depth are somewhat larger for $V_g = 4 \times 10^{-6}$ m^3/mol, while $V_g = 12 \times 10^{-6}$ m^3/mol results in a monotonic decrease in grain size at all depths. The grain size profiles predict the asthenosphere to be dominated by dislocation creep down to at least ~400 km, which is consistent with the observation of radial anisotropy in the oceanic upper mantle (*Nishimura & Forsyth*, 1989; *Gaherty et al.*, 1996; *Tan & Helmberger*, 2007; *Nettles & Dziewonski*, 2008). However, greater values of V_g will push the dislocation-diffusion creep boundaries to shallower upper mantle depths. Plate velocity also influences grain-size, with slower velocities producing lower strain rates and thus larger grain-sizes (e.g., U_p = 1, 5, 10 cm/yr result in d = 35, 21, 15 mm at 150 km depth for $V_g = 8 \times 10^{-6}$ m^3/mol).

Eq. (7) can be used to determine the time scale over which the grain size evolves from an initial value, d_o, to the steady state value, d_{ss} (*Hall & Parmentier*, 2003). For all cases, the time-scale to achieve steady state is < 0.1 Myrs at depths below the base of the thermal boundary layer (~75 km) and are very small compared to the age of the plate (Figure 4D). This implies that in the absence of vigorous small-scale convection, the steady state value provides a good estimate of the grain size below the base of the lithosphere. To achieve a steady-state grain size in the lithosphere, however, requires times that are greater than the age of the plate and thus our calculations are not appropriate for estimating grain size in these regions (shown in grey in Figure 4). Furthermore, as olivine grain size approaches ~10 cm or greater, grain boundary pinning associated with the presence of secondary phases such as pyroxene likely control the maximum grain size (*Evans et al.*, 2001).

All 3 activation volumes for grain growth (V_g) result in a mantle viscosity of ~10^{19} Pa·s at the center of the asthenosphere increasing to ~10^{20}–10^{21} Pa·s at 400 km (Figure 4B). Because deformation is dominated by dislocation creep in all 3 cases (Figure 4C), the increase in viscosity with depth reflects the activation volume for dislocation creep. These values of asthenospheric viscosity are similar to estimates from post-seismic relaxation (*Pollitz & Sacks*, 1996; *Freed & Bürgmann*, 2004) and geoid (*Craig & McKenzie*, 1986; *Hager*, 1991) studies, as well as estimates of the viscosity at the base of the olivine stability field based on post-glacial rebound (*Peltier*, 1998).

To further test the sensitivity of our results, we examined the steady state grain size and mantle viscosity at a depth of 150 km as a function of mantle potential temperature and olivine water content (Figure 5). As expected elevated water contents result in larger grain sizes, due to the higher grain boundary mobility under hydrous conditions. Warmer temperatures also produce larger grain sizes. This occurs because higher temperatures promote grain growth, while simultaneously reducing asthenospheric viscosity, which in turn reduces the stress available to drive recrystallization. For example, at 150 km depth values of T_m of 1300, 1350, 1400ºC result in $d = 12$, 15, and 22, respectively. Thus, for the range of potential temperatures and olivine water contents typical of the Earth's upper mantle (1300–1450ºC and 50–2000 H/10^6Si), we find grain sizes and viscosities at the center of the asthenosphere in the range of 1–100 mm and 0.3–10 × 10^{19} Pa·s, respectively.

Fig. 5

Lastly, we tested the effect of imposing a rapid change in water content (50 to 1000 H/10^6Si) at 70 km depth to simulate the dehydration boundary associated with the onset of dry melting beneath a ridge axis (*Hirth & Kohlstedt*, 1996). Intriguingly, our grain size profiles are essentially independent of a dehydration boundary for plate ages > 10 Myr, and are sensitive only to the water content of the mantle below 70 km. The reason for this can be seen from examination of Eq. (9), in which the steady state grain size is proportional to $C_{OH}^{p/p_{ref}}\dot{\varepsilon}_{disl}^{-1}$. Just below the dehydration boundary there is a rapid increase in strain-rate due to the decrease in viscosity for wet olivine. However, the elevated water content below the dehydration boundary simultaneously enhances grain growth. These two effects almost perfectly offset in our simple 1-D model, however future work is necessary to determine how these processes interact during corner flow beneath a ridge axis.

