

THE DYNAMICAL INFLUENCES FROM PHYSICAL PROPERTIES IN THE LOWER MANTLE AND POST-PEROVSKITE PHASE TRANSITION

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ABSTRACT

The discovery of post-perovskite phase transition near the core-mantle boundary(CMB) has turned our heads to the potentially important role played by the increasing complexity of the physical properties in the lower-mantle models. In this study we have investigated the influences on lower mantle dynamics by the strongly depth-dependent coefficient of thermal expansion and radiative thermal conductivity together with the post-perovskite transition within the framework of isochemical models. We have carried out the simulations in both 2-D and 3-D Cartesian geometries. First, we review the basic connection between the temperature profile and the Clapeyron slope, calling attention to the special relationship between the temperature intercept of the post-perovskite phase change and the temperature at the core-mantle boundary. Double-crossing of the post-perovskite boundary takes place only, when the temperature of the CMB is greater than the temperature intercept of the phase change. We find that mantle plumes become multiscale in nature because of the combined effects exerted by variable mantle viscosity, strongly depth-dependent thermal expansivity, radiative thermal conductivity at the bottom of the mantle, the spinel to perovskite phase transition and the perovskite to post-perovskite phase change in the deep mantle. Both radiative thermal conductivity and strongly decreasing thermal expansivity in the lower mantle can help to induce partially layered convection with slabs stagnating in the transition zone. In our isochemical models a second low viscosity zone is created under the transition zone accompanied by intense shear heating. Secondary mantle plumes emerge from this region at the base of the transition zone. Large-scale upwellings in the lower mantle are induced mainly by both the style of lower-mantle stratification and the decrease in thermal expansivity. They control the location and the local dynamics of the upper-mantle plumes. In these models with variable thermal conductivity and viscosity, an increase in the temperature of the CMB causes a greater tendency for layered convection. From the same depth-dependent thermal expansivity, we can deduce the 3-D density anomalies from the seismic velocity anomalies inferred from seismic tomographic inversion. Using these density distributions, we can calculate the viscous responses of the Earth due to these density anomalies for a given viscosity structure. We then focus on the lateral viscosity variations of the deep mantle on the solution of the inverse problem involving the inferences of the viscosity from the long-wavelength geoid. Our solution for the large-scale lateral viscosity structure in the

lowermost mantle shows that the region underneath hot spots have significantly higher viscosity in the deep mantle than the region below subduction regions. Recent inferences from first-principles calculations and laboratory experiments on analogue post-perovskite material also surmise the rheology of post-perovskite would be dominated by dislocation mechanism and be softer than perovskite. We put forth a hypothetical scenario in which the bottom portions of the superplumes in the deep mantle are stiffer than the adjacent post-perovskite mantle and are held fixed by the surrounding horizontal flow of post-perovskite.

Keywords: post-perovskite, mantle convection, thermal expansivity, lateral viscosity, radiative thermal conductivity.

1. INTRODUCTION

The new discovery of the post-perovskite (PPV) transition (Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004) is indeed quite exciting (Hirose et al., 2006) and has already provided new constraints on the thermo-mechanical structure and physical properties of the lower mantle, because of its proximity to the core-mantle boundary (CMB) (e.g. Wentzcovitch et al., 2007). The occurrence of post-perovskite bearing rock in the bottom 300 km of the mantle may explain the presence of discontinuous jumps in the seismic velocity found in some regions above the D" layer (Lay and Helmberger, 1983) as well as other lowermost mantle seismic properties (Wookey et al., 2005). The Clapeyron slope of this exothermic phase transition has been inferred to be quite large, around 10 MPa/K, which allows for significant lateral variations of the phase boundary (Wentzcovitch et al., 2006) and also gives it the possibility for the locally steep geotherms near the CMB to intersect the Clapeyron slope more than once (Hernlund et al, 2005). Discontinuity pairs in the deep mantle under the Cocos plate have been detected from body-wave seismology (Thomas et al., 2004) in accordance to the “double-crossing” idea put forth by Hernlund et al. (2005). High-resolution seismological investigations (Lay et al., 2006, van der Hilst et al, 2007) have made use of the thermodynamic properties of the PPV transition to estimate the temperatures just above the CMB to be around 4000 K. Three-dimensional simulations in a spherical model (Monnereau and Yuen, 2007) have also placed constraints on the temperature above the CMB by using the thermodynamic constraint of the temperature of the PPV transition at the CMB and monitoring the distribution in the two depths (Hernlund et al, 2005), where the local geotherms would intersect the PPV phase boundary. Figure 1 below shows the basic idea behind the possible intersections between the curved boundary-layer geotherm and the phase boundary which has two parameters, the Clapeyron slope and the temperature intercept, T_{int} , which is the temperature of the PPV transition at the pressure corresponding to the CMB.

From a dynamical standpoint, the reaction to this recent finding has also been enthusiastic, as shown by the rapid responses of Nakagawa and Tackley (2004) and Matyska and Yuen (2005), where they showed within the framework of 2-D models that the exothermic PPV transition can be destabilizing for the bottom thermal boundary layer. Nakagawa and Tackley (2005, 2006) have investigated the PPV transition together with a thermal-chemical convection model. They found that there remains still a significant signature coming from the PPV component. In our study we will take the end-member position of thermal or isochemical convection and will develop our arguments from this stance. We recognize fully well the potential importance of thermal-chemical convection. The key issue here is the relative trade-off

between the PPV phase transition and chemical heterogeneities (see also contribution by Peltier in this volume) in explaining the unique seismological and other physical properties, such as rheology of the D" layer and thermal conductivity, which may be influenced greatly by iron (Manga and Jeanloz, 1996). The constraints imposed by the double-crossing and the PPV lens-like structure under the Cocos plate (van der Hilst et al., 2007) are quite important in this regard, since they place tight constraints on the depth interval of the double crossing (Monnereau and Yuen, 2007).

In this paper we will devote our attention on the dynamical influences of physical properties in the lower mantle, such as variable thermal conductivity and pressure-dependent thermal expansivity, with the post-perovskite phase change. We will also discuss about the nature of the rheological structure of the D" layer in view of recent laboratory work carried out by Yamazaki et al. (2006) on post-perovskite analogue materials and inferences of the lateral variations in the deep mantle viscosity by Čadež and Fleitout (2006) based on long-wavelength geoid anomalies. In section 2 we will describe the two numerical models, the physical model of the PPV phase transition and the nature of the variable physical properties in the lower mantle. In the next section we will go over the 2-D results from the Cartesian model of Matyska and Yuen (2005, 2006, 2007). We will present in section 4 the 3-D results from the model of Kameyama and Yuen (2006) with some new findings for pressure-dependent thermal expansivity. In section 5 we will discuss about the rheological structure of the D" layer. Finally, we summarize our results and discuss the implications of the PPV transition on mantle dynamics and mantle rheology.

2. PHYSICAL BACKGROUND AND MODEL DESCRIPTION

In this section we first discuss the physical-chemical characteristics of the PPV transition and its relationship to the thermal boundaries of the core-mantle boundary (CMB). Then we will briefly review the governing equations and the numerical treatment of the phase boundaries and the physical properties of the lower mantle on which we will be concentrating.

2.1 PPV phase transition

From the earliest days (Schubert and Turcotte, 1971) mantle phase transition has always been discussed only in terms of its Clapeyron slope T' , even though an equation for a line has a slope and an intercept. The reason for this picture is that a half-space model was employed and the phase transitions were far away from the boundaries. The post-perovskite phase transition has now been determined to be exothermic (Murakami et al., 2004) and has a steep Clapeyron slope of around 10 MPa/K (Hirose et al., 2006). Because of its close proximity to the CMB, we must introduce another parameter besides the Clapeyron slope into the description of the phase change. This quantity is called the temperature intercept T_{int} , the temperature of the PPV transition at the pressure of the CMB. These quantities are displayed in Fig.1 along with a thermal profile $\langle T \rangle$, characteristic of a thermal boundary layer. We see that there can be a double crossing of the phase boundary by $\langle T \rangle$, if the temperature of the CMB, T_{CMB} , is slightly greater than T_{int} . That is to say, there can be a slab of post-perovskite being sandwiched in by two perovskite layers. The thickness of this post-perovskite slab is marked by E – D in Figure 1 and can be estimated by seismic imaging (van der Hilst et al.; 2007, Lay et al., 2006). In principle, there is now a new constraint imposed on the T_{CMB} , if one can obtain from experimental or theoretical means an idea of T_{int} . However, there is still a substantial uncertainty, around 400 K,

in determining the magnitude of T_{int} . For $T_{\text{CMB}} < T_{\text{int}}$, there is no double crossing (Kameyama and Yuen, 2006) and the entire D" layer is covered with post-perovskite of varying thickness, depending on the local geotherm. The morphology of the PPV layer above the CMB changes with the cooling of the mantle (Oganov and Ono, 2005), going from a purely perovskite layer to islands of post-perovskite to eventually a post-perovskite hilly terrain (Monnereau and Yuen, 2007).

2.2 Governing equations

We have employed two Cartesian models in obtaining the results presented in this paper. They come from the two-dimensional model of Matyska and Yuen (2005, 2006) in which the phase transition is assumed to occur at a certain depth by the use of the effective thermal expansivity procedure of Christensen and Yuen (1985) and the 3-D model of Kameyama and Yuen (2006), which accounts for the influence of phase-boundary distortion, see Figure 2. The phase-boundary perturbations are influential for the dynamics of the PPV boundary, which can disappear altogether inside hot plumes, see left-hand panel of Fig. 2. The phase boundary distortion comes from the linear relationship between the temperature and the hydrostatic pressure, from which one can determine the sensitivity of the depth of the PPV phase transition locally to a change in the local temperature. We have employed the extended Boussinesq equations for thermal convection with phase transitions. The depth of the mantle is taken to be 2900 km. The mantle density is assumed to be constant except at the sites of the two phase transitions, which include the spinel to perovskite transition at the interface between the upper and lower mantles and the perovskite to post-perovskite transition in the deep mantle right above the CMB. The viscosity is taken to be temperature- and depth-dependent. We have not incorporated any change in the rheology, when PPV transition takes place in the convection calculations. The volumetric thermal coefficient of expansion or thermal expansivity decreases with depth and we will focus on this particular aspect. We will study the influence of radiative thermal conductivity of the lower mantle in the 2-D models and use a temperature-dependent thermal conductivity following Hofmeister (1999) in the 3-D model.

