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Three-dimensional structures and dynamics in the deep mantle: Effects of post-perovskite phase change and deep mantle layering

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[1] Three-dimensional numerical simulations of thermo-chemical mantle convection with multiple phase transitions (olivine-spinel-perovskite-post perovskite) are used to investigate the morphology of compositional and post-perovskite (PPV) boundary structures above the core-mantle boundary (CMB). Compositionally-dense subducted MORB partially segregates above the CMB forming ridge-like dense piles, morphologically similar to structures in previous spherical or Cartesian studies in which a dense layer was inserted a priori. An anti-correlation is observed between regions where a thick post-perovskite layer occurs and regions containing piles of dense material, as in our previous two-dimensional study. Lateral variations in the thickness or occurrence of a PPV layer cause very strong seismic shear-wave velocity anomalies which may dominate thermal or composition-related seismic heterogeneity in the depth range where the variable PPV boundary occurs, and also generate sharp-sided structures as observed seismologically. Both compositional and PPV effects may be necessary to simultaneously explain large-scale heterogeneity and the global distribution of the discontinuity atop D″.

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1. Introduction

[2] In the core-mantle boundary (CMB) region, structures of quite different scale coexist, including large-scale (i.e., spherical harmonic degree two) high-amplitude structures which may be sharp-sided [*Ni et al.*, 2002], a seismic discontinuity at the top D″ which varies between ~50–350 km above the CMB, small-scale scattering within D″, and ultra-low-velocity zones (ULVZs) of up to 50 km thick [e.g., *Wysession et al.*, 1998; *Lay et al.*, 2004]. Although a number of 'cartoon' interpretations of these exist, they have not been simultaneously reproduced by any numerical models of mantle convection, although some individual aspects of them have. For example, large-scale heterogeneity with an anti-correlation of bulk and shear wave velocity and sharp sides can be produced if compositionally-dense material forms "piles" above the CMB [*Tackley*, 2002; *Deschamps et al.*, 2006], but it is difficult to explain the D″ discontinuity in such a manner. Instead, a strongly exothermic phase change interacting with cold subducted slabs provides a good explanation for the seismically observed topography of the D″ discontinuity [*Sidorin et al.*, 1999], and such a phase change was subsequently discovered [*Murakami et al.*, 2004; *Oganov and Ono*, 2004]. That mechanism does not, however, explain strong, smaller-scale heterogeneities above the CMB.

[3] In our previous study [*Nakagawa and Tackley*, 2005], two-dimensional numerical convection calculations were used to characterize the structures generated by the interaction of the perovskite-post perovskite phase change with thermo-chemical convection, and compare them to the velocity anomalies inferred from global seismic tomography. The main findings were: an anti-correlation between the location of post-perovskite regions and the location of "piles" of dense material, and the relatively flat spectrum of compositional heterogeneity, meaning that compositional heterogeneity dominates at short wavelengths, and possibly, in the CMB region, at long wavelengths. The coexistence and anticorrelation of dense "piles" and the PPV phase transition may explain both large-scale heterogeneity and the global variability of the D″ discontinuity.

[4] However, this previous study considered only two-dimensional cases, whereas three-dimensional geometry is necessary to determine the planform of thermo-chemical structures in CMB region for comparison with seismological constraints. Additionally, the heterogeneity amplitude and spectrum associated with lateral variations in the depth of the PPV transition was not calculated. Thus, in the present study, three-dimensional numerical calculations of thermo-chemical mantle convection with multiple phase changes including the post-perovskite phase change are used to investigate the morphology of features and spectra of deep mantle compositional and post-perovskite seismic velocity anomalies.

2. Model and Parameters

[5] The physical model and numerical details are described in detail in our previous paper [*Nakagawa and Tackley*, 2005], so due to space limitations only differences to that are described here. The main difference is geometry: a three-dimensional Cartesian box with an aspect ratio of four (instead of a two-dimensional half-cylindrical shell) and a numerical resolution is 128(x) × 128(y) × 64(z) cells with 16 tracer particles per grid cell to track chemical composition. Vertical grid refinement is used to improve the resolution in boundary layers near the surface, 660 km depth and CMB.