3. Seismic Structure of the Oceanic Upper Mantle

The resultant grain size profiles are used to calculate shear wave velocity (V_S) and seismic quality factor (Q) as a function of depth. Following *Karato* (2003), we estimate V_S as:

$$V_S = V_\infty(T,P)\left[1 - F\cdot Q^{-1}(\omega,T,P,C_{OH},d)\right] \qquad (11)$$

where ω is frequency, V_∞ is the velocity at infinite frequency, $F = (1/2)\cdot\cot(\pi\alpha/2)$ and α is a non-dimensional constant (*Minster & Anderson*, 1980). In this formulation, the influences of water and grain size on V_S enter through the anelastic term (enclosed in square brackets), while the effects of temperature and pressure influence both the anelastic and anharmonic terms. We calculate the velocity at infinite frequency, V_∞, following *Stixrude & Lithgow-Bertelloni* (2005):

$$V_\infty(T,P) = 4.77 + 0.038P - 0.000378(T - 300) \qquad (12)$$

in which pressure and temperature are given in GPa and °K, respectively. This expression incorporates the modal mineralogy of a pyrolytic bulk composition appropriate for the oceanic upper mantle.

The anelastic effects are approximated by:

$$Q^{-1}(\omega,T,P,C_{OH},d) = \left(Bd^{-p_Q}\omega^{-1}\exp\left(-\frac{(E_Q + PV_Q)}{RT}\right)\right)^{\alpha} \qquad (13)$$

where

$$B = B_o d_{Qref}^{p_Q - p_{Qref}} \left(\frac{C_{OH}}{C_{OH(Qref)}}\right)^{r_Q} \exp\left(\frac{(E_Q + P_{Qref}V_Q) - (E_{Qref} + P_{Qref}V_{Qref})}{RT_{Qref}}\right). \qquad (14)$$

The reference values, p_{Qref}, E_{Qref}, and V_{Qref}, are taken from *Faul & Jackson* (2005) and d_{Qref}, T_{Qref}, P_{Qref}, and $C_{OH(Qref)}$ are given in Supplemental Table S3. To estimate the value of B consistent with Eq. (13) we fit the attenuation data of *Tan et al.* (2001) and *Jackson et al.* (2002) at a fixed period of 8.2 s with $\alpha = 0.27$. We find that $p_Q = 1$ and $E_Q = 420$ kJ mol^{-1} results in the best fit the data (Figure 6), consistent with *Faul & Jackson* (2005) and *Jackson et al.* (2002), respectively. The resulting parameters for calculating Q and V_S are given in Supplemental Table S3. As hypothesized by *Karato* (1995), the influence of hydrogen on attenuation is justified by the correlation between steady state creep rates and transient creep observed in deformation experiments (e.g., *Gribb & Cooper*, 1998). Exploratory experiments on hydrous olivine suggest that water can influence anelastic properties, but more quantitative analyses await further experimental work (*Aizawa et al.*, 2008)

Fig. 6

Our approach for calculating V_S differs from *Faul & Jackson* (2005) in two ways. First, *Faul & Jackson* (2005) assumed a pure olivine upper mantle in their calculations of V_S. By utilizing the *Stixrude & Lithgow-Bertelloni* (2005) expression for V_∞ in Eq. (12) we account for the addition presence of pyroxene, garnet, and spinel, which can account for >30% of the oceanic upper mantle by volume. Second, unlike *Faul & Jackson* (2005), who allow grain size to influence both the anelastic and anharmonic terms (see Eq. (7) of *Faul & Jackson* (2005)), we include the grain-size dependence of V_S only in the anelastic term (Eq. 13) as grain size should not effect the unrelaxed properties of olivine. The net effect of our approach is to reduce the influence of grain size on V_S in our calculations as compared to those of *Faul & Jackson* (2005).