The background of the extended Boussinesq equations can be found described in Christensen and Yuen (1985) and more completely in Matyska and Yuen (2007). In the extended Boussinesq approximation the mantle compressibility in the continuity equation is neglected. Therefore, the conservation of mass is just

$$\nabla \cdot \mathbf{v} = 0, \quad (1)$$

where $\mathbf{v}$ is the fluid velocity vector. For an infinite Prandtl number fluid such as appropriate for mantle rocks, this means that inertial terms can be neglected. Then the dimensionless momentum equation is given by

$$-\nabla \Pi + \nabla \cdot [(\eta/\eta_s)(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)] + Ra_s(\alpha/\alpha_s)(T - T_0) \mathbf{e}_r = 0, \quad (2)$$

where Π is the perturbation pressure, η_s is the surface value of the viscosity η , α_s is the surface value of the thermal expansion coefficient α , which contains the influence of phase transitions, T is the dimensionless temperature scaled by the difference between T_{CMB} and the surface temperature T_s and equal to zero at the surface, T_0 is a reference dimensionless temperature, $\mathbf{e}_r$ is the vertical unit vector, Ra_s is the Rayleigh number based on surface values and the superscript T

denotes the transpose operation. We note here that α includes both the normal thermal expansivity, which decreases with pressure (Chopelas and Boehler, 1992), and also the effects from phase transitions, which induce sharp localized changes of a few per cent in the density. (Richter, 1973; Christensen and Yuen, 1985). We note that α in sensu stricto is a function of both temperature and pressure, which can be constructed from the first-principles of quantum mechanics (Wentzcovitch et al., 2006). This function can be thus available as a look-up table, which would be extremely suitable for parallel computing. In the 2-D models, we will make use of the approximation where the phase transition is assumed to take place at a given depth (Christensen and Yuen, 1985) and α becomes a function of depth only, with sharp changes at the prescribed depths of the two phase changes in the model. The Newtonian viscosity η is a function of both temperature and depth.

The conservation of energy equation has latent heat release, mechanical heating terms and radiogenic heating contributions. The dimensionless form is given by

$$\begin{aligned} \partial T / \partial t = & \nabla \cdot ((k/k_s) \nabla T) - \mathbf{v} \cdot \nabla T + R - \\ & - Di_s (\alpha/\alpha_s) (T + T_s / (T_{\text{CMB}} - T_s)) v_r + (Di_s / Ra_s) (\eta/\eta_s) (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) : \nabla \mathbf{v}, \end{aligned} \quad (3)$$

where we introduced the thermal conductivity k , the dimensionless radiogenic heating term R and the surface dissipation number Di_s . We note that $R = Qd^2/k_s(T_b - T_s)$, where Q is the rate of radiogenic heating per unit volume and d is the mantle thickness. For chondritic heating abundance R is around 12 (Leitch and Yuen, 1989).

2.3 Phase change formulation

Solid-state phase transitions in multi-component systems, such as found in the Earth's mantle, are characterized by zones involving mixed phases (e.g. Schubert et al., 2001). We will assume that the depth range of these zones can be neglected and that we may describe the overall phase change behavior which involves sharp jumps in both the density and entropy. Lateral variations in the temperature produce undulations in the phase boundary, which represent significant additional buoyancy force due to the density change. There is also release or consumption of latent heat from the jump in the entropy. In the two dimensional models we will assume that the phase boundary occurs at a given dimensionless depth z_p (scaled by d) and we can replace the dimensionless thermal expansivity α/α_s by

$$(\alpha/\alpha_s) + P \delta(z - z_p) \quad (4)$$

where the dimensionless quantity $P = \Gamma(\Delta\rho)/(\alpha_s \rho_0^2 g_0 d)$ is called the phase buoyancy parameter (Christensen and Yuen, 1985) (Γ is the slope of the Clapeyron curve, $\Delta\rho$ is the density jump across the phase interface, ρ_0 is a reference density and g_0 gravity acceleration) and $\delta(z - z_p)$ is a localized compact-support function with a sharp peak at $z = z_p$ approximating the Dirac δ -function.

In the three-dimensional models, we have employed the phase function approach of (Richter, 1973) to describe the distribution of the two phases in a zone with a finite-width w . A hyperbolic tangent function, whose argument depends on the difference between the local geotherm and the phase boundary equation shown in Fig. 1, is used to describe the percentage of the particular phase at a given point in 3-D. In this way one can determine the topology of the

phase boundary surface between the two phases and the local enhancement of the buoyancy force due to the phase transition.

In Fig. 2 we illustrate schematically the dynamical influences of the phase boundary distortions by a sketch of the phase boundary of PPV (dashed curve) in the hot upwellings and the cold downwellings. For T_{CMB} greater than T_{int} , we note that underneath the hot plumes there can exist a patch of hot perovskite. Only when the Earth starts to cool down, does the perovskite hole disappears and is filled with PPV. The buoyancy of the hot plumes is increased by the deflection of the lighter perovskite phase downward, albeit it is only 1 to 1.5 %, but this is equivalent to several hundred degrees of thermal contribution because of the low thermal expansivity near the CMB. In the downwelling we observe also the greater negative buoyancy provided by the phase boundary being pushed upwards by the negative thermal contrast. Underneath the isotherm T_3 , there may appear another zone of perovskite right above the CMB, marking what has become to be known as the “double-crossing” phenomenon (Hernlund et al., 2005; Hernlund and Labrosse, 2007), for T_{CMB} greater than T_{int} .

2.4 Viscosity, thermal conductivity and thermal expansivity

In its major importance mantle viscosity is both temperature- and depth-dependent. In two-dimensions we have taken the form of a depth-dependence (see Hanyk et al., 1995), given by

$$\eta_0(z)/\eta_s = 1 + 214.3 z \exp(-16.7(0.7-z)^2), \quad (5)$$

which produces a viscosity maximum at around 1800 km depth, consistent with the geoid inversion results of Ricard and Wuming (1991) and Mitrovica and Forte (2004). For the temperature-dependent portion we have used the dependence

$$f(T) = \exp(10.0(0.6/(0.2+T)-1.0)) \quad (6)$$

according to the Arrhenius form of a thermally activated process for mantle rheology (Ranalli, 1995). The composite temperature- and depth-dependent viscosity in the two-dimensional models is given by

$$\eta(z, T)/\eta_s = \eta_0(z)/\eta_s \min\{100, \max\{0.01, f(T)\}\}, \quad (7)$$

which means the temperature-dependence of the dimensionless viscosity lies between the interval of 0.01 and 100. In 3-D we have used a Frank-Kamenetzky form for a temperature- and depth-dependent viscosity of the form

$$\eta(z, T)/\eta_s = \exp(-E_T T + E_p z) \quad (8)$$

with $E_T = \ln(10^{3.5})$ and $E_p = \ln(10^2)$.

Thermal conductivity is a transport property in the lower mantle, whose subtle effects have not been well appreciated in most modeling efforts. In the 2-D models we have employed a thermal conductivity model, which focuses mainly on the radiative portion of the thermal conductivity, because the phonon contribution to temperature-dependence saturates out at temperatures around the Debye temperature (Hofmeister and Yuen, 2007) and the pressure-

dependence of thermal conductivity does not give rise to any feedback in the temperature equation. This thermal conductivity takes the form

$$k(z, T)/k_s = 1 + g(z)(T + T_s / (T_{\text{CMB}} - T_s))^3, \quad (9)$$

where $g(z)=0$ in the models without radiative transfer of heat and $g(z)=5$ in a layer approximating D" in the models with radiative thermal conductivity. We must recognize that mantle thermal conductivity is still in a nascent stage of development and more work is needed for verifying certain assumptions, such as the influence of impurities (D.J. Stevenson, private communication, 2004) and grain-boundaries (Hofmeister, 2005). In three-dimensional model we take into account another temperature-dependence of thermal conductivity, which can also simulate the effects of radiative heat transfer expected to be dominant in a hot lower mantle. Then we assume,

$$k(z, T)/k_s = 1 + c(-2T^3 + 3T^2). \quad (10)$$

In this study the constant c is chosen to be either 0 or 3. In the dimensionless temperature range of $0 \leq T \leq 1$, the derivative dk/dT is always non-negative, which is in accordance of basic laws of photon physics. By choosing $c=3$ we can mimick to some extent the functional form of the radiative heat transfer up to 2800 K proposed by Hofmeister (1999).

The depth-dependence of thermal expansivity is now recognized as being influential in lower mantle dynamics (Anderson, 2002) because any decrease in the thermal buoyancy would change the style of lower mantle convection to circulations with longer wavelengths (Hansen et al., 1993). We have employed two types of thermal expansivity profiles. The first model has been parameterized to

$$\alpha/\alpha_s = 8/(2+z)^3, \quad (11)$$

where the thermal expansivity drops by $8/27$ across the entire mantle (Zhao and Yuen, 1987). Recently Katsura et al. (2005) found from measurements that Anderson-Grueneisen parameter of perovskite up to 30 GPa is close to 10, thus implying a stronger decrease of the thermal coefficient of expansion in the lower mantle. By approximating a linear dependent increase in density for both the upper- and lower-mantles, and assuming the Anderson-Grueneisen parameter of upper-mantle materials is close to 5, which fits the estimates for olivine (Chopelas and Boehler, 1992), we arrive at the following relations for thermal expansivity in the whole mantle:

$$\alpha/\alpha_s = (1+0.78z)^{-5} \quad \text{if } 0 \leq z \leq 0.23, \quad (12)$$

$$\alpha/\alpha_s = 0.44(1+0.35(z-0.23))^{-10} \quad \text{if } 0.23 < z \leq 1.00, \quad (13)$$

We note that the magnitude of coefficient of thermal expansion should be around $3.5 \times 10^{-5} \text{ K}^{-1}$ at the top of the lower mantle according to Katsura et al. (2005). In this model there is a greater decrease in the thermal expansivity in the lower mantle.

