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Effects of the post-perovskite phase transition properties on the stability and structure of primordial reservoirs in the lower mantle of the Earth

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ABSTRACT

Two key features of the lowermost Earth's mantle are the presence of Large Low Shear Velocity Provinces (LLSVPs), which may be reservoirs of primordial, chemically distinct material, and the phase change from perovskite (pv) to post-perovskite (pPv), which may occur at lowermost mantle conditions. However, the influence of this phase change on the shape, dynamics, and stability of chemically distinct reservoirs is not well constrained. Here, we performed numerical experiments of thermo-chemical convection in 2-D spherical annulus geometry to investigate the effects on thermo-chemical structure in the lower mantle of three parameters affecting the pPv phase change: the core–mantle boundary (CMB) temperature (T_{CMB}), the viscosity ratio between pv and pPv ($\Delta\eta_{pPv}$), and the Clapeyron slope of the pPv phase transition (Γ_{pPv}). Our results indicate that increasing CMB temperature increases the wavelength of the primordial reservoirs. Furthermore, a high CMB temperature promotes the development of plumes outside the reservoir of primordial material. High CMB temperature and large Clapeyron slope both favour the formation of pPv patches and of a double-crossing of the phase boundary, thus preventing the formation of continuous layer of pPv above the CMB. Combined with a low CMB temperature and/or a low Clapeyron slope of the pPv phase transition, a full layer of weak pPv above the CMB strongly enhances the mixing efficiency of primordial material with ambient regular mantle material, which may not allow the generation of large reservoirs. Based on our experiments, we conclude that the models of convection best describing the Earth's mantle dynamics include a large pPv Clapeyron slope (typically in the range of 13–16 MPa/K), and a moderate CMB temperature (around 3750 K). Our models do not provide further constraints on the value of the pPv viscosity, both regular and low values giving similar results on stability and structure of large primordial reservoirs for models with a moderate CMB temperature and large Clapeyron slope, but more plumes can be observed outside these large reservoirs in the cases with regular pPv than those in the cases with weak pPv.

1. Introduction

One of the most important discoveries of the past decade in mineral physics is the phase change from perovskite (pv) to post-perovskite (pPv), which may occur under the conditions of the lowermost mantle of the Earth (Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004). This phase transition was predicted by Sidorin et al. (1999), who noted that an exothermic phase change above the core–mantle boundary (CMB) would explain the D'' discontinuity observed by seismologists better than a chemically distinct layer. Since its discovery, post-perovskite was found to bear properties compatible with the properties of the D'' region. In particular, the shear modulus of pPv is larger than that of pv, implying that shear-waves travel faster in pPv regions (e.g., Caracas and Cohen, 2005; Mao et al., 2007; Stackhouse and Brodholt, 2007). Recent seismic observations (Cobden and Thomas, 2013) suggest that the D'' discontinuity may however have different origins depending on the polarities of P- and S-waves, and that the pPv phase transition may be a good candidate for regions where these polarities are opposite. A key property of the pPv phase transition is its large Clapeyron slope, around 8–10 MPa/K (Oganov and Ono, 2004), or even more according to recent estimates (Tateno et al., 2009; Hernlund, 2010), implying that pPv should not be stable in hot regions, which would explain why the

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seismic discontinuity atop D'' is not ubiquitous. Interestingly, pPv is a strongly anisotropic mineral, and its presence may thus explain the anisotropy observed in the D'' region (Wookey et al., 2005).

Seismic tomography models further reveal two Large Low Shear Velocity Provinces (LLSVPs) in the lowermost mantle beneath Africa and the Pacific (e.g., Masters et al., 2000; Trampert et al., 2004; Ni et al., 2002; He and Wen, 2012). Cluster analysis (Lekic et al., 2012) and the fact that they are also observed by normal mode tomography (Ishii and Tromp, 1999; Trampert et al., 2004; Mosca et al., 2012) indicate that LLSVPs are robust features, not artifacts. Furthermore, probabilistic tomography (Trampert et al., 2004; Mosca et al., 2012) suggest that they are hotter and chemically distinct compared to the ambient mantle. Since the phase change from perovskite (pv) to post-perovskite (pPv) is mainly expected to occur in cold regions of the lowermost mantle, pPv may not be found within LLSVPs. This is in agreement with the most recent thermo-chemical distributions deduced from probabilistic tomography (Mosca et al., 2012). If it is present outside LLSVPs, pPv may explain the anti-correlation between shear-wave and bulk sound velocity anomalies (Hutko et al., 2008; Davies et al., 2012).

The presence of post-perovskite may have some substantial influences on mantle dynamics. It has been pointed out, for instance, that the distributions of dense material and post-perovskite are anti-correlated (Nakagawa and Tackley, 2005, 2006), and the spectra of chemical anomalies are strongly influenced by the topography of the post-perovskite phase transition (Nakagawa and Tackley, 2006). Furthermore, due to its large Clapeyron slope, the post-perovskite phase transition may be responsible for specific structures such as double-crossings in warm regions (Hernlund et al., 2005). It is therefore important to properly describe the interactions between the pPv phase transition and the LLSVPs. This, in turn, requires a good knowledge of the properties of pPv and of the conditions under which it appears, including the temperature at the CMB, the Clapeyron slope of the pPv phase transition, and the viscosity of the pPv relative to that of pv. These parameters, however, remain poorly constrained.