To assess the influence of grain size and olivine water content on V_S and Q, we compared two cases with grain-size profiles calculated for a dry (50 H/10^6Si) and wet (1000 H/10^6Si) mantle at 60 Myrs (Figure 7). Both cases result in V_S minima at a depth of ~130 km, which corresponds closely to the depth of the LVZ for intermediate oceanic plate ages (25–100 Myr) (e.g., *Nettles and Dziewonski*, 2008). Because the difference in water content has a greater effect on V_S than does the calculated change in grain size, the dry case predicts a slightly higher V_S (~4.4 km/s) at 130 km than does the wet case (~V_S = 4.3 km/s). Comparing these results to available seismic models for the oceanic upper mantle we find that the wet case results in a slightly better fit to the observed LVZ. However, we note that there are considerable differences in the amplitude and depth of the LVZ between the seismic models resulting from the different spatial distribution and frequency content of the data used in constructing each model. Thus, given these uncertainties it is difficult to distinguish between the wet and dry cases from the seismic data alone.

Fig. 7

We also identify two discrepancies between our model predictions and the available constraints on the seismic structure of the upper oceanic mantle. First, our models predict a smaller velocity gradient at the base of the mantle than is observed (Figure 7B). One possible explanation for this difference is that we have underestimated V_Q in our calculations. Alternatively the composition of the mantle may not be constant near the transition zone. Second, the modeled V_S profiles lack the fast and constant velocity lid above 60–70 km depth that is observed in PA-5 (*Gaherty et al.*, 1996) and other recent studies that incorporate reverberation phases (e.g., *Tan & Helmberger*, 2007). The low temperatures (and associated high Q values) in this depth range make it unlikely that the rapid change in V_S at the base of the lid (also referred to as the Gutenberg or G- discontinuity) is generated by an anelastic mechanism unless our thermal models vastly underestimate temperature at this depth. In the following section we speculate on possible origins for the G-discontinuity in the oceanic upper mantle.

4. Discussion

We use our model to investigate the variation in upper mantle properties as a function of oceanic plate age by examining a series of 1-D calculations with different imposed temperature structures (Figure 8). While this approach ignores complications associated with buoyancy-driven flow and ridge corner flow, it provides a first-order approximation of the variations in upper mantle structure with age. A combination of petrological (*Dixon et al*., 1988; *Michael et al*., 1995; *Hirth & Kohlstedt*, 1996; *Hirshmann et al*., 2005) and geophysical observations (e.g., *Evans et al*., 2005) indicate that there is 125 +/- 75 ppm by weight of water in the oceanic mantle; this value results in approximately 1000 H/10^6Si in olivine given the partition coefficient of hydrogen between the mantle phases (*Hauri et al*., 2006). Based on these observations, and the fact that water content has only a limited influence on upper mantle grain size (Figures 5A & Figure 7A), we consider a series of calculations with ~1000 H/10^6Si and a mantle potential temperature of 1350°C.

Fig. 8

For all plate ages, grain size is minimized at the depth corresponding to the maximum dislocation creep strain rate. Further, the grain size at a given depth decreases with increasing plate age, owing to the overall cooling of the mantle (Figure 8A). This positive gradient in grain size from the center of the asthenosphere to the base of the upper mantle is consistent with that proposed by *Faul & Jackson* (2005). However, the magnitude of the variations calculated from our model are significantly smaller; for a plate age of 100 Myr we predict an increase from 15 to 22 mm between 150 and 400 km depth, while *Faul & Jackson* (2005) propose an increase on the order of 1 to 50 mm. Although *Faul & Jackson* (2005) used a lower mantle potential temperature (1300°C) than was considered here, we calculate a minimum grain size of 12 mm at the center of the asthenosphere for 1300°C —still more than an order of magnitude larger than their minimum grain size of 1 mm. As discussed below these differences have important implications for the permeability and anisotropic structure of the upper mantle.