2.5 Numerical Methods for Convection

In the two-dimension Cartesian convection models, we integrate the set of coupled elliptic (for momentum) - nonlinear parabolic (for the temperature) partial differential equations for the stream-function ψ and temperature T with the associated boundary conditions appropriate for an impermeable, stress-free boundary conditions for the velocity and a given temperature difference across the mantle with reflecting temperature conditions at the side walls (see Matyska and Yuen (2005, 2007) for details). The depth-dependence of thermal expansivity causes a dramatic decrease in the buoyancy forcing term in the lower mantle and also in the adiabatic heating and cooling terms in the time-dependent temperature equation. We have carried out the computations in a wide box with an aspect-ratio of 10 to avoid edge effects from the reflecting boundary conditions. We have employed 1281 (horizontal) x 129 (vertical) equally spaced nodal points within the framework of a second-order finite-difference scheme. The fourth-order elliptic equation has been solved by a conjugate gradient iterative scheme and the temperature equation is integrated in time by a second-order Runge-Kutta method.

In the three-dimensional Cartesian model, we solve the set of conservation of mass, momentum and temperature equation, using the primitive variables of velocity $\mathbf{v}$, dynamical pressure P and temperature T . A description of this parallelized multigrid-based code, which runs on many nodes on the Earth Simulator can be found in Kameyama et al. (2005) and Kameyama (2006). We have employed 64 points in the vertical and 256 x 256 on the horizontal plane, using a second-order finite-volume scheme and a second-order time-stepping method. Each run has been carried out to over 200,000 time-steps.

3. RESULTS

3.1 Two-dimensional models

We have put two phase transitions in all models. The endothermic spinel to perovskite phase transition in the upper- and lower mantle boundary and the PPV transition near the bottom of the lower mantle. The first set of the 2-D numerical experiments is focused on the role played by the Clapeyron slope of the PPV transition. We have varied the Clapeyron slope from negative to positive values in Plate 1 in order to illustrate the physics played by the sign of the Clapeyron slope. One can clearly see in the five panels that the positive Clapeyron slope results in a prevalence of thermal instabilities at the lower boundary layer and, consequently, in the creation of small lower mantle plumes, which are attracted to each other by plume-plume collisions (Vincent and Yuen, 1988) in the region between the cold downwellings. This continuously running scenario is thus responsible for chaotically repeated plume-plume interactions in the D'' layer. We observe that the plumes are efficiently cooled by the adiabatic cooling and by the latent heat absorbed by the post-perovskite to perovskite transition in the upward flowing plume. Since the boundary between the upper and the lower mantle is only partially permeable, convection is partially layered and upper mantle plumes are very thin in comparison with their lower mantle counterparts, which are thicker because of the depth-dependent viscosity and thermal expansion coefficient (Hansen et al., 1993). In a similar manner as in the lower mantle, the upper mantle plumes are attracted toward the central position, which is then characterized by a variable intensity of hot upward flow. On the other hand, the absence of the PPV transition (center panel) or a negative Clapeyron slope of the PPV (fourth panel) phase transition, as was suggested earlier by Shim et al. (2004), would strongly induce the creation of the lower mantle superplumes due to the combined effect of the increase of viscosity in the mid lower-mantle and

the decrease of thermal expansivity in the lower mantle. But the behavior of the upper mantle plumes does not change substantially. We emphasize here the strong mechanical coupling at the 670 km boundary in that the nearly horizontal flow at 670 km boundary produces very intense shear heating, which can result in a very interesting physical phenomenon: material at the top of the lower mantle plume is relatively not very hot but it is heated due to viscous dissipation, when it is horizontally transported below the 670 km boundary, and finally it becomes very hot below the source region of the upper mantle plumes.

However, both laboratory experiments (Hirose, 2006) and *ab initio* quantum mechanical calculations (Tsuchiya et al., 2004) show that the PPV phase transition has a positive Clapeyron slope with a magnitude of around 10 MPa/K. Therefore, the question arises as to the existence of the lower mantle superplumes under these conditions. We demonstrated in the bottom panel that this puzzle might be solved by taking into account the radiative transfer of heat at the bottom of the mantle. Its magnitude is a matter of controversy but if the conduction of heat in the D" layer is dominated by radiative photon transfer, upward flow in the lower mantle is dominated by broad but relatively fast upwellings. The main consequence of a small vertical temperature gradient in D" is that the whole lower mantle outside downwelling becomes rather hot with only small lateral temperature gradients. High lateral temperature gradients thus mark the regions bounding cold downwellings. It is interesting that situation in the upper mantle is not very sensitive to such a substantial change of convection in the lower mantle, and especially, to the increase of temperature in the lower mantle. As to the upper mantle plumes temperature, the key role is played by the temperature at the source region of the upper mantle plumes. We recall that in the previous models without the radiative thermal conductivity in the D" layer the material penetrating the 670 km boundary is also sufficiently heated and the amount of material passing through the 670 km boundary is probably controlled by the cold downwellings, which are not very much influenced by the changes confined to the D" region. Consequently, the situation in the upper mantle is not very sensitive to the changes in the D" in these models. Fig. 3 shows the corresponding streamlines of the panels displayed in Plate 1. We see from the streamlines the presence of partially layered convection in all cases, but in particular the case with radiative thermal conductivity in the D" layer (bottom panel).

The panels in Plate 2 show the influence from varying the temperature of the core-mantle boundary (CMB). This quantity can impact mantle convection nonlinearly through the change in the Rayleigh number, dimensionless surface temperature, temperature-dependence of viscosity and radiative thermal conductivity, and the vertical shift of the PV to PPV phase interface. We supposed that this shift is about 100 km if the temperature of the CMB is changed by 20 %. The main effect, which is visible here, is the stabilization of mantle convection, when the CMB temperature is lowered (top two panels in Fig. 3). In the model without any radiative thermal conductivity, the cold downwellings become very thick, convection is sluggish and is dominated by hot plumes with vertical velocities about one order of magnitude higher in comparison to the velocities of cold downwellings. If radiative heat transfer in the D" layer is added, this extreme difference is reduced substantially and temperatures of hot mantle regions are "homogenized" again. When the temperature of the CMB is increased, the PPV phase transition is closer to the CMB in our model and thus its role in destabilizing the lower thermal boundary layer appears to be reduced. We then obtained very hot regions in the upper mantle in this case with a higher CMB temperature (bottom 3 panels). From the streamlines in Fig. 4, one can discern from comparing the second and last two panels that there is a greater tendency toward layered convection, for higher temperature at the CMB in the case of radiative thermal

conductivity in the D" layer. This scenario fits well with the geochemical evidence of greater amounts of layering in the distant geological past than at the present time (e.g. Allegre et al., 1997), due to the cooling of the Earth's core and the decrease in the convective strength of mantle convection.

3.2 Three-dimensional model

In the first part of this subsection we will illustrate the influence of varying CMB temperature for a thermal expansivity which decreases moderately by a factor of 8/27 across the mantle according to eqn. (11). Plate 3 shows a snapshot of the planform, as shown by the lateral temperature field and distribution of the post-perovskite phase obtained for a case with the temperature of the CMB, T_{CMB} , equal to 2800 K and a density change of 2 % due to the PPV phase transition. The time instant taken is at a statistically equilibrated stage. We have displayed here the isosurfaces of the lateral thermal anomalies $\Delta T = T - \langle T \rangle$, where $\langle T \rangle$ is the horizontally averaged temperature at each depth. Bounded by the yellow surfaces are the hot thermal anomalies with a magnitude greater than 75 K, while the green surfaces represent the cold anomalies with a magnitude less than -125 K. The transparent red surfaces denote the isosurfaces of the phase function equal to 0.5 for the PPV phase, i.e. half of the total mineral assemblage has been transformed to PPV. We note that the T_{CMB} is lower than the T_{int} , which means that the entire D" layer has already been transformed to PPV. In Fig. 5 we show the three characteristic temperature profiles from this 3-D simulation: the horizontally-averaged temperature $\langle T \rangle$, the maximum temperature profile and the minimum temperature profiles. Also shown schematically are the two phase transitions along with their Clapeyron slopes. For each phase transition, the hatched regions indicate the regions of the transitions, while the thick dashed lines indicate the relations of the phase boundaries, where there is no excess pressure difference (see Christensen and Yuen, 1985). The profiles show that the $\langle T \rangle$ lies only a couple of hundred degrees below the maximum temperature profile and is well above the minimum temperature profile by 800 degrees. One can see the latent heat effect of around 100 K on the minimum temperature profile.

We then change the T_{CMB} from 2800 to 3800 K, which represents an increase close to 35 %. This higher temperature is now above the T_{int} so the CMB is not covered completely with a post-perovskite layer, as in the case of a lower T_{CMB} . This situation is shown in Plate 4, where we can see the black space at the bottom of the mantle, indicating perovskite material atop the CMB. We see that the PPV pools (red color) lie close to the cold downwellings. These red pools of PPV do not touch the CMB surface because T_{CMB} is greater than the T_{int} of the PPV transition (see the temperature profiles in Fig. 5). Thus there is a thin layer of perovskite lying underneath the red "carpet" of PPV. The convective planforms have a longer wavelength than the convection cells with a lower T_{CMB} . In Fig. 6 we show the corresponding temperature profiles depicting the maximum, the horizontally averaged and the minimum temperature profiles. There is no visible effect from the latent heat release for this case with a higher T_{CMB} . The averaged temperature profile shows greater degree of adiabaticity throughout the entire mantle, more than the case with a lower T_{CMB} , because T_{CMB} lies above the T_{int} .

