Effects of a perovskite-post perovskite phase change near core-mantle boundary in compressible mantle convection

Takashi Nakagawa[1] and Paul J. Tackley[2]

[1]   Numerical simulations of compressible, isochemical mantle convection are used to investigate the effect of the perovskite to post-perovskite phase transition at around 2700 km depth, which has recently been discovered by high-pressure experiments and ab initio calculations, on the convective planform, temperature, and heat transport characteristics of the mantle. The usual phase transitions at 410 km (olivine-spinel) and 660 km (spinel-perovskite) are also included. The exothermic post-perovskite phase change at 2700 km depth destabilizes the lower thermal boundary layer, increasing the heat flow, increasing interior mantle temperature, and increasing the number and time-dependence of upwelling plumes. The resulting weak, highly time-dependent upwellings also have a smaller horizontal spacing than the plumes that occur in the absence of the phase transition. While the influence of post-perovskite phase change may be smaller than that of some other complexities, such as compositional stratification, it appears to have an important enough effect that it should not be ignored in dynamical studies of mantle convection.   *INDEX TERMS:* 8121 Tectonophysics: Dynamics, convection currents and mantle plumes; 8124 Tectonophysics: Earth's interior—composition and state (1212); 8147 Tectonophysics: Planetary interiors (5430, 5724). **Citation:** Nakagawa, T., and P. J. Tackley (2004), Effects of a perovskite-post perovskite phase change near core-mantle boundary in compressible mantle convection, *Geophys. Res. Lett.*, *31*, L16611, doi:10.1029/2004GL020648.

1. Introduction

[2]   Recent mineral physics experiments and ab initio calculations [*Murakami et al.*, 2004; *Oganov and Ono*, 2004; *Tsuchiya et al.*, 2004] have indicated that perovskite undergoes an exothermic phase change to a post-perovskite structure just above the core-mantle boundary (CMB). While the density change of this proposed phase change is small, at 1.0–1.2%, the Clapeyron slope is estimated to be large, in the range 8 to 9.6 MPa/K [*Murakami et al.*, 2004; *Oganov and Ono*, 2004; *Tsuchiya et al.*, 2004]. Thus the phase transition could have an important dynamical effect.

[3]   Although there have been many mantle convection modeling studies that have focused on structure in the deep mantle, they have mostly been concerned with the heterogeneous structures that are generated from possible compositional layering in that region [e.g., *Davies and Gurnis*, 1986; *Hansen and Yuen*, 1988; *Montague and Kellogg*, 2000; *Tackley*, 2002]. A deep phase transition has been considered in only one Earth-related modeling study [*Sidorin et al.*, 1999], which focused on the seismic signature associated with such a phase transition, and concluded that it offered the best explanation of observed seismic structures such as the "Lay discontinuity", but did not investigate the dynamical effects of such a transition. The only studies on the dynamical effects of deep phase transitions were modeling Mars, which, due to its smaller size and lower gravity, has the equivalent of Earth's transition zone in its' deep mantle. While [*Weinstein*, 1995; *Harder and Christensen*, 1996] found that the endothermic spinel to perovskite transition just above the CMB focuses upwellings into fewer big features, *Breuer et al.* [1998] appeared to find a similar effect with an exothermic phase transition 20% of the mantle depth above the CMB due to latent heat effects. Given this apparent contradiction and the fact that these models were set up to study Mars, there is a clear need for new calculations with a more Earth-like model, in order to clarify the effects that this deep exothermic post-perovskite phase transition has in Earth's mantle. Here, an exploratory set of three model calculations is presented to give a first order characterization these effects.

2. Model

[4]   The new feature of the model is the proposed exothermic perovskite-post perovskite at 2700 km depth, which is approximately 200 km above the CMB. Additionally the usual olivine-system phase changes at 410 km (+2.5 MPa/K) and 660 km (−2.5 MPa/K) depth are included. The properties of the perovskite-post perovskite phase change, listed in Table 1, are based on recent discoveries [*Murakami et al.*, 2004; *Oganov and Ono*, 2004; *Tsuchiya et al.*, 2004]. The physical and numerical model are similar to that described in other publications [*Tackley*, 1996], so only the key details are described here. The isochemical and compressible anelastic approximation are used, which naturally incorporates reasonable depth-dependence of the physical properties thermal expansivity, conductivity, and density; depth-dependence of physical properties. Viscosity is moderately dependent on temperature and depth, following the formulation of *Tackley* [1996], with viscosity varying by three orders of magnitude with temperature and two orders of magnitude with depth. In

[1]Department of Geophysical Sciences, University of Chicago, Chicago, Illinois, USA.
[2]Department of Earth and Space Sciences and Institute of Geophysics and Planetary Physics, University of California, Los Angeles, California, USA.