Grain sizes of 10–20 mm in the asthenosphere are consistent with available constraints on grain size in the upper mantle. Although few xenoliths from oceanic environments are available, xenoliths from continental extension zones, where upper mantle temperatures are likely be similar to those in the oceanic upper mantle, record grain sizes on the order of 1–20 mm (e.g., *Ave Lallemant et al*., 1980). Moreover, olivine in harzburgite and dunite bodies outside of mylonitic shear zones in the Oman ophiolite display grain sizes of 1–20 mm (*Boudier & Coleman*, 1981; *Braun*, 2004). While these grain sizes are slightly smaller than our predictions, the fabrics preserved in ophiolites are formed in the shallowest portions of the upper mantle, which is most strongly influenced by ridge corner flow, and have additionally undergone late stage deformation associated with exhumation. Finally, these estimates are generally consistent with previous inversions for grain size at 100 km depth and 1550°K from global attenuation models (*Cammarano & Romanowicz*, 2008), which suggest grain sizes of ~10 mm based on *Faul & Jackson's* (2005) parameterization for the effect of grain size on Q.

The calculated S-wave velocity structure predicts the depth of the low velocity zone (LVZ) to increase with increasing plate age, with the slowest velocities near the ridge axis where the shallow temperature structure is warmest (Figure 8B). Comparing the 1-D velocity structure at 100 Myr with seismic models for old oceanic upper mantle, we find a good correspondence between the depth and minimum velocity of the LVZ (Figure 8D). We also calculated grain size and V_S at 100 Myr using temperatures derived from a plate-cooling model (*Parsons & Slater*, 1977; *Stein & Stein*, 1992) assuming a plate thickness of 125 km and a mantle potential temperature of 1350°C (red curves in Figures 8C & 8D). The warmer temperatures calculated from the plate model produce slightly larger grain sizes and a slower, shallower LVZ compared to the half-space cooling model. However, again the available seismic constraints are not sufficient to distinguish between these two models and as discussed below neither model displays a fast, constant velocity lid above ~70 km.

Fig. 9

The diffusion and dislocation creep rates calculated from the composite rheology (Eq. 4) can be used to infer the anisotropic structure of the oceanic upper mantle (Figure 9). Because anisotropy develops due to dislocation creep, but is destroyed (or at least does not form) in the diffusion creep regime, we assume that the mantle in our 1-D model will be strongly anisotropic when $\dot{\varepsilon}_{disl} > \dot{\varepsilon}_{diff}$ and $\varepsilon_{disl} > 1$ (Figure 9C). Based on this criterion, we find that the maximum depth-extent of anisotropy deepens with plate age, consistent with radial anisotropy models for the Pacific derived from surface waves (e.g., *Nishimura & Forsyth*, 1989; *Nettles & Dziewonski*, 2008). However, while the peak amplitude of radial anisotropy increases slightly with plate age in the ocean basins (e.g., Figure 1B), the coherence between azimuthal anisotropy and the fossil seafloor fabric decays with age (*Nishimura & Forsyth*, 1989). This breakdown in coherence at old ages is not predicted by our simple 1-D model in which flow is driven solely by ridge-normal plate motion. Older regions of the oceanic mantle have likely experienced additional shear associated with small-scale convection and/or larger-scale buoyancy-driven flow, which will tend to re-align the orientation of shear in the asthenosphere relative to the fossil seafloor fabric.

For comparison, we also determined the region of the mantle dominated by dislocation creep based on the grain size distribution of *Faul & Jackson* (2005). To do this we used the composite rheology to calculate stress and strain-rates in the upper mantle for a fixed grain size profile. Assuming a linear increase in grain size from 1 to 50 mm between 165 and 350 km depth and a mantle potential temperature of 1300ºC as proposed by *Faul & Jackson* (2005), we find that diffusion creep is the dominant deformation mechanism above ~180 km (Figure 9F). Similarly, their hot mantle grain size profile with a linear increase from 5 to 100 mm and T_p = 1400ºC, predicts the upper 80 km of the mantle to be dominated by diffusion creep. Both of these models are inconsistent with the observation of radial anisotropy in old oceanic upper mantle, and thus argue that the minimum grain size in the oceanic upper mantle must be greater than 1–5 mm in order to promote dislocation creep. Therefore, while our modeled grain size profiles are consistent with the gradient in grain size in the upper oceanic model proposed by *Faul & Jackson* (2005), at face value directly inverting isotropic S-wave velocities for grain size at dry conditions results in values that are inconsistent with the anisotropic velocity structure.