The CMB temperature provides important constrains on the thermal structure of Earth's mantle. Previous laser-heated diamond-anvil cell (DAC) experiments indicated that the solidus temperature of primitive mantle is about 4200 K at the CMB (e.g., Zerr et al., 1998; Fiquet et al., 2010; Andrault et al., 2011). This high CMB temperature indicates that part of the CMB region is in the perovskite stability field, thus preventing a global layer of pPv covering the CMB. However, a recent study by Nomura et al. (2014) suggests that a natural primitive mantle (pyrolite) with 400 ppm H_2O could result in a much lower CMB temperature (3570 ± 200 K) compared to the previously assumed range of values.

The viscosity contrast between pv and pPv remains a matter of debate. Some experimental studies (e.g., Yoshino and Yamazaki, 2007; Hunt et al., 2009), as well as theoretical calculations by Ammann et al. (2010) based on the first-principle methods, reported a weak pPv viscosity, by a factor of $O(10^3)$ to $O(10^4)$ lower than that of pv. A low viscosity of pPv is consistent with recent geoid modelling, which requires colder regions of the deepest lower mantle to be weaker than hotter regions (Cadek and Fleitout, 2006). Meanwhile, some other studies give opposite results favouring more viscous pPv (Karato, 2011).

The Clapeyron slope of the phase transition from pv to pPv also varies in different experimental studies from early measured values of 8–10 MPa/K (e.g., Oganov and Ono, 2004) to the current preferred value of 13 MPa/K or higher (e.g., Tateno et al., 2009; Hernlund, 2010).

In this study, we perform a series of numerical experiments of thermo-chemical convection to investigate the influence of each of the three parameters discussed above on mantle convection. We focus in particular on their effects on the stability and structure of the primordial reservoirs in the lower mantle.

2. Numerical experiments set up

The numerical experiments are performed with StagYY (Tackley, 2008), which solves the conservation equations of mass, momentum, energy, and composition for an anelastic compressible fluid with infinite Prandtl number. Calculations are performed in 2-D spherical annulus geometry (Hernlund and Tackley, 2008) with a ratio between inner and outer radii of $f = 0.55$, matching the Earth's mantle.

The viscosity is assumed to depend on temperature, depth, phase, and yield stress. A viscosity jump of 30 is imposed at the boundary between upper and lower mantles. Viscosity is thus given by

$$\begin{aligned} \eta_b(z, T, \Gamma_{pPv}) &= \eta_0\left[1 + 29H(z - 660)\right] \\ &\quad \times \exp\left[\Gamma_{pPv}\ln(\Delta\eta_{pPv}) + V_a\frac{z}{D} + E_a\frac{\Delta T_S}{(T + T_{off})}\right] \\ \eta_Y &= \frac{\sigma_0 + \sigma_i P}{2\dot{e}} \\ \eta &= \frac{1}{\left(\frac{1}{\eta_b(z,T,\Gamma_{pPv})} + \frac{1}{\eta_Y}\right)} \end{aligned} \quad (1)$$

where η_0 is the reference viscosity (taken at temperature $T = 1600$ K and depth $z = 0$ km), H is the Heaviside step function, and $\Delta\eta_{pPv}$ is the viscosity jump between perovskite and post-perovskite, which is equal to 1 for regular pPv, and 1/1000 in the case of weak pPv. V_a and E_a are the non-dimensional activation volume and energy, controlling viscosity variations with depth and temperature, respectively. T_{off} is the offset temperature, which reduces the viscosity jump through the top thermal boundary layer. Here, we set the value of this parameter to $0.88\Delta T_S$. The yield stress helps to build plate-like behaviour at the top of the domain. Here, we define the yield stress by imposing its surface value σ_0, and its pressure gradient σ_i. The yield viscosity η_Y, is defined as the ratio between the yield stress and the second invariant of the strain rate tensor $\dot{e}$. To avoid numerical difficulties, the viscosity is truncated between 10^{-3} and 10^5 of the reference viscosity.

The reference Rayleigh number is defined as:

$$Ra_{ref} = \frac{\alpha_s g \rho_s \Delta T_s D^3}{\eta_0 \kappa_s} \quad (2)$$

where α_s is the surface thermal expansivity, g the acceleration of gravity, ΔT_s the super-adiabatic temperature difference, D the mantle thickness, η_0 the reference viscosity obtained using the potential temperature of 1600 K at the surface, and κ_s the surface thermal diffusivity. This reference Rayleigh number remains constant during the entire experiment, and in this study we prescribed $Ra_{ref} = 10^8$ for all experiments. The effective Rayleigh number Ra_{eff}, calculated with volume-averaged properties, varies with time but remains around 3×10^6 in all our calculations.

We use a phase function approach to model the perovskite to post-perovskite phase transition. This phase function is based on that in Christensen and Yuen (1985), and is defined by

$$\Gamma_{pPv}(T, z) = 0.5 + 0.5\tanh\frac{z - z_{pPv} - \gamma_{pPv}(T - T_{pPv})}{w} \quad (3)$$

where Γ_{pPv} is the phase function for post-perovskite, varying from 0 for perovskite to 1 for post-perovskite, T and z are temperature and depth, respectively, (T_{pPv}, z_{pPv}) is a point on the phase boundary, γ_{pPv} is the Clapeyron slope and w is the width of the phase