Next we employ in the simulations the sharper decreasing thermal expansivity by Katsura et al (2005) in order to see the changes in the style of 3-D mantle convection. We have used an effective thermal expansivity for describing the phase changes, as in the 2-D models. Thus there is no distortion in the depth of the phase transition from thermal anomalies. In Fig. 7 we can see from the 4 snapshots in time some dramatic changes in the planforms by the

temperature isosurfaces with a value of $T = 0.65$. We see the upwellings become sheet-like, as in the 3-D spherical solutions found by Yuen et al. (2007) and Roberts and Zhong (2006) in the presence of steep viscosity stratification in the mantle. Thus sharp changes in thermal expansion coefficient can also exert a similar effect on the upwellings. The accompanying temperature profiles show a much cooler mantle along with a nearly isothermal lower mantle, as shown by the $\langle T \rangle$ profile, because of the low value of α . We display in Fig. 8 the associated lateral temperature fields for the hot and cold thermal anomalies, both bounded by a magnitude of 0.05 or around 200 K. The wall-like scaffold of connecting hot anomalies is very distinct in this temperature representation. The cold anomalies are fragmented with many of them trapped above the spinel to perovskite phase change at 670 km depth. These results show that the dynamical impact from a sharply decreasing coefficient of thermal expansion may be as important as the viscosity stratification in the lower mantle. The style of layered convection can be better appreciated visually by plotting the vertical velocity contours along a given vertical 2-D cross-section. We show this for the last two time instants in Figs. 9 and 10, where 4 vertical planes are chosen for each time frame. We can clearly discern that the convective system is partially layered with smaller cells in the upper mantle and large weak circulations in the lower mantle. The upper mantle plumes are the fastest entities in this type of mantle flow. The lower mantle plumes are relatively sluggish in comparison to flows in the upper mantle.

3.3 Lateral viscosity variations in the deep mantle

Seismic studies already revealed that the lower mantle is laterally heterogeneous over short and global length scales. It is no wonder then to expect significant lateral variations in the viscosity in the deep mantle above the CMB. Čadek and Fleitout (2006) have inferred the lateral viscosity variations above the CMB based on predictions of the long wavelength geoid. Their parameter for scaling between the density perturbation to seismic velocity anomaly was taken to be a constant with depth. They found that presence of the lateral viscosity variations in the deep mantle can greatly help to increase the percentage of predicted free-air gravity (e.g., eqn. (18) in Čadek and Fleitout, 2003) from 42 to 70 %, while the basic features of the radial mantle viscosity profile, remains relatively unchanged as in the case of the best-fitting laterally homogeneous viscosity models. What they found is quite interesting in that region in the deep mantle under hot spots have a higher than average viscosity. This result shows that for a hot deep mantle, where there is no post-perovskite the viscosity is greater than the adjacent deep mantle, which is presumably colder and contains post-perovskite. First-principle calculations by Oganov and Ono (2005) and Carrez et al. (2007) show that strong dislocation properties should predominate in the PPV phase. Similar conclusions are also reached by Yamazaki et al. (2006) on the basis of experiments of elastic deformation of analogue PPV materials.

We have used the laterally-dependent viscous incompressible, spherical model of Čadek and Fleitout (2003) for inferring the laterally varying viscosity in the deep mantle from the long-wavelength geoid anomalies. Different from the previous work of Čadek and Fleitout (2006), we have employed a more recent seismic tomographic model by Becker and Boschi (2002) and a depth-dependent scaling parameter between the density and seismic velocity scaling based on the depth-dependence of the thermal expansivity of Katsura et al. (2005). We have assumed the viscosity is Newtonian and the boundary conditions prescribed at the surface, the 660 km discontinuity and the CMB are the same as in Čadek and Fleitout (2003). This model prescribes the observed plate velocities on thin membranes, while stress-free and impermeable boundaries are prescribed at the CMB. The flow situation at the 670 km boundary is characterized by a

parameter λ , which determines the percentage of layered flow in the mantle flow (see Čadek and Fleitout, 1999, 2003). Here λ is treated as a free parameter, it hovers around 0.6.

This mantle model is characterized by the following parameters: the layering coefficient λ , and the parameters describing the viscosity structure. The velocity-to-density scaling factor depends now on depth. According to a depth-dependent thermal expansivity, in the lower mantle this is given by

$$d(\ln \rho)/d(\ln V_S) = C[1+0.35(z-0.23)]^{-10}, \quad (14)$$

where we have made use of the chain-rule in calculus and the temperature-dependent derivatives of the density and seismic velocity. The dimensionless depth z is scaled by the thickness of the mantle and C is a free constant parameter, which is close to 1 in the optimal models. The value of the conversion parameter in the upper mantle is considered to be a relatively small constant; typically around 0.05. The scaling between density and V_S in equation (14) does not include the influences of compositional differences, e.g., some iron infiltration into the D" layer from the core (Petford et al., 2005; Kanda and Stevenson, 2006; Sakai et al., 2006). There is no lateral viscosity variation in each of the top three viscosity layers. Each layer is characterized by a single viscosity value. They include the asthenosphere, which is 100 km thick, the upper mantle, 460 km thick and the lower mantle with a thickness of 2040 km. The bottom layer is 200 km thick and has both radial and lateral variations in the viscosity. The viscosity in this layer is parameterized in the logarithmic scale in terms of a spherical harmonic expansion truncated at degree and order 4:

$$\log_{10} \eta_{\text{CMB}}(\vartheta, \varphi) = \sum_{l=0}^4 \sum_{m=-l}^l \eta_{lm} Y_{lm}(\vartheta, \varphi) \quad (15)$$

where Y_{lm} are the complex spherical harmonics and η_{lm} are spherical harmonic coefficients to be determined. These coefficients are assumed to be constant in radius above the CMB region. The objective of the inversion is to determine the magnitudes of the parameter values that best fit the long-wavelength geoid. The details of the inversion can be found in Čadek and Fleitout (2003, 2006). Basically the inversion problem is formulated as a least-squares minimization and is nonlinear. The values of the model parameters that fulfills this minimum requirement must be found numerically by methods of global search.

The best model found by the global inverse search predicts around 90% of the geoid and 70% of the free-air gravity. We can discern the significant role played by lateral viscosity variations above the CMB region in helping to fit the data. The best fitting viscosity model has a strongly increasing trend with depth ($\eta_{\text{asth}} = 1 \times 10^{19}$ Pa s, $\eta_{\text{um}} = 2 \times 10^{20}$ Pa s, $\eta_{\text{lm}} = 7 \times 10^{21}$ Pa s) and a layering coefficient λ of 0.65. The fit to the data can further be improved (see Plate 5) if the tomography based density anomalies in the upper mantle are replaced by a density structure obtained from reconstruction of subduction in the past (Ricard et al., 1993). In this case, the best fit is obtained for λ equal to 0.75. In comparison with the results of Čadek and Fleitout (2006), our model is characterized by a lower value of viscosity in the lower mantle and more layered circulation.

In Plate 6 we show the predicted pattern of the lateral viscosity variations in the CMB region. The lateral viscosity contrasts shown in Plate 6 amount to about three and half orders in

magnitude, ranging from a low under Central America and the Indian Ocean to the highs under South Pacific and Africa. The maximum viscosity values are found in the core-mantle boundary region beneath the South Atlantic, Africa and the Pacific. These areas are characterized by many hotspots on the surface and slow anomalies in the lower mantle. In Fig. 11 we plot the histogram showing the number of hotspots, which are binned according to the viscosity value of the CMB region underneath them. From Fig. 11 it is clear that there is a correlation in the relationship between the hotspot distribution at the surface and the lateral viscosity anomalies in the deep mantle. Very strikingly, most hotspots are located right above the regions of higher-than-average viscosity, while only a few hotspots are found above the lowest viscosity regions. There is a large difference in the surface density of hotspots between those which lie above the low viscosity region atop the CMB and the ones above the high viscosity portion at the bottom of the mantle.

Oganov et al. (2005) suggested from theoretical considerations, based on first-principles metadynamics calculations, that post-perovskite may have a greater tendency for having a dislocation-like or non-Newtonian behavior than perovskite on the basis of greater degree of anisotropy developed from its slip system. This proposal was also confirmed by the recent work of Carrez et al. (2007) on the basis of hybrid mesoscopic simulations using DFT combined with the continuum dislocation core model of Peierls and Nabarro. Their paper showed that plastic flow or strongly dislocation-creep is characteristic of deformation in PPV crystals. From their shear-deformation experimental studies Yamazaki et al. (2006) analyzed the fabric information of analogue post-perovskite phase of CaIrO_3 . In concert with their interpretation of lattice preferred orientation (LPO), they also concluded that dislocation creep is the dominant deformation mechanism associated with the PPV crystal structure with MgO also contributing substantially by the change in the slip-system (see also accompanying article by Yamazaki and Karato in this volume).

Thus there is now accumulating sufficient theoretical and experimental evidence to support the idea that there is a change in the deformation mechanism associated with the perovskite to post-perovskite phase transition. This change will be toward a mechanism with more dislocation-like behavior. For the sake of modeling the resultant dynamics, we may assume as a first approximation that a change from Newtonian to non-Newtonian rheology accompanies the phase change of PV to PPV. Such a change in the rheology of mantle material upon a phase change is unusual for the phase transitions in the upper mantle where there are no compelling reasons for this kind of suggestion as in the case for the deep mantle phase transition. This proposal is primarily driven by the observation of a sudden appearance of splitting and azimuthal seismic anisotropy in the D" layer.