The largest discrepancy between the modeled and observed velocity structures is the inability of our model to predict the high velocity lid above 60–70 km (G-discontinuity) for old ages that is observed in reverberation phases (e.g., *Gaherty et al*., 1996; *Tan & Helmberger*, 2007). If this high velocity lid is caused by anelastic effects, it would require a sharp change in mantle properties at ~70 km depth that are not predicted by our model. Moreover, given the existing thermal models for the oceanic upper mantle it is difficult to invoke an anelastic origin for the G-discontinuity. To illustrate this point, we calculated the change in grain size or water content that is required to produce a 3% decrease in velocity at 70 km as a function of mantle temperature (Figure 10). For relatively hot temperatures (>1250ºC) characteristic of young oceanic mantle, the variation in grain size (~10 mm) and/or water content (~2000 H/10^6Si) needed to produce the G-discontinuity remains reasonable. However, for temperatures of 650º–850ºC predicted from half-space cooling at an age of 100 Myr lithosphere (the average age of PA-5) grain size and/or water content would have to vary by ~10 orders of magnitude in order to generate a 3% change in V_S (Figures 10A & 10B). In the case of water content, this would require values well above the solubility of water in olivine (*Zhao et al.*, 2004; Figure 10B&D). Furthermore, even the warmest published plate model (1400ºC at 90 km; *Stein & Stein* (1992)) predicts a temperature of only ~1100ºC at 70 km depth at 100 Myr, which would still require unreasonably large variations in grain size and/or water content to produce the G-discontinuity. Intriguingly, these warmer temperatures predicted from the *Stein & Stein* (1992) plate model do approach the damp (*Asimow et al.*, 2004) and carbonated (*Dasgupta & Hirshmann*, 2006) mantle solidi at 2–3 GPa, implying that melt could be present at these depths in old oceanic mantle. Thus, we conclude that either the temperature structure of old oceanic lithosphere is similar to or even hotter than the warmest published plate models, or an alternative mechanism such as compositional changes and/or scattering are required to explain the existence of the G-discontinuity.

Fig. 10

The grain size profiles predicted by our model are also relevant for estimating the permeability of the oceanic mantle to melt migration. Melt permeability scales with d^2 (e.g., *von Bargen & Waff*, 1986; *Wark et al.*, 2003), thus an accurate estimate of grain size is necessary for determining the rate of melt migration. Some recent geodynamical studies have assumed permeabilities consistent with a mantle grain size of ~1 mm (e.g., *Braun et al.*, 2000; *Choblet & Parmentier*, 2001; *Spiegelman & Kelemen*, 2003; *Cagnioncle et al.*, 2007). However, our calculations predict minimum grain sizes of 10–20 mm, resulting in an increase in permeability by more than a factor of 100 compared to these previous studies. This will result in more rapid melt ascent velocities and in turn a smaller effect of melt buoyancy on mantle flow beneath ridges and plumes.

5. Conclusions

In this study, we have coupled laboratory based grain size evolution models with a 1-D channel flow model for the oceanic upper mantle assuming a composite diffusion-dislocation creep rheology. We evaluated both the *Hall & Parmentier* (2003) and the *Austin & Evans* (2007) grain size evolution models and found that the *Austin & Evans* (2007) model does a better job at reproducing the available laboratory data over a range of experimental conditions (e.g., temperature and olivine water content). Applying the *Austin & Evans* (2007) model to the oceanic upper mantle we find that for ages >60 Myr and an olivine water content of 1000 $H/10^6Si$, grain size reaches a minimum of 15–20 mm at ~150 km depth, increasing to 20–30 mm at 400 km. This grain size structure produces a good fit to the low seismic shear wave velocity zone (LVZ) in oceanic upper mantle, and predicts dislocation creep to be the dominant deformation mechanism at all depths throughout the upper mantle. Our results predict larger grain sizes than proposed by *Faul & Jackson* [2005], who suggested that the LVZ could be explained by a dry mantle and a minimum grain size of 1 mm. However, for a grain size of 1 mm diffusion creep is the dominant deformation mechanism above 100–200 km depth, inconsistent with abundant observations of seismic anisotropy from surface wave studies. These results indicate that a combination of grain size evolution and a hydrated upper mantle is a likely explanation for the oceanic LVZ.

