Sensitivity study of the thermal state in the lower mantle by 3-D convection with post-perovskite phase transition

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The influences of the post-perovskite (PPV) phase transition on the thermal state in the lower mantle are studied with a three-dimensional model of mantle convection in a Cartesian domain under the extended Boussinesq approximation with variable viscosity and temperature-dependent thermal conductivity. We have varied (i) the rate of density change associated with the PPV transition which determines the intensity of latent heat exchange and (ii) the temperature at the core-mantle boundary (CMB) which determines the stability field of the PPV phase through the relative positioning with the phase transition temperature at the CMB. We found that the actual PPV phase transition hardly affects the thermal structure in the lower mantle, although it has a tendency to bend the vertical temperature profile toward the equilibrium thermodynamic conditions of the transition in extreme cases for large density changes.
1. Introduction

The experimental discovery of the post-perovskite (PPV) phase by Murakami et al. [2004] has greatly stimulated new research directions in many areas in the earth sciences (see Hirose et al. [2006a] for a review), such as theoretical mineral physics (e.g. Tsuchiya et al. [2004]; Iitaka et al. [2004]; Oganov and Ono [2004]; Oganov et al. [2005]), seismology (Lay et al. [2005]; Hernlund et al. [2005]), and geodynamics (Nakagawa and Tackley [2004, 2005]; Matyska and Yuen [2005a, b]). Up to now, the geodynamical studies on the PPV transition have been focused on the destabilizing nature of the D" layer from the phase transition (Matyska and Yuen [2005a]) and the core-mantle interaction (Nakagawa and Tackley [2004, 2005]). In these earlier studies, the influences of the PPV transition were estimated mainly by varying the Clapeyron slope of the transition. However, there has been scant attention devoted so far to the influences of the variation of other thermodynamic parameters, such as the rate of density change $\Delta \rho/\rho$ associated with the phase transition and the temperature $T_{\text{int}}$ of the transition at the pressure of the core-mantle boundary (CMB). Indeed, the thermodynamic parameters of the PPV transition are also fraught with at least 50% uncertainties in the Clapeyron slope (Hirose et al. [2006b]), and 500 to 1000K in the transition temperature at the CMB pressure (Hirose, private communication, 2006). Since $\Delta \rho/\rho$ determines the intensity of the latent heat exchange during the phase transition, it is most likely to affect the thermal state near the phase transition regions. On the other hand, the stability field of the PPV phase near the CMB, which is roughly estimated by the relative positioning between the CMB temperature $T_{\text{CMB}}$ and the temperature $T_{\text{int}}$ of the PPV phase transition there, is expected to control the po-
sitions of the phase transition as well as the number of crossing the phase boundaries (Hernlund et al. [2005]). In this paper we will study the sensitivity of the thermal state in the lower mantle, by a three-dimensional model of mantle convection in a rectangular domain, with special emphasis to the influence of the variations in $T_{\text{CMB}}$ and $\Delta \rho/\rho$.

2. Model Description

A time-dependent convection model in a basally-heated three-dimensional rectangular box of 3000km height and aspect ratio of $6 \times 6 \times 1$ is considered. We employed an extended Boussinesq approximation (e.g. Christensen and Yuen [1985]), where the effects of latent heat, adiabatic heating and viscous dissipation are explicitly included in the energy transport. Temperature is fixed to be $T_{\text{top}} (=300\text{K})$ and $T_{\text{CMB}}$ at the top and bottom boundaries, respectively. The value of $T_{\text{CMB}}$ is taken to be either 2800K or 3800K in this study: The former is lower than the temperature of the PPV transition at the bottom surface (assumed to be 3155K in this study), while the latter is higher (see below for the meanings). The viscosity $\eta$ of mantle materials exponentially depends on temperature and depth, with the viscosity variation of $10^{3.5}$ by the temperature change of $\Delta T (=2500\text{K})$ and that of $10^2$ with depth. We also take into account a temperature-dependence of thermal diffusivity $\kappa$, which mimics the effects of radiative heat transfer expected to be dominant in the hotter part of the mantle (Hofmeister [1999]). Here we assume that $\kappa$ increases by a factor of 4 with temperature $T$, as a third-order polynomial of $T$. Other physical properties, such as thermal expansivity, are kept constant in the entire domain. In all of the calculations presented in this paper we used the Rayleigh number $Ra_{\text{top}} = 8 \times 10^6$.
In this study we take into account an exothermic phase transition between perovskite to PPV as well as an endothermic transition between spinel and perovskite. Their mechanical and thermodynamical effects are modeled by a phase function $\Gamma$ (Christensen and Yuen [1985]). In nondimensional forms they are defined by,