With this Ansatz we may be able to explain the paradoxical pattern in the lateral viscosity in the D" layer discovered by Čadež and Fleitout (2006). The PPV layer being non-Newtonian is softer than the Newtonian PV hot plume because of the large stress suffered by the cold downwelling upon phase transformation to PPV and being forced to bend upon impacting the CMB. Thus the strong stress-dependence of the PPV rheology enables it to become much softer than the hot, rising, Newtonian PV plume. This scenario is clearly illustrated in Fig. 12, where we have drawn a possible scenario in which the hot but hard rising plume rises through a softer PPV horizontal flows. The peculiar dynamics of a hot but harder PV plume rising through a softer PPV layer in the deep mantle is reminiscent of the Rayleigh-Taylor experiments of Whitehead and Luther (1975), where thicker mantle plumes would be produced, thus resembling superplumes (Maruyama, 1994). Korenaga (2005) also proposed a mechanism for generating

superplumes based on the grain-size reduction associated with the phase transition (Riedel and Karato, 1997) and the consequent reduction in the viscosity of the material after the phase transition. We note here that this softening mechanism of PPV proposed here is not due to grain-size changes but due to the change in the availability of the dislocation vectors. We must investigate further by numerical experiments whether a thermal attractor of a stationary plume can be maintained dynamically by this type of interaction involving a phase-dependent rheology. This novel mechanism, as envisioned in Fig. 12, may be an attractive alternative toward explaining the elusive concept of a fixed lower mantle plume, first proposed by Morgan (1971). Work is currently in progress to demonstrate this phenomenon. Without bringing in new physical effects such as radiative thermal conductivity (Matyska and Yuen, 2005), grain-size sensitive rheology (Korenaga, 2005), or chemical piles (Mc Namara and Zhong, 2004) it is extremely difficult to explain the fixity of lower-mantle plumes in thermal convection at high Rayleigh numbers.

4. CONCLUSIONS

In this paper we have gone over several ideas about the potential effects of physical properties in the lower mantle on its dynamics. These findings are intimately tied to the presence of a PPV layer in the D" layer. The conclusions would have been quite different without considering PPV. The halcyon era in the lower mantle with only perovskite present might have prevailed in the Archean era, when the temperature was hotter in the lower mantle. There is now gathering more evidence to support the idea that today the PPV transition has taken place in the D" layer. Therefore we must take on a holistic view in this endeavor of understanding lower mantle dynamics. This means including the PPV transition in dynamical considerations, because this mechanism ties in strongly with the thermal boundary layer above the CMB. However, we should note that many of the physical effects presented still have great uncertainties and that the magnitudes of variations in thermal expansivity, thermal conductivity and rheology in the deep mantle are not well constrained. We still need more research in mineral physics from both experimental and computational arenas to elucidate these salient points.

As we have seen in section 3.1 the nature of the phase boundary does influence the boundary layer dynamics for variable viscosity convection. The exothermic nature of the phase transition with the steep Clapeyron slope causes many boundary layer instabilities and brings up the presence of these sandwiched-in PPV layers in the D" layer under subducting regions. In order to reconcile with the existence of superplumes, we must invoke some new physics, be it radiative thermal conductivity (section 3.1) or non-Newtonian rheology (section 3.3). The influence of strongly depth-dependent thermal expansivity in the lower mantle, though not directly related to the PPV issue, also induces partially layered convection (section 3.2). It also impacts on the relationship between seismic velocity anomalies and density anomalies. Using this new constraint for geoid inversion, in section 3.3 we found that the lower mantle viscosity becomes lower than before, and mantle circulation more layered. It also reinforced the earlier result (Čadež and Fleitout, 2006) that hot upwellings in the deep mantle have higher viscosity than the adjacent horizontal flows in the D" layer, which, from both theoretical and experimental evidence, appear to have non-Newtonian rheology. Indeed, mantle dynamics now enter a new era of new dynamical complexity with the discovery of the PPV transition.

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FIGURE CAPTIONS

Fig. 1 Schematic portrayal of the thermal profile and the Clapeyron slope. The thermal profile is representative of an horizontally averaged temperature profile $\langle T \rangle$. The Clapeyron slope has a slope Γ and an intercept T_{int} at the core-mantle boundary (CMB). The Clapeyron slope is crossed by $\langle T \rangle$ profile at two different depths E, D. This is called „double crossing“ (Hernlund et al., 2005) and is possible only when T_{CMB} is higher than T_{int} . The depth interval (E,D) is an important constraint for dynamical modelling (Monnereau and Yuen, 2007) and can be measured from seismic imaging (van der Hilst et al., 2007).

Fig. 2 Cartoon showing the isotherms and the PPV phase boundaries in regions of hot upwelling and cold downwelling. The isotherms in terms of decreasing temperature are given by T_1, T_2, T_3 and T_4 , with T_4 being the coldest. We note that beneath hot upwellings, only the perovskite phase may exist, as shown by the steeply falling dashed phase boundary intersecting the core-mantle boundary. The phase boundary (dashed curve) is elevated in regions of cold downwelling because of the positive Clapeyron slope of the PPV phase transition.

Plate 1 Typical snapshots of the temperature field for a long time scale. The depth-dependent thermal expansivity according to formulas (12), (13) was considered. Viscosity was both the depth- and temperature-dependent, see eqns. (5)–(7). An endothermic phase change with $P=-0.08$ at the depth of 670 km was included, which corresponds to the Clapeyron slope multiplied by $\Delta\rho/\rho_0$ equal to about -0.3 Mpa/K. The surface Rayleigh and dissipation numbers were 10^7 and 0.5, respectively. Thermal conductivity was considered in the form (9), where $g(z)=0$ (no radiative heat transfer) in all panels except the bottom one, where radiative heat transfer is considered below the depth 2650 km with g equal to 5.

Fig. 3 Streamlines of the model flow for the cases shown in Fig. 4. The streamfunction is equal to zero on all sides of the box and the contour interval of streamlines is 20 in dimensionless units. The contour interval is kept the same in all panels. The solid lines display the zero and negative values and the dashed lines show the positive values of the streamfunction.

Plate 2 Typical snapshots of the temperature field for a long time scale. The depth-dependent thermal expansivity according to formulas (12), (13) was considered. Viscosity was both the depth- and temperature-dependent, see eqns. (5)–(7). An endothermic phase change with $P=-0.08$ at the depth of 670 km was included, which corresponds to the Clapeyron slope multiplied by $\Delta\rho/\rho_0$ equal to about -0.3 Mpa/K. An exothermic phase change with $P=0.05$ at the top of D" was chosen as the fixed parameter. The surface Rayleigh and dissipation numbers were 10^7 and 0.5, respectively. Thermal conductivity was considered in the form (9), where $g(z)=0$ above D" in all panels and $g(z)$ was equal to either 0 or 5 in D". The dimensionless temperature of the CMB was 0.8 or 1.2. We used a periodic color scale, i.e., dark blue below the transition zone shows the places, where dimensionless temperatures are slightly higher than 1.2.

Fig. 4 Streamlines of the model flow for the cases shown in Fig. 4. The streamfunction is equal to zero on all sides of the box and the contour interval of streamlines is 20 (50) in dimensionless units in the models with dimensionless temperature of the CMB equal to 0.8 (1.2). The solid lines display the zero and negative values and the dashed lines show the positive values of the streamfunction.

Plate 3 A snapshot of convective flow pattern and distribution of post-perovskite (PPV) phase obtained for a case with the temperature at the bottom surface $T_{\text{CMB}} = 2800\text{K} < T_{\text{int}}$ and the density jump of the PPV phase transition of 2%. Indicated by opaque surfaces are the isosurfaces of the lateral thermal anomalies $\Delta T = T - \langle T \rangle$, where $\langle T \rangle$ is the horizontal average of temperature

at each depth. Bounded by yellow surfaces are the hot thermal anomalies with $\Delta T > 75\text{K}$, while by green surfaces are the cold anomalies with $\Delta T < -125\text{K}$. The transparent red surfaces are the isosurfaces of the phase function of 0.5 for the PPv phase transition. In the figure the isosurfaces of ΔT are not shown in the thermal boundary layer along the top surface.

Fig. 5 Plots of the horizontally-averaged $\langle T \rangle$, maximum $T_{\max}$ and minimum $T_{\min}$ temperatures against dimensionless height z obtained for the snapshot shown in Fig. 7. Also schematically shown are the phase relations assumed in this calculation. For each phase transition, the hatched regions indicate the regions of intense transitions, while the thick dashed lines indicate the relations of the phase boundaries (i.e., the two phases are in equilibrium).

Plate 4 The same as in Fig. 7 but for the case with the temperature at the bottom surface $T_{\text{CMB}} = 3800\text{K} > T_{\text{int}}$.

Fig. 6 The same as in Fig. 8 but for the snapshots shown in Fig. 9.

Fig. 7 Snapshots of convective flow patterns for four different elapsed times indicated in the figure. In the left column the isosurfaces of the dimensionless temperature $T=0.65$ are shown. In the right column there are the horizontally-averaged $\langle T \rangle$, maximum $T_{\max}$ and minimum $T_{\min}$ temperatures as functions of the dimensionless height z . Moreover, the phase relations assumed in this calculation are schematically shown in the right column. For each phase transition, the hatched regions indicate the regions of intense transitions, while the thick dashed lines indicate the relations of the phase boundaries (i.e., the two phases are in equilibrium).

Fig. 8 Snapshots of convective flow patterns obtained for four different elapsed times indicated in the figure. The distributions of the lateral thermal anomaly ΔT are shown in the figure. The cold anomalies with $\Delta T < -0.05$ and the hot anomalies with $\Delta T > 0.05$ are indicated.

Fig. 9 Three cross-sections of the vertical velocity v_z in upward or downward direction for snapshot (c) in Fig. 11. The plotted values of v_z are scaled by its maximum of $|v_z|$ ($=5.105 \times 10^5$ at this instance).

Fig. 10 The same as in Fig. 13 but for snapshot (d) in Fig. 11. The plotted values of v_z are scaled by its maximum of $|v_z|$ (3.285×10^5 at this instance).