Table 1. Physical Parameters for the Post-Perovskite Phase Change[a]

Symbol	Meaning	Dim. Values
$\Delta\rho_{ppv}$	Den.var.	66.4 kg m^{-3}
γ_{ppv}	Clapeyron slope	See text
T_{ppv}	Temp. at phase boundary	2650 K
d_{ppv}	Depth at phase boundary	2700 km

[a]The density jump is calculated by using experimental data [*Murakami et al.*, 2004].

order to emphasize the dynamics of instabilities in the CMB region, no internal heating is included. All physical parameters are listed in Table 2.

[5] For this initial exploratory study, a two-dimensional half-cylindrical geometry is used, with periodic side boundaries and free slip, impermeable and isothermal upper and lower boundaries. The numerical resolution is 256 (azimuthal) by 128 (radial) cells, with radial grid refinement near the top and bottom boundaries and the 410 and 660 km discontinuities. The temperature field is initialized to an adiabat (1800 K potential temperature) with small random perturbations and error function boundary layers at top and bottom. In order to reach such a secular equilibrium and establish long-enough time series for the highly time-dependent diagnostics (heat flow etc.), time integration is performed for 200,000 steps, which correspond to around t = 0.073 (27.6 Gyrs of dimensional time). For this initial exploration, three cases are presented with different Clapeyron slopes for the perovskite-post perovskite phase change: (1) a reference case with 0 MPa/K Clapeyron slope, (2) a ''predicted'' case with 8 MPa/K slope and (3) an ''exaggerated'' case in which the Clapeyron slope is artificially doubled to 16 MPa/K.

3. Results

[6] Time variations of the temperature field for the reference case (with no post-perovskite phase change) are shown in Figure 1a. Cold downwellings penetrate into the lower mantle, sometimes in the form of mantle ''avalanches'' caused by the endothermic phase change at 660 km depth. There is typically only one upwelling plume, which seems to be a relatively stationary feature, although some time-dependence is induced by episodic mantle avalanches. These cold downwellings sometimes generate a secondary plume from CMB, which subsequently merges into the main plume. Figure 1b shows time variations of the temperature field for the exaggerated case with a Clapeyron slope of +16 MPa/K. The most noticeable difference is in the upwelling plumes: instead of one large, steady plume there are now several smaller plumes that are very time-

dependent and typically do not travel across the whole mantle. Sometimes small plumes merge to make what temporarily appears to be a larger, branching plume, for example at t = 0.0726. Mantle avalanches induced by the endothermic phase change at 660 km occur, as in the reference case. Figure 1c shows time variations of temperature field for the ''predicted'' case with a Clapeyron slope of +8 MPa/K. The convective planform is still strongly time-dependent compared to the reference case (Figure 1a). However, the horizontal scale of upwelling plumes is relatively larger than in the exaggerated case (Figure 1b).

[7] Comparing the two cases with a deep phase transition to the reference case, it is clear that the main effect of the phase transition is to make upwelling plumes strongly unstationary and have a smaller horizontal scale. Boundary-layer instabilities occur more easily when an exothermic phase change is taken into account. The exothermic phase change thus destabilizes the lower thermal boundary layer, making instabilities grow more rapidly and be smaller, generating small-scale plumes. Because of this, the lower mantle temperature is higher.

[8] The time variation of heat flow through the surface and CMB, scaled to spherical shell geometry, is plotted in Figure 2 for the two extreme cases (reference and exaggerated). The heat flow is highly time-dependent, probably due to the action of the endothermic '660 km' phase transition and the relatively high Rayleigh number. The cases also have reached a secular equilibrium, in which quantities fluctuate about a mean value but there is no long-term trend. The important finding here is that the deep exothermic phase change enhances heat transport. This is indicated by the time averaged heat flows through surface and CMB: 41 TW for the reference case, 47 TW for the ''realistic'' case and 49 TW for the exaggerated case.