$$
\Gamma^{(i)} = \frac{1}{2} \left[ 1 + \tanh \left( \frac{\pi^{(i)}}{\Delta z^{(i)}} \right) \right],
$$

$$
\pi^{(i)} \equiv -z - \gamma^{(i)}(T - T_{\text{int}}^{(i)}).
$$

\(i\) is the index classifying the phase transitions (\(i = 1\) for spinel-perovskite and \(i = 2\) for PPV transitions), \(\pi\) is the excess pressure, \(z\) is the vertical coordinate pointing upward, \(T\) is temperature, \(\gamma\) is the Clapeyron slope, \(\Delta z (=0.05)\) is the depth range for phase transitions, and \(T_{\text{int}}\) is the temperature of phase transition at the bottom surface \((z = 0)\). This formulation describes the undulation of the phase boundaries and, in particular, allows the possibilities of double-crossing expected for the PPV transition (Hernlund et al. [2005]).

The density change due to phase transition is expressed by another nondimensional parameter called phase boundary Rayleigh number $Rb$ (Christensen and Yuen [1985]), whose ratio to $Ra_{\text{top}}$ equals the ratio of the density change due to the phase transition and that due to the thermal expansion by a unit temperature change ($\Delta T$). In this study, the spinel-perovskite phase transition \((i = 1)\) is modeled by a transition at around 660km depth with $\gamma = -0.12$ and $Rb/Ra_{\text{top}} = 1.25$, which correspond to the Clapeyron slope of around $-4.3\text{MPa/K}$ and the density jump of around 10%, respectively. On the other hand, the PPV phase transition \((i = 2)\) is modeled by a transition with $\gamma = 0.36$ and
$T_{\text{int}} = 1.26 \ (\sim 3155 \text{K})$, while $Rb/Ra_{\text{top}}$ is taken to be a free parameter ranging from 0 to 1.25 ($\sim 10\%$ density jump). We note that the above values of adopted parameters are larger than those derived from theoretical or experimental studies (e.g. Hirose [2002]; Murakami et al. [2004]; Tsuchiya et al. [2004]; Oganov and Ono [2004]; Fei et al. [2004]; Hirose et al. [2006b]), in order to emphasize the extreme roles played by these parameters in the PPV phase transition.

The computational domain is divided uniformly into $512 \times 512 \times 128$ meshes based on a finite-volume scheme. The calculations are carried out by our newly developed code for the Earth Simulator (Kameyama et al. [2005]; Kameyama [2005]) using a primitive variable formulation (velocity, pressure and temperature), whose numerical validity has been already verified. In each run, we continued time-marching calculations until the initial transient behavior disappeared. Each run typically requires 200,000 time steps, and takes about 100 wall-clock hours, using 16 nodes or 128 processors of the Earth Simulator. Although the actual calculations are carried out in a nondimensional form, the results are presented in a dimensional form using a temperature scale of $\Delta T = 2500 \text{K}$.

3. Results

3.1. Influence of the density jump associated with the PPV transition

We first present the results of the calculations of the series L where $T_{\text{CMB}} = 2800 \text{K}$ (see Table 1) is kept and, hence, the PPV phase is dominant at the bottom surface (i.e. $T_{\text{CMB}} < T_{\text{int}}^{(2)}$). In Figure 1 we show for three cases (a) the three-dimensional distributions of lateral thermal anomalies $\delta T \equiv T - \langle T \rangle$, and (b) the plots against height $z$ of the horizontally-averaged $\langle T \rangle$ (red), maximum $T_{\text{max}}$ (green) and minimum $T_{\text{min}}$ (blue)
values of temperature at height $z$. The values of $T_{\text{max}}$ and $T_{\text{min}}$ roughly represent the temperature of ascending and descending flows, respectively. The case L02 is the case with $Rb^{(2)}/Ra_{\text{top}} = 0.25$, which approximately corresponds to the density jump of 2% associated with the PPV transition and is close to the value obtained by theoretical and experimental studies (Tsuchiya et al. [2004]; Murakami et al. [2004]), while the values of $Rb^{(2)}/Ra_{\text{top}}$ adopted in cases L00 and L02 are 0 and 1.25, respectively. Namely, in case L00 the PPV transition does not affect the convective nature at all, while in case L10 the effect of density jump associated with the phase transition is significantly exaggerated. Also shown in Figure 1b are the phase relations assumed in these calculations, as functions of temperature $T$ and height $z$. The dotted lines indicate the relations of phase boundaries ($\Gamma^{(i)} = 0.5$ or $\pi^{(i)} = 0$), while the hatched regions indicate the phase transition regions marked by $|\pi^{(i)}| \leq \Delta z^{(i)}$. The intersection of the temperature profiles and the hatched regions means that the phase transition occurs over the depth range.