Plate 5 Comparison between observed and predicted geoids. (a) Observed nonhydrostatic geoid (degrees 2-8) corrected for the lithospheric effects (Doin et al., 1996). (b) Dynamic geoid predicted for a viscosity model including laterally variable viscosity in the CMB region.

Plate 6 Lateral viscosity variations in the core-mantle boundary region obtained from inverse modeling of the geoid. The white circles indicate the positions of known hotspots (hotspot list adopted from Nataf and Ricard, 1996). The viscosity (in Pa s) is plotted in logarithmic scale.

Fig. 11 Density of hotspots plotted as a function of viscosity in the CMB region (Fig. 16). The density is defined as a number of hotspots located in the region of a given viscosity divided by the relative area of the region. The total area of the surface is assumed to be 1.

Fig. 12 Cartoon showing a possible scenario in the deep mantle. The hot perovskite plume, being stiffer than the adjacent post-perovskite deep mantle, is surrounded by softer material associated with the horizontal flow, which originated from the cold slabs.

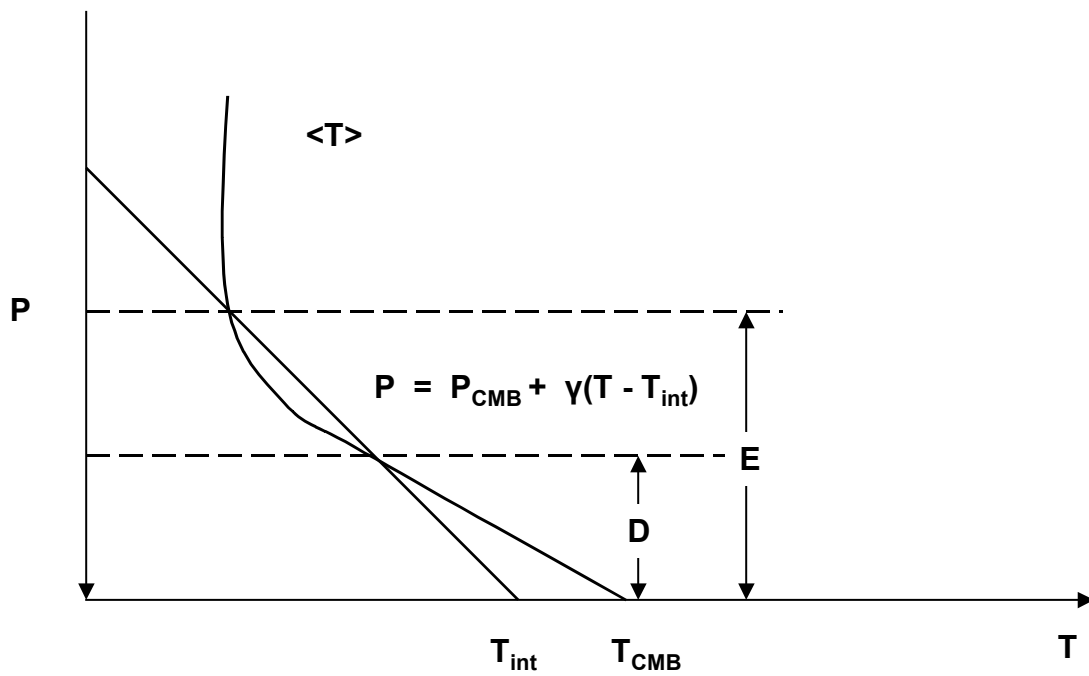


Fig. 1

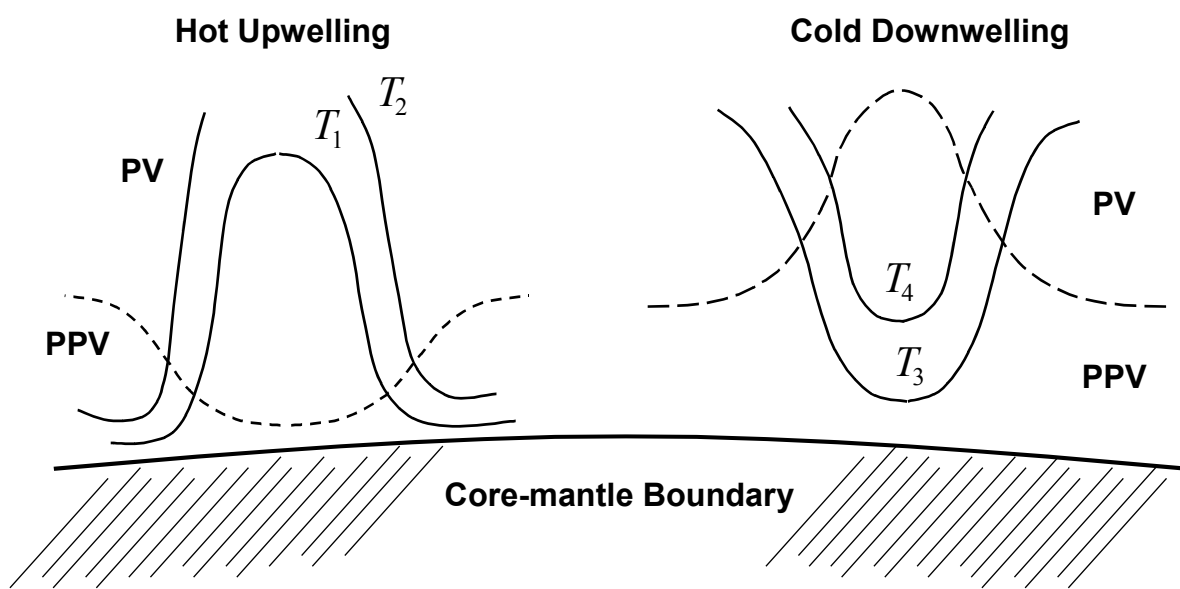
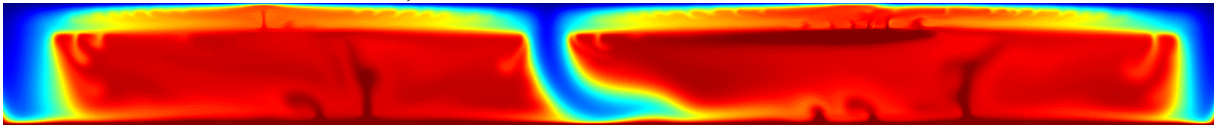


Fig. 2

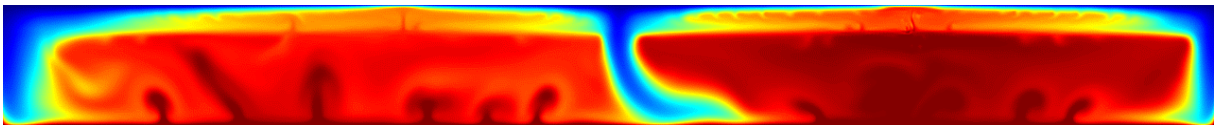
Change of the ppv Clapeyron slope sign and the thermal conductivity in D''

new thermal expansivity ; depth- and temperature-dependent viscosity
 $P_{670} = -0.08$; $T_{\text{CMB}} = 1.0$

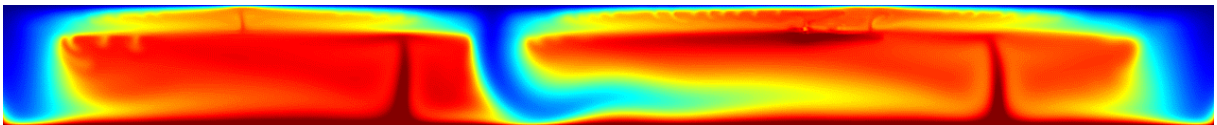
$k=1$ in the whole mantle ; $P_{D''} = 0.10$



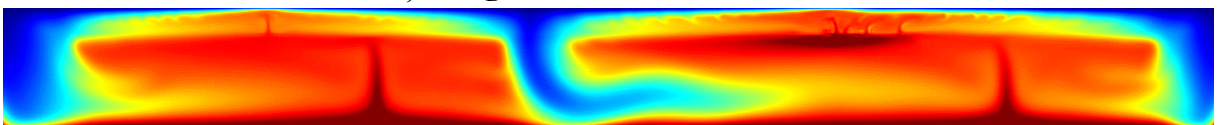
$k=1$ in the whole mantle ; $P_{D''} = 0.05$



$k=1$ in the whole mantle ; $P_{D''} = 0.00$



$k=1$ in the whole mantle ; $P_{D''} = -0.05$



$k=1+5(T_0+T)^3$ in D'' $k=1$ above D'' ; $P_{D''} = 0.05$

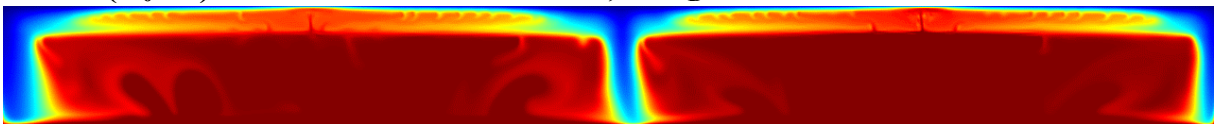


Plate 1

Change of the ppv Clapeyron slope sign
and the thermal conductivity in D''

new thermal expansivity
depth- and temperature-dependent viscosity
 $P_{670}=-0.08$; $T_{\text{CMB}}=1.0$; $ci=20$