[6] We here focus on the effect of chemical density contrast, the value of which in the deep mantle is

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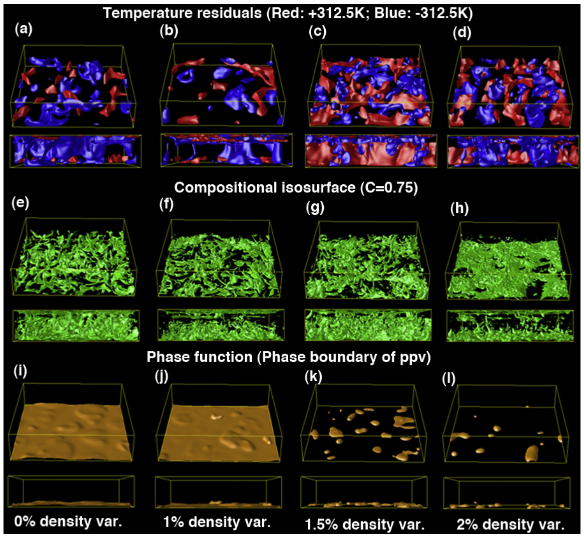

Figure 1. Snapshots at the present time (i.e., end of calculation) for all four cases. In the top images of Figures 1a–1h, the upper half of the domain has been removed otherwise deep mantle structures are obscured by shallower structures. (a–d) Temperature residuals, with red indicating 312.5 K higher and blue 312.5 K lower than the average temperature at that depth. (e–h) Compositional isosurfaces showing where C = 0.75. (i–l) The post-perovskite phase boundary (i.e., phase function = 2.5).

apparently much more uncertain than the values of PPV phase change parameters. Thus, the Clapeyron slope of the post-perovskite phase transition is fixed at +8 MPa/K, which is within the range determined by mineral physics experiments and modeling, and temperature for the post-perovskite phase change at the CMB is estimated as 3340 K using a experimental data (density variation and reference temperature) and Clapeyron slope that is used in this study, while the compositional density variation is varied. Four compositional variations are considered: 0%, 1%, 1.5% and 2%, where this refers to the chemical density variation between the endmember compositions of harzburgite (composition C = 0) and MORB (C = 1). As before, the internal heating rate is higher in the MORB endmember to crudely account for the fractionation of incompatible heat-producing elements into the melt, and the core cools with time due to the heat removed by the mantle. Also as before, cases are started from an initial condition in which the temperature field is adiabatic with a potential temperature of 1800 K except for thin error function thermal boundary layers at the top and the bottom plus small random perturbations, and the compositional field is initialized at a constant C = 0.3, with all compositional variations arising through melting-induced differentiation over the 4.5 billion year run time. The convective vigor is somewhat lower than Earth-like, with a present-day surface heat flow and root-mean-square surface velocity in the range 21–29 TW and 0.9–1.3 cm/yr, respectively, values are a factor of ~2 and ~3 lower than realistic. Temperature at CMB is 3040 K (0%), 3173 K (1%), 3692 K (1.5%) and 3432 K (2%) at t = 4.5 Gyrs (at the end of calculations). Comparing with temperature at the phase boundary, 0% and 1% would be single-crossing, while double-crossing expects the case for 1.5% and 2%.