The plots in Figure 1b show that the vertical temperature profiles have single intersection with each phase boundary. In other words, the dominant phase monotonously changes from spinel to perovskite and from perovskite to PPV with increasing depth. This also implies that the double-crossing of the PPV transition (Hernlund et al. [2005]) never occurs in these calculations. The plots also show that the PPV transition takes place not near the core-mantle boundary but at a much shallower part. In case L02, for example, the vertical profiles of $T_{\text{min}}, T_{\text{max}}$ and $\langle T \rangle$ intersect with the perovskite to PPV phase boundary at $z \sim 0.3, 0.1$ and 0.2, respectively. All of these phenomena described above come from the low $T_{\text{CMB}} < T_{\text{int}}^{(2)}$ and thus resulting low overall mantle temperature.
Figure 1 shows that the thermal state at depth is significantly influenced by a sufficiently large density jump associated with the PPV transition. From a comparison of the three cases we can clearly discern that the thermal state is significantly different in case L10 \((Rb^{(2)}/Ra_{\text{top}} = 1.25)\), while it is basically the same in case L02 \((Rb^{(2)}/Ra_{\text{top}} = 0.25)\) with that in case L00. The thermal state obtained in case L10 is characterized by (i) a thick transition region (ranging about \(0.1 \leq z \leq 0.3\)) between the perovskite to PPV phases and (ii) the vertical profile of \(\langle T \rangle\) bent toward the phase equilibrium relations over the depth range. This is due to the steep positive Clapeyron slope as well as the large density jump associated with the PPV phase transition. Because the Clapeyron slope is steep and positive, the PPV phase transition is allowed to occur over the broad range of pressure (or depth) according to the temperature variation. In addition, when a significant amount of latent heat is exchanged during the phase transition, the thermal state in the phase transition region tends to be controlled by the thermodynamic \(p-T\) condition, as in the cases with solid-liquid phase transitions in melt dynamics (e.g. Kameyama et al. [1996]). Since the rate of latent heat exchange is proportional to the density jump of the phase transition \((Rb/Ra_{\text{top}})\), a significant amount of latent heat is exchanged in the case L10 and, hence, the thermal state in the PPV phase transition region becomes close to the phase equilibrium condition. We also carried out (though not shown here) similar calculations with several values of \(Rb^{(2)}/Ra_{\text{top}}\) ranging from 0.5 to 1, and confirmed that the above tendency is more prominent for a larger \(Rb^{(2)}\) or, in other words, a higher rate of latent heat exchange.
The snapshot of case L10 in Figure 1 also shows other influences of the exaggerated latent heat exchange by a large $Rb^{(2)}$. First is the occurrence of a superadiabatic region in the bottom third of the mantle, which would concur with earlier studies in mineral physics (e.g. da Silva et al. [2000]). This is because the vertical temperature gradient in the PPV phase transition region becomes close to that of the equilibrium condition of the transition. Second is the “necking” of the surfaces of the cold thermal anomalies at around the depth of $z \sim 0.2$, which approximately corresponds to the mean height of the PPV transition (see Figure 1b). As can be seen from the vertical profile of $T_{\text{min}}$ in Figure 1b, cold descending flows are heated up at the perovskite to PPV phase transition because of the latent heat release due to the exothermic transition. This reduces the temperature contrast between the cold descending flows and the surroundings, and hence, results in the “necking” of the cold thermal anomalies. The latter phenomenon is quite similar to “slab detachment” by the exothermic olivine to spinel transition in the upper mantle, suggested by Brunet et al. [1998].

3.2. Influence of the bottom temperature $T_{\text{CMB}}$

In Figure 2 we present the results of the several cases of the calculations of the series H where $T_{\text{CMB}} = 3800\text{K}$ is assumed. In this series, in contrast to the series L, the PPV phase is not dominant at the bottom surface, since $T_{\text{CMB}} > T_{\text{int}}^{(2)}$. Shown in Figure 2 are the snapshots obtained for the cases H02 and H10 where the values of $Rb^{(2)}/Ra_{\text{top}}$ are 0.25 and 1.25, respectively.

The snapshot of case H02 shows that the manner of the PPV phase transition is quite different from that in case L02 (see Figure 1). The vertical profile of $\langle T \rangle$ for the case
H02 (Figure 2) shows that the PPV phase transition takes place on average at around $z \sim 0.05$, much deeper than in case L02 (see also Figure 1b). Moreover, the profile of $T_{\min}$ has two intersections with the phase boundary between perovskite and PPV phases (i.e. double crossing; Hernlund et al. [2005]) while that of $T_{\max}$ does not at all. This indicates that the PPV phase as well as the double crossing of the phase transition are associated only with the regions near cold descending flows in the lowermost mantle (Nakagawa and Tackley [2005]). Figure 2b also shows that the vertical thermal profiles at depth in case H02 are very similar to those expected in cases without the influences of the PPV transition, implying that the influence of the PPV transition with small density jump is rather minor, as also observed in case L02 (see Figure 1).