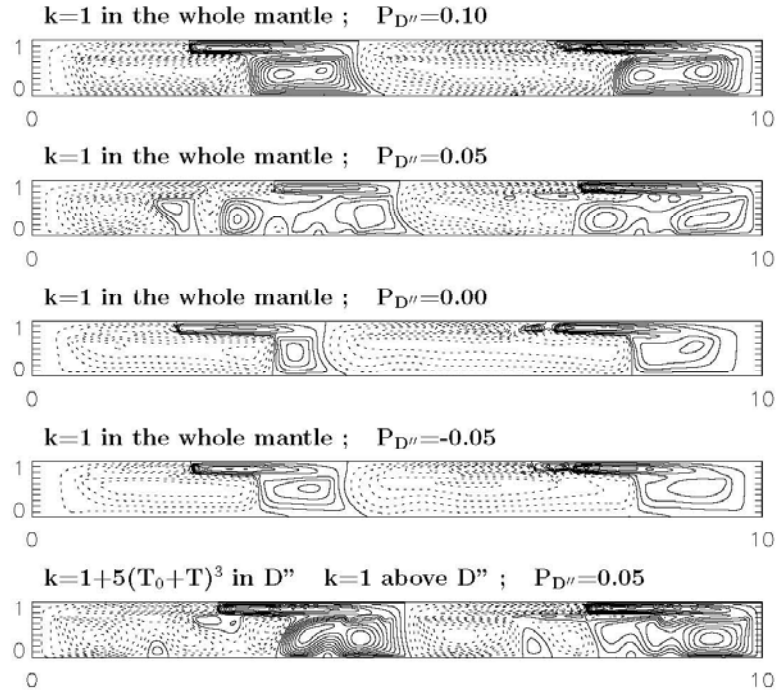
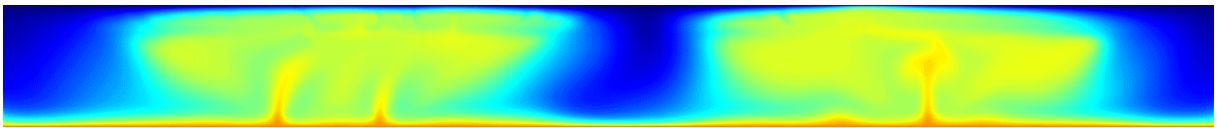


Fig. 3

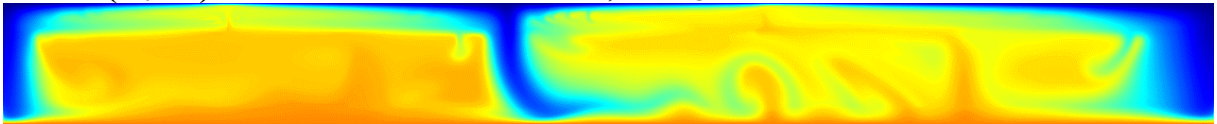
Change of the CMB temperature and the thermal conductivity in D''

new thermal expansivity ; depth- and temperature-dependent viscosity
 $P_{670} = -0.08$; $P_{D''} = 0.05$

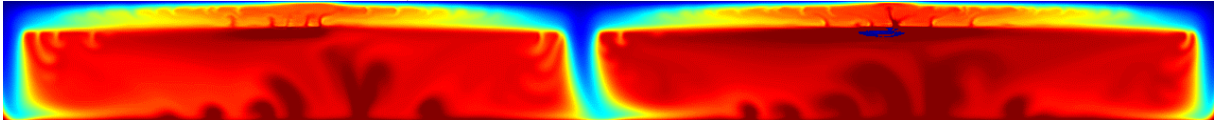
$k=1$ in the whole mantle ; $T_{CMB}=0.8$



$k=1+5(T_0+T)^3$ in D'' $k=1$ above D'' ; $T_{CMB}=0.8$



$k=1$ in the whole mantle ; $T_{CMB}=1.2$



$k=1+5(T_0+T)^3$ in D'' $k=1$ above D'' ; $T_{CMB}=1.2$

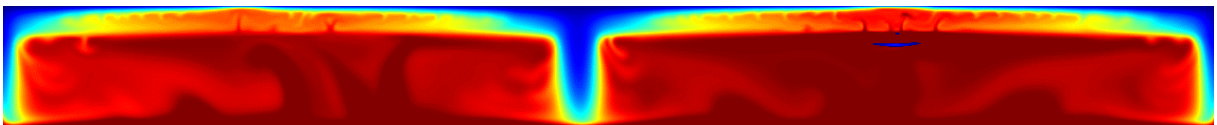
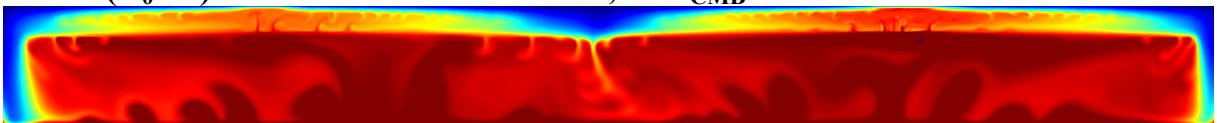


Plate 2

Change of the CMB temperature
and the thermal conductivity in D''

new thermal expansivity
depth- and temperature-dependent viscosity
 $P_{670}=-0.08$; $P_{D''}=0.05$