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Figure Captions

Figure 1. **A)** Average S-wave velocity and **B)** radial anisotropy for oceanic regions from *Gaherty et al.* (1996) (G96) and *Nettles and Dziewonski* (2008) (ND08). **C)** Seismic *Q* factor from the models of *Dziewonski & Anderson* (1981) (PREM), *Romanowicz* (1995) (R95), and *Selby & Woodhouse* (2002) (SW02). Note the region of low S-wave velocity, low Q, and high radial anisotropy in the center of the asthenosphere at 100–200 km depth.

Figure 2. **A)** Model setup and **B)** imposed upper mantle temperature structure for plate ages of 20, 60, and 120 Myrs assuming a mantle potential temperature of 1350ºC.

Figure 3. Grain size as a function of stress calculated from the grain-size evolution models of *Hall & Parmentier* (2003) and *Austin & Evans* (2007) under (**A & B**) wet (1250ºC, 600 $H/10^6Si$) and (**C & D**) dry (1650ºC, 50 $H/10^6Si$) experimental conditions. Open circles and black triangles show the experimental data of *Van der Wal et al.* (1993) and *Karato et al.* (1980). Blue and red lines show model predictions for grain growth exponents (p_g) of 2 and 3, respectively. Multiple curves in **C & D** are for activation enthalpies of 200, 350, and 500 kJ/mol. All other parameters for grain growth under wet and dry conditions are given in Table 2.

Figure 4. Example calculation of grain size evolution in a 1-D channel flow model beneath a 60 Myr plate moving at 10 cm/yr assuming a mantle potential temperature of 1350ºC and an olivine water content of 1000 $H/10^6$ Si. Model setup and solution follows *Podolefsky et al.* (2004), using the *Austin & Evans* (2007) model (Eq. 9) to solve for the **(A)** steady state grain size, d_{ss} and **(B)** composite mantle viscosity. Black, blue, and red curves show solutions with activation volumes for grain growth of 4, 8, and 12×10^{-6} m^3/mol, respectively. Dashed and dash-dot curves show predictions of grain size from the piezometric relationships of *Karato et al.* (1980) and *Van der Wal et al.* (1993), respectively. **(C)** Calculated shear stress (dashed) and transition stress where $\dot{\varepsilon}_{diff} = \dot{\varepsilon}_{disl}$ (solid). Dislocation creep is the dominant deformation mechanism in regions where the calculated shear stress exceeds the transition stress. **(D)** Equilibration time for grain size to reach d_{ss}. Grey regions in all panels denote depths where $t_{eq} > 60$ Myr, and d_{ss} is not a good estimate of the true grain size.

Figure 5. **(A)** Steady state grain size and **(B)** mantle viscosity at a depth of 150 km and plate age of 60 Ma as a function of mantle potential temperature and water content. Calculations assume a plate velocity of 10 cm/yr and $V_g = 8 \times 10^{-6}$ m^3/mol. Typical values of mantle temperature and olivine water content in the Earth's upper mantle (1300–1450ºC and 50–2000 $H/10^6Si$), result in grain sizes and viscosities in the range of 1–100 mm and $0.3–10 \times 10^{19}$ Pa·s, respectively.

Figure 6. Grain-size dependence of *Q* predicted by Eq. (13) compared to the attenuation data of *Tan et al.* (2001) and *Jackson et al.* (2002) (filled dots) at a fixed period of 8.2 s. Fit is achieved by adjusting p_Q, E_Q, and V_Q to best fit the data, holding p_{Qref}, E_{Qref}, and V_{Qref}, constant to the values given by *Faul & Jackson* (2005).