From the comparison between the cases H02 ($Rb^{(2)}/Ra_{\text{top}} = 0.25$) and H10 (1.25), we can see that the influence of increasing $Rb^{(2)}$ is apparent only near the cold thermal anomalies. The three-dimensional distributions of lateral thermal anomalies $\delta T$ (Figure 2a) show that in case H10 they are rounded-off above the bottom surface instead of reaching there, while in case H02 they are spread along the bottom surface after having reached there. This is similar to the “necking” of descending flows observed in case L10. Indeed, as can be seen in Figure 2b, the vertical profile of $T_{\min}$ in case H10 is bent toward the phase equilibrium relations between the perovskite and PPV phases. This is also due to the significant latent heat exchange during the PPV phase transition introduced by the exaggerated $Rb^{(2)}$. In contrast, the profiles of $T_{\max}$ are very similar in cases H02 and H10. This reflects the fact that the PPV phase transition never occurs in the hot anomalies.
The comparison between the series L and H clearly indicates that the influence of increasing $Rb^{(2)}$ on the thermal state becomes smaller for higher $T_{CMB}$. As can be seen in Figures 1b and 2b, the vertical profiles of $\langle T \rangle$ are raised by increasing $Rb^{(2)}$ only slightly over a rather narrow depth range just above the bottom surface for $T_{CMB} = 3800K$, while they are significantly affected over a broad depth range for $T_{CMB} = 2800K$. The difference comes from the difference in the extent of the occurrence of the PPV transition. The vertical profiles of $T_{max}$ and $T_{min}$ show that for high $T_{CMB} > T^{(2)}_{int}$ (series H) the PPV phase transition takes place only in the cold regions, while for low $T_{CMB} < T^{(2)}_{int}$ (series L) it occurs both in hot and cold regions. Owing to the reduced extent of the PPV transition, the influence of increasing $Rb^{(2)}$ on the thermal state becomes smaller for higher $T_{CMB}$. In other words, the influence of a higher $T_{CMB}$ is to diminish the tendency toward superadiabaticity. We may expect more superadiabatic situations in a secularly-cooled lower mantle.

4. Concluding Remarks

We studied by three-dimensional numerical model of mantle convection in a rectangular domain the possible influences of the post-perovskite (PPV) phase transition on the thermal state in the lowermost mantle. In this paper we carried out several calculations by varying two parameters: (i) $Rb^{(2)}/Ra_{top}$ describing the density jump associated with the PPV phase transition and (ii) the temperature $T_{CMB}$ at the bottom surface which determine the stability field of PPV phase around there. We found that the influence of the phase transition is prominent only in the cases where $Rb^{(2)}/Ra_{top}$ is sufficiently large and $T_{CMB}$ is lower than the temperature at the PPV phase transition $T^{(2)}_{int}$ at the bottom.
surface. The former condition requires a sufficient amount of latent heat exchange during
the phase transition, while the latter requires that the PPV phase transition takes place
not only in cold but also in hot regions at depth. When the above conditions are met, the
vertical temperature profile tends to be bent toward the equilibrium relations of the PPV
phase transition owing to the buffering effect of latent heat exchange. We also found that,
for realistic values of the density jump associated with the PPV phase transition (\(\sim 1.5\%\);
Tsuchiya et al. [2004]), the transition is not likely to exert significant influences on the
thermal state at depth. However, this finding may underestimate the potential influence of
the PPV transition, owing to our insufficient treatment of the depth-dependence of phys-
ical properties. Indeed, earlier studies based on fully compressible model (Nakagawa and
Tackley [2004, 2005]) reported that the PPV transition can affect the convective patterns
even with a density change of a few percent. In particular, a strong depth-dependence
of thermal expansivity, as recently suggested by Katsura et al. [2005], may significantly
amplify the influence of PPV transition.

Our results also demonstrate that, in addition to other thermodynamics parameters,
the density change of the phase transition can control the position of the phase transition
and, in particular, the number of crossing the PPV phase boundary. In earlier studies
(Hernlund et al. [2005]; Nakagawa and Tackley [2005]), the possibility of “double crossing”
of the PPV boundary has been discussed only in terms of the Clapeyron slope and the
stability field of the PPV phase near the CMB. However, our results indicate that the
above conjecture is valid only when the influence of the latent heat exchange is minor (see

DRAFT January 12, 2006, 11:59am DRAFT
Figure 2). We thus conclude that the latent heat energetics is another important agent which may control the nature of phase transitions in the deep mantle.

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