[9] Time-averaged vertical profiles of temperature for all cases are shown in Figure 3. The most striking feature is the increase of interior temperature with increasing strength of the post-perovskite phase transition, with a difference of about 400 K between the reference and exaggerated cases.

Table 2. Physical Mantle Parameters, $Ra_0 = \rho_0 g \alpha_0 \Delta T_{sa} d^3 / \kappa_0 \eta_0$

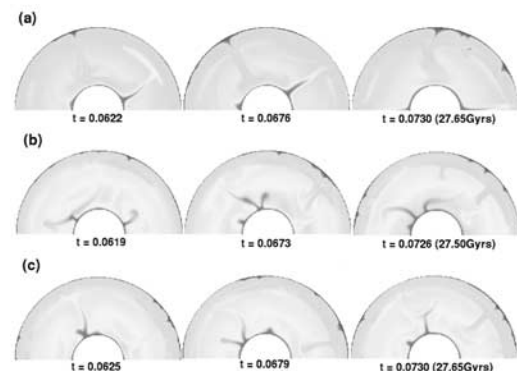| Symbol	Meaning	Non-D. Value	Dim. Values
Ra_0	Rayleigh #	6×10^7	N/A
d	Thickness	1	2890 km
η_0	Ref. visc.	1	1.4×10^{22} Pa s
ρ_0	Ref. (surface) density	1	3300 kgm^{-3}
g	Gravity	1	9.8 ms^{-2}
α_0	Ref. (surf.) th. expan.	1	5×10^{-5} K^{-1}
κ_0	Ref. (surf.) th. diff.	1	7×10^{-7} m^2 s
ΔT_{sa}	Temp. scale	1	2500 K
T_s	Surf. temp.	0.12	300 K

Figure 1. Time variation of the temperature field for (a) reference case with no post-perovskite transition (b) exaggerated case with doubled Clapeyron slope and (c) case with predicted Clapeyron slope. Quoted times are nondimensional, with a dimensional equivalent given for the final frame. Red indicates high temperature and blue indicates low temperature. See color version of this figure in the HTML.
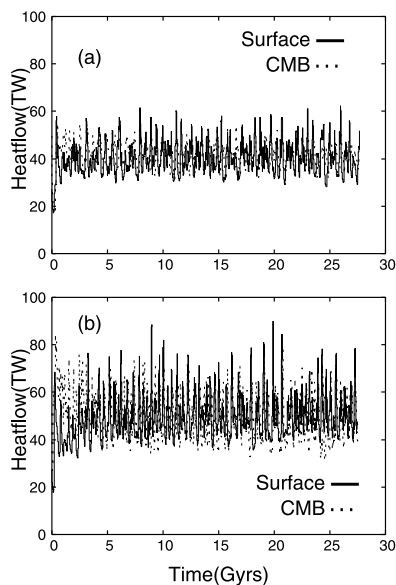
Figure 2. Heat flow through surface and CMB as a function of time. (a) No post-perovskite transition. (b) Exaggerated Clapeyron slope case.

Of course, the temperature difference that would occur under real Earth conditions would be lower because of the much stronger temperature-dependence of viscosity in the real Earth, which tends to buffer the mantle temperature through a feedback mechanism [*Tozer*, 1972]. Curiously, this temperature trend is opposite to what would be expected from latent heat effects, indicating that the phase change buoyancy effect is dominating the dynamics. This is not surprising, as the temperature change due to latent heat is only about 40 K. The higher mantle temperature has two consequences: it results in lower viscosity, which enhances convective vigor hence heat transport, but at the same time results in a lower temperature contrast for mantle plumes, reducing their strength.

4. Discussion

[10] It is useful to compare and contrast the present findings with previous results that were oriented towards understanding Mars. *Weinstein* [1995] studied the effect of a deep endothermic phase change (γ-spinel to perovskite) in a two-dimensional cylindrical geometry with the Boussinesq approximation, and found that it focuses plumes, resulting in fewer, stronger upwellings and a longer flow wavelength. This was confirmed in a three-dimensional spherical geometry by *Harder and Christensen* [1996], who found that one to two large upwelling plumes was a typical configuration. These findings, although treating a phase change of the opposite Clapeyron slope, form a consistent trend with the present study, in which a deep exothermic phase transition results in a larger number of weaker upwellings.