Figure 7. **(A)** Grain size, **(B)** V_S, and **(C)** *Q* for a 60 Myr plate moving assuming olivine water contents of 50 (red) and 1000 (blue) $H/10^6$ Si. Calculations assume a plate velocity of 10 cm/yr,

a mantle potential temperature of 1350ºC and $V_g = 8 \times 10^{-6}$ m^3/mol. Black, dashed, and grey lines in **B** correspond to V_S models PA-5 (*Gaherty et al*., 1996), ND08 (*Nettles & Dziewonski*, 2008) for intermediate oceanic plate ages (25–100 Myr), and NF89 (*Nishimura & Forsyth*, 1989) for 52–110 Myr, respectively. Q models shown in **C** are same as in Figure 1C.

Figure 8. **(A)** Grain size and **(B)** V_S as a function of plate age beneath a plate moving at a velocity of 10 cm/yr. Calculations assume a mantle potential temperature of 1350ºC, an olivine water content of 1000 H/10^6 Si, and $V_g = 8 \times 10^{-6}$ m^3/mol. Grey curve denotes depth above which t_{eq} is greater than the age of the plate. Black curves show V_S from *Nishimura & Forsyth* (1989) for 3 age intervals: 4–20 Myr, 20–52 Myr, and 52–110 Myr plotted at the center of each interval. **(C)** Grain size and **(D)** V_S as a function of depth for a plate age of 100 Myr. Blue and red curves show solutions for half-space cooling and plate models. Plate model assumes a plate thickness of 125 km. Grey region denotes depths where $t_{eq} > 100$ Myr. Black, dashed, and grey lines in **B** correspond to V_S models PA-5 (*Gaherty et al*., 1996), ND08 (*Nettles & Dziewonski*, 2008) for old oceanic plate ages (>100 Myr), and NF89 (*Nishimura & Forsyth*, 1989) for 52–110 Myr, respectively.

Figure 9. Total strain accumulated in the **(A)** dislocation creep and **(B)** diffusion creep regimes as a function of plate age. Model parameters are the same as Figure 8. (**C**) Grey area denotes portion of the upper mantle predicted to be anisotropic ($\dot{\varepsilon}_{disl} > \dot{\varepsilon}_{diff}$ and $\varepsilon_{disl} > 1$). Red curves show the anisotropic parameter, $\xi = (V_{SH}/V_{SV})^2$, of *Nishimura & Forsyth* (1989) for 3 age intervals: 4–20 Myr, 20–52 Myr, and 52–110 Myr plotted at the center of each interval. Total accumulated **(D)** dislocation and **(E)** diffusion creep strain as a function of depth for a plate age of 100 Myr (blue curves). Dashed curve in **D** shows radial anisotropy for ocean plate ages >100 Myr from *Nettles & Dziewonski* (2008). (**F**) Calculated shear stress (dashed) and transition stress where $\dot{\varepsilon}_{diff} = \dot{\varepsilon}_{disl}$ (solid) at a plate age of 100 Myr. Curves correspond to calculations for a dry (50 H/10^6 Si , red) and wet (1000 H/10^6 Si, dark blue) mantle as well as for the imposed grain size distribution of *Faul & Jackson* (2005) (light blue). Dislocation creep is the dominant deformation mechanism in regions where the calculated shear stress exceeds the transition stress. Note that for the *Faul & Jackson* (2005) grain size distribution most of the upper mantle above 200 km is in the diffusion creep regime.

Figure 10. **(A,C)** Grain size and **(B,D)** water content in olivine required to decrease V_S by 3% at 70 km depth as a function of mantle temperature. Thin dashed lines show initial grain size, d_o, and water content, COH_o, respectively. Red and blue curves in (A&C) show calculations for olivine water contents of 50 and 1000 H/10^{6}Si, while red, blue, and black curves in (B&D) assume grain sizes of 1, 10, and 100 mm, respectively. Thick dary grey lines in (B&D) show water saturation in Fo_{90} olivine calculated from *Zhao et al.* (2004). Grey region illustrates range of mantle temperatures between 50 and 70 km depth calculated from a half-space cooling model for a 100 Myr plate. Grey boxes in (A&B) show enlarged regions illustrated in (C&D).