3. Results

[7] Figure 1 shows isosurfaces of residual temperature, composition and phase function at the end of the simulated time (for examples of time evolution the reader is referred to our previous study). Most of the features and trends are as observed previously, but new information about planforms is obtained. With no compositional density contrast subducted MORB is, as expected, present through the entire mantle depth (Figure 1e) but as density contrast is increased 'ridges' (Figures 1f and 1g, 1–1.5%) or 'pools' (Figure 1h, 2%) of dense material form above the CMB, with exposed patches of core existing in all cases. The presence of dense material with high internal heating above the CMB reduces the core cooling rate, resulting in a higher final CMB temperature for higher compositional density contrast. In the cases with a 0 or 1% density contrast the present-day CMB temperature is low enough that a 'single crossing' of the PPV transition occurs globally (Figures 1i and 1j), but with a 1.5 or 2% density contrast the CMB is hot enough to be in the perovskite stability field, resulting in either a "double-crossing" or no crossing of the PPV phase transition (Figures 1k and 1l), that is, isolated patches of PPV above the CMB occurring in cold regions [*Hernlund et al.*, 2005]. As observed in [*Nakagawa and Tackley*, 2005], there is an inverse correlation between PPV thickness or occurrence (for single or double crossing respectively) and the location of ridges or piles of compositionally-dense material. Regarding the temperature field (Figures 1a–1d), hot upwellings are more prevalent in cases with a hot abyssal layer of dense material, both because the material itself is hot and also because the CMB is hotter.

[8] These trends and features are further evidenced in Figure 2, which shows horizontal slices at 2700 km depth (i.e., 190 km above the CMB) and vertical slices at y = 2. With zero density contrast (Figures 2a, 2e, 2i, and 2m), 'blobs' of subducted MORB tend to occur within cold regions above the CMB (i.e., related to subducted slabs that are in the process of heating up) whereas when MORB is dense enough that some fraction of it settles above the CMB, it occurs in hot ridges or regions above the CMB. Comparing T and C planforms to the planform of PPV occurrence confirms that when subducted MORB is dense, there is an anticorrelation between C and PPV, whereas when C is passive, the correlation is much weaker and may even be positive. PPV regions have a rounded to elongated shape depending on parameters. In order to compare with seismic tomography, calculated seismic anomalies are useful (Figures 2m–2p). It is clear to find sharp-sided structures [e.g. *Lay et al.*, 2004] when MORB is denser but, for the case that the MORB is 2% denser, sharp-sided structures are hard to see because the basaltic pool covers with huge area of CMB region.

[9] Figure 3 shows power spectra plotted as a function of nondimensional spatial frequency [*Tackley*, 2002]. The conversion between T or C and Vs is as given in [*Nakagawa and Tackley*, 2005] but the contribution of PPV to Vs was not previously considered. Here it is assumed that the

transition to PPV increases Vs by 2%, within the seismologically-determined range for the velocity jump across the discontinuity atop D″ [*Lay et al.*, 2004] and consistent with recent mineral physics studies of the PPV transition [*Tsuchiya et al.*, 2004; *Wentzcovitch et al.*, 2006; *Wookey et al.*, 2005].

[10] The startling observation from Figure 3 is that lateral variations in the occurrence of PPV are generally the dominant contributor to seismic heterogeneity in the D″ region. This is true at long wavelengths for all cases except the 2% density contrast case, where T, C, and PPV have roughly equal contributions at the longest wavelengths. This is understandable because the 2% Vs change associated with the transition is larger than that caused by a 1000 K temperature change (2.3%) or by a change from C = 0 to C = 1 (0.1%) at this depth.

4. Discussion and Summary

[11] The use of three-dimensional geometry allows the morphology and planform of features to be determined. *McNamara and Zhong* [2004] investigated the morphology of a pre-existing chemically-dense layer in a three-dimensional spherical shell without any phase changes and found that the dense material forms ridge-like features above the CMB, similar to earlier results in Cartesian geometry [*Tackley*, 1998]. In the present results, in which compositional anomalies are generated entirely by melt-induced differentiation and multiple phase changes are present, similar features are obtained, which indicates a robustness to exact physical parameters and approach.