[11] *Zhou et al.* [1995] found that the two exothermic phase transitions, which are olivine to β-spinel and β-spinel to γ-spinel phase transitions near lower boundary layer in the Martian mantle, accelerate downwellings and boost plumes, resulting in stronger plumes. Such models were further explored by *Breuer et al.* [1997], who found that

latent heat can have a strong effect, tending to inhibit plumes from crossing the phase transition, in opposition to the phase change buoyancy effect which boosts plumes. The competition between these two effects resulted in oscillations between flow amplification and flow inhibition by the phase transitions. In all of the above studies the system was in a state of secular evolution throughout the calculations, unlike the present study where the focus is on the long-term statistical equilibrium state.

[12] In any case, it is expected that latent heat effects will be relatively more important on Mars than on Earth, because of the low excess temperature of upwellings and downwellings in the Martian mantle due to the rigid lid mode of convection. Quantitatively, in Mars the temperature change due to latent heat release by olivine to β-spinel or β-spinel to γ-spinel transitions is about 80 K, compared to a temperature contrast that participates in convection of 700–1000 K [*Breuer et al.*, 1998] or less [*Reese et al.*, 2002]. In contrast, the temperature change across the proposed post-perovskite transition in Earth is about 40 K, compared to a convection-participating temperature contrast of perhaps 2500 K. This suggests that the buoyancy effect of the deep exothermic phase transition will be dominant on Earth, as it is for the well-known transitions in the range 410 to 660 km depth, and as is observed in the present study. The present results indicate that a deep exothermic phase transition in Earth destabilizes the lower boundary layer, increasing the efficiency of heat transport through the CMB and decreasing the horizontal scale of upwelling plumes from the CMB region, as indicated by the clear trend observed in as the Clayeron slope is increased from 0 to 8 MPa/K then 16 MPa/K.

[13] The destabilization of the lower boundary layer slightly increases the heat flow through the CMB, indicating more rapid core cooling in a secular cooling Earth. This further reinforces the need for a heat buffer in the CMB region in order to obtain a thermal evolution that matches the available constraints (the present-day radius of the inner core and the need to maintain sufficient heat flux to power of the geodynamo). A heat buffer can be provided by a dense, compositionally-distinct layer above the CMB [*Nakagawa and Tackley*, 2004], radiogenic potassium in the core alloy [e.g., *Nimmo et al.*, 2004] and radiative thermal conductivity of deep mantle material (C. Matyska and D. A. Yuen, The importance of radiative heat transfer for superplumes with a deep mantle phase transition, submitted to *Earth and Planetary Science Letters*, 2004).
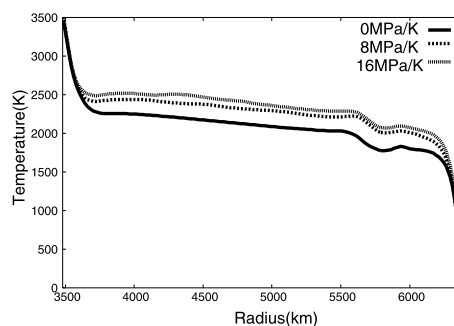

Figure 3. Vertical temperature profiles for all cases.

[14] In this study, the phase transition depth is fixed at 2700 km as predicted from experimental and theoretical approaches [*Murakami et al.*, 2004; *Oganov and Ono*, 2004]. Earlier in Earth's evolution, it would have been shallower while the thermal boundary layer would have been thinner, and the effects of this should be checked in a future study.

[15] The smaller horizontal scale of upwelling plumes in cases that include the new phase transition (e.g., compare Figures 1a and 1b) appears to make it more difficult to match the very long-wavelength, degree-two dominated heterogeneity in the CMB region observed in global seismic tomography models [e.g., *Masters et al.*, 2000] and may change the horizontal scale of thermo-chemical plumes found in numerical model of thermo-chemical mantle convection [e.g., *Tackley*, 2002].

[16] However, in the present study, various important complicating processes, such as extreme rheological behavior that results in plate tectonics, compositional variations and secular core-cooling, are not included. Such processes may dominate the change induced by the post-perovskite phase transition, and thus further investigation is necessary before reaching firm conclusions. The different anisotopic properties of the post perovskite phase may modify the seismic anisotropy predicted from slab interacting with the CMB [*McNamara et al.*, 2003].

References

Breuer, D., D. A. Yuen, and T. Spohn (1997), Phase transition in the Martian mantle: Implications for partially layered convection, *Earth Planet. Sci. Lett.*, *148*, 457–469.

Breuer, D., D. A. Yuen, T. Spohn, and S. Zhang (1998), Three dimensional models of Martian mantle convection with phase transitions, *Geophys. Res. Lett.*, *25*, 229–232.

Davies, G. F., and M. Gurnis (1986), Interaction of mantle dregs with convection-lateral heterogeneity at the core-mantle boundary, *Geophys. Res. Lett.*, *13*, 1527–1530.

Hansen, U., and D. A. Yuen (1988), Numerical simulations of thermal-chemical instabilities at the core mantle boundary, *Nature*, *334*, 237–240.

Harder, H., and U. R. Christensen (1996), A one-plume model of Martian mantle convection, *Nature*, *380*, 507–509.

Masters, G., G. Laske, H. Bolton, and A. Dziewonski (2000), The relative behavior of shear velocity, bulk sound speed, and compressional velocity in the mantle: Implications for chemical and thermal structure, in *Earth's Deep Interior: Mineral Physics and Tomography From the Atomic to the Global Scale*, Geophys. Monogr. Ser., vol. 117, edited by S. Karato et al., pp. 63–87, AGU, Washington, D. C.

McNamara, A. K., P. E. van Keken, and S.-I. Karato (2003), Development of finite strain in the convection lower mantle and its implications for seismic anisotropy, *J. Geophys. Res.*, *108*(B5), 2230, doi:10.1029/2002JB001970.

Montague, N. L., and L. H. Kellogg (2000), Numerical models of a dense layer at the base of the mantle and implication for the geodynamics of D″, *J. Geophys. Res.*, *105*, 1101–1114.

Murakami, M., K. Hirose, N. Sata, Y. Ohishi, and K. Kawamura (2004), Phase transition of $MgSiO_3$ perovskite in the deep lower mantle, *Science*, *304*, 855–858.

Nakagawa, T., and P. J. Tackley (2004), Effects of thermo-chemical mantle convection on the thermal evolution of the Earth's core, *Earth Planet. Sci. Lett.*, *220*, 107–119.

Nimmo, F., G. D. Price, J. Brodholt, and D. Gubbins (2004), The influence of potassium on core and geodynamo evolution, *Geophys. J. Int.*, *156*, 363–376.

Oganov, A. R., and S. Ono (2004), Theoretical and experimental evidence for a post-perovskite phase of $MgSiO_3$ in Earth's D″ layer, *Nature*, *430*, 445–448.

Reese, C. C., V. S. Solomatov, and J. R. Baumgardner (2002), Survival of impact-induced thermal anomalies in the Martian mantle, *J. Geophys. Res.*, *107*(E10), 5082, doi:10.1029/2000JE001474.

Sidorin, I., M. Gurnis, and D. V. Helmberger (1999), Dynamics of a phase change at the base of the mantle consistent with seismological observations, *J. Geophys. Res.*, *104*, 15,005–15,023.

Tackley, P. J. (1996), Effects of strong variable viscosity on three-dimensional compressible convection in planetary mantles, *J. Geophys. Res.*, *101*, 3311–3332.

Tackley, P. J. (2002), Strong heterogeneity caused by deep mantle layering, *Geochem. Geophys. Geosyst.*, *3*, 1024, doi:10.1029/2001GC000167.

Tozer, D. C. (1972), The present thermal state of the terrestrial planets, *Phys. Earth Planet. Inter.*, *6*, 182–197.

Tsuchiya, T., J. Tsuchiya, K. Umemoto, and R. M. Wentzcovitch (2004), Phase transition in $MgSiO_3$ perovskite in the earth's lower mantle, *Earth Planet. Sci. Lett.*, *224*, 241–248.

Weinstein, S. A. (1995), The effects of a deep mantle endothermic phase change on the structure of thermal convection in silicate planets, *J. Geophys. Res.*, *100*, 1719–1728.

Zhou, H., D. Breuer, D. A. Yuen, and T. Spohn (1995), Phase transition in the Martian mantle and the generation of megaplumes, *Geophys. Res. Lett.*, *22*, 1945–1948.

————————————

T. Nakagawa, Department of Geophysical Sciences, University of Chicago, 5734 S. Ellis Ave., Chicago, IL 60637, USA. (takashi@geosci.uchicago.edu)

P. J. Tackley, Department of Earth and Space Sciences and Institute of Geophysics and Planetary Physics, University of California, Los Angeles, CA, USA.