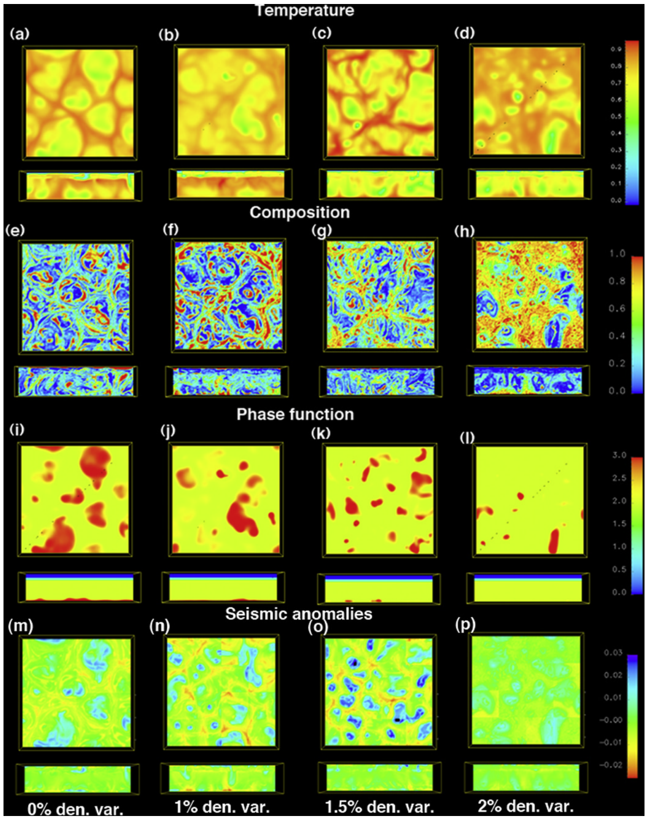

Figure 2. Horizontal and vertical slices of temperature, composition and phase function for all cases. (a–d) Temperature. (e–i) Composition. (i–l) Phase function. (m–p) Seismic anomalies. The top image in Figures 2a–2p shows a horizontal slice at 2700 km depth and bottom one shows the vertical slice.

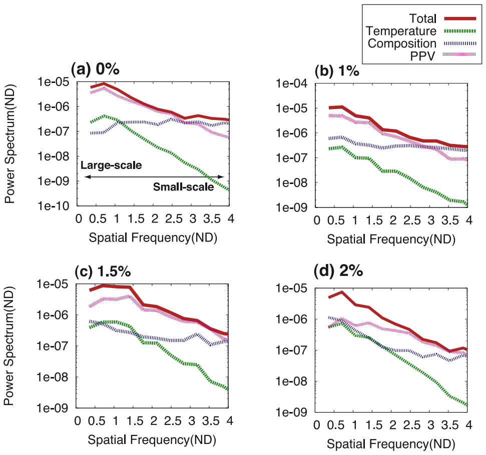

Figure 3. Spectral profiles as a function of spatial frequency of seismic anomalies at 2700 km calculated by using $d\ln V_s = a\delta T + b\delta C + c\delta\Gamma$ where the coefficients a and b are determined from mineral physical constraints [*Trampert et al.*, 2001] and the coefficient c is set to 0.02. (a) 0% compositional density variation, (b) 1%, (c) 1.5%, and (d) 2%.

[12] Regarding the distribution of the seismic discontinuity above D″, if this is explained by the PPV transition then it should be at shallower depth in regions where cold slabs pool above the CMB, and at greater depth or absent (if the CMB is hot enough to be in the perovskite stability field) in hot regions. Unfortunately the global sampling of this discontinuity [e.g., *Lay et al.*, 2004] appears insufficient to constrain this in detail. In the latter case, a possible explanation for sharp-sided structures observed in the deep mantle is the "edge" of a PPV region.

[13] In summary, the main conclusions are: (1) Lateral variations in the depth or occurrence of PPV can dominate the lateral heterogeneity spectrum in the depth range they occur as well as cause sharp-sided structures. (2) Previous findings in 2D such as the anticorrelation of PPV and accumulations of chemically-dense material are robust in 3D. In order to check it quantitatively, the cross-correlation between compositional field and phase function of PPV should be calculated but it will be done in the future. (3) The planform of such accumulations in a system where heterogeneity is introduced through differentiation is similar to that obtained in spherical or cartesian calculations in which a layer is inserted a priori and which have differing approximations and parameters. (4) A combination of the PPV transition and dense piles of dense basaltic material, anticorrelated with each other, may both be necessary for simultaneously understanding the distribution of the D″ discontinuity as well as long-wavelength heterogeneity in the CMB region.

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