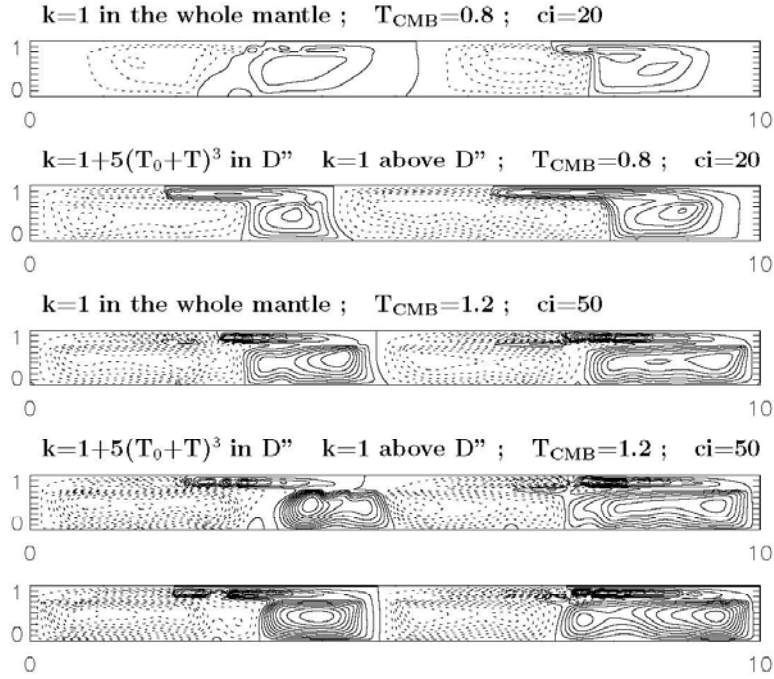


Fig. 4

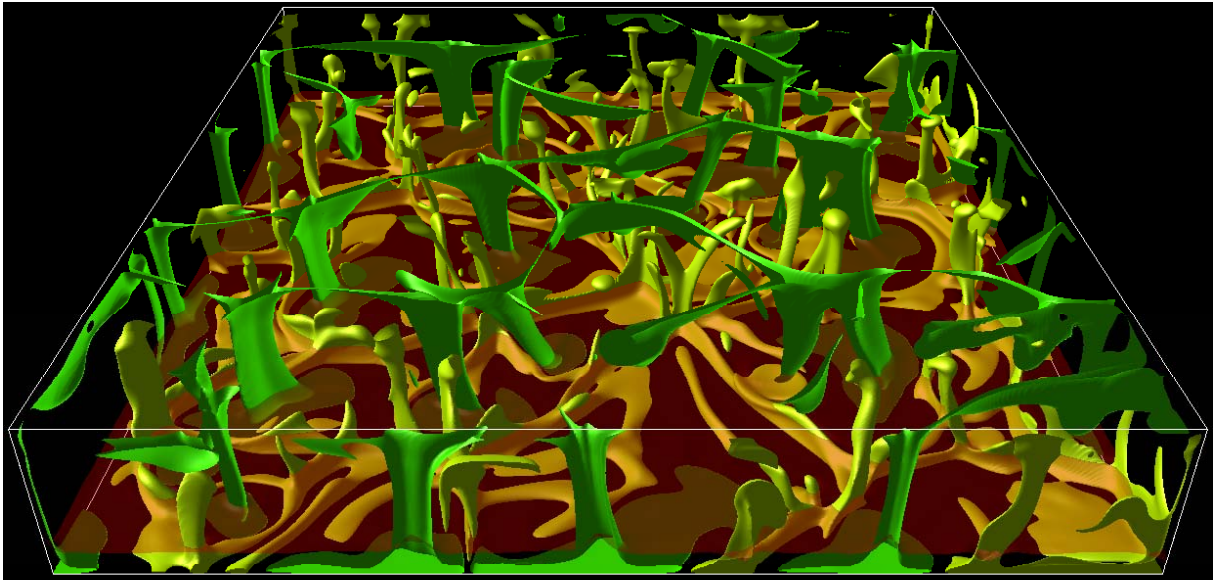


Plate 3

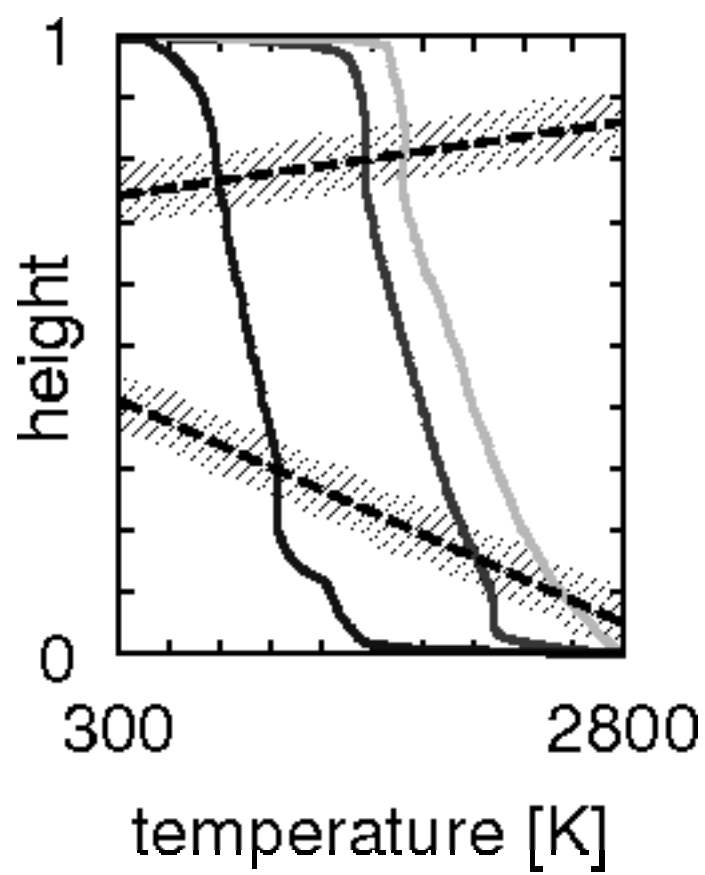


Fig. 5

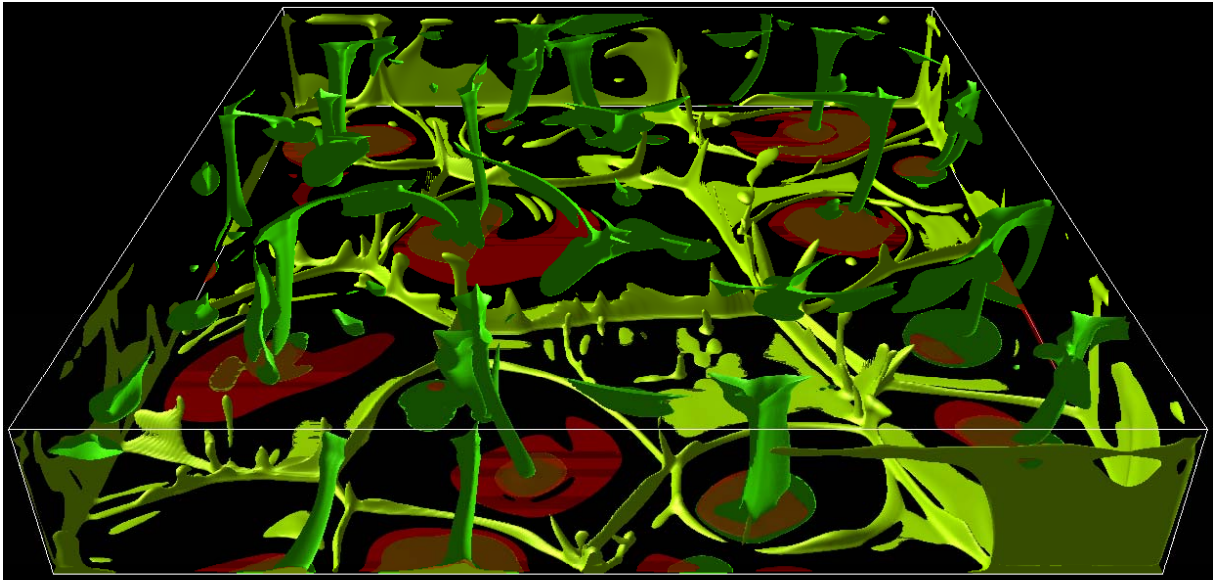


Plate 4

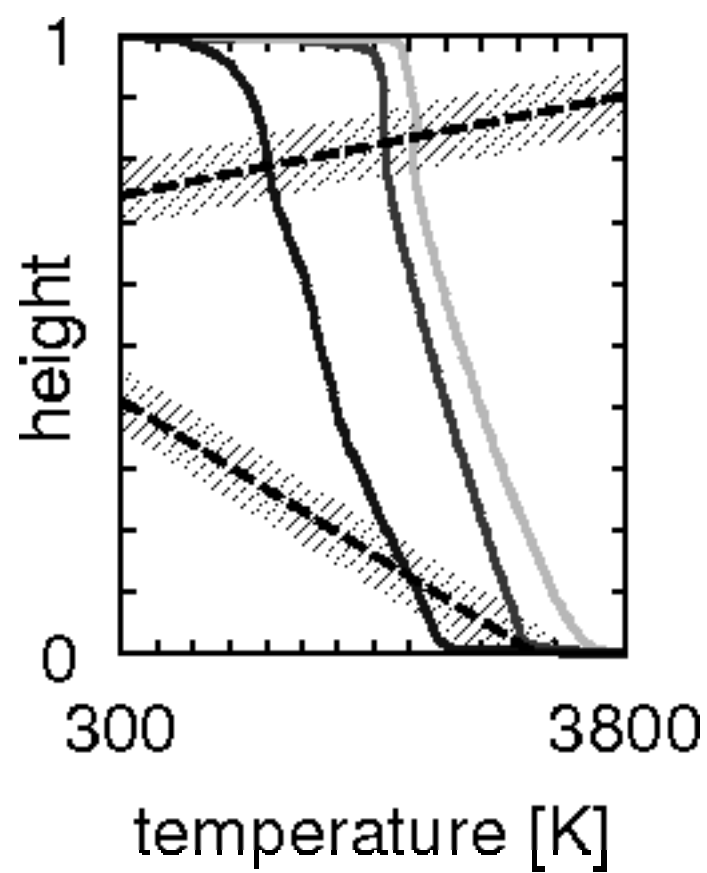
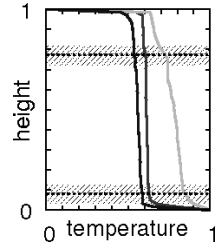
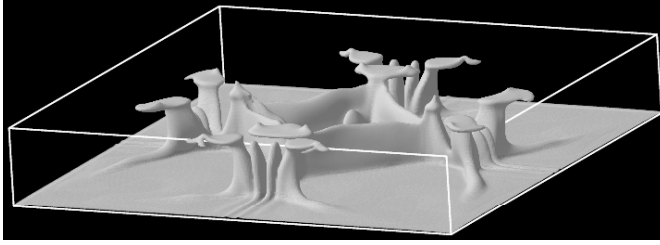


Fig. 6

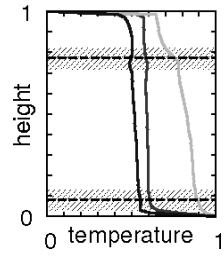
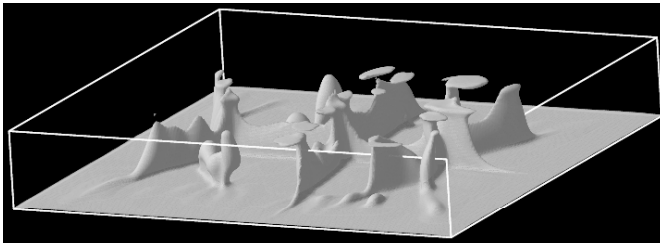
isosurfaces of $T=0.65$

$\langle T \rangle$ $T_{\max}$ $T_{\min}$

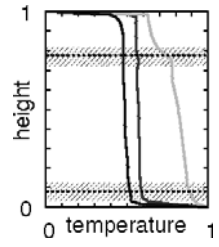
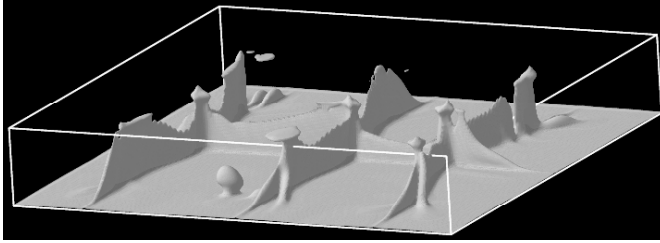
(a) $t=2.68471441 \times 10^{-4}$



(b) $t=6.94067556 \times 10^{-4}$



(c) $t=1.35916630 \times 10^{-3}$



(d) $t=2.02965442 \times 10^{-3}$

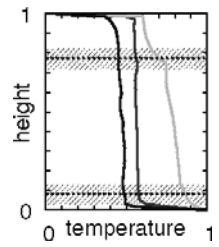
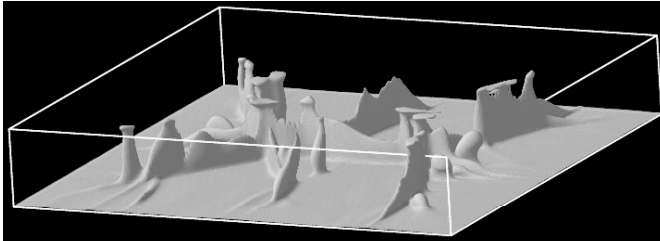
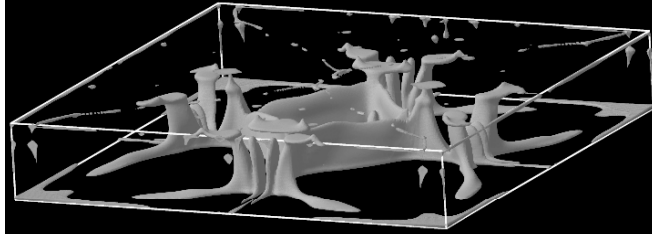


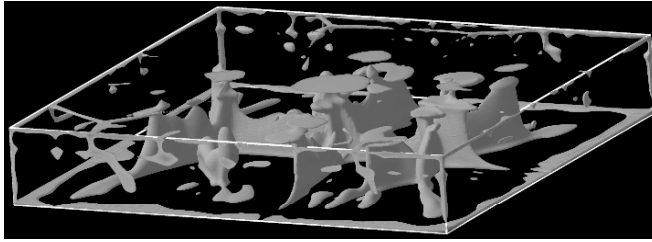
Fig. 7

$$\Delta T = T - \langle T \rangle \text{ with } |\Delta T| > 0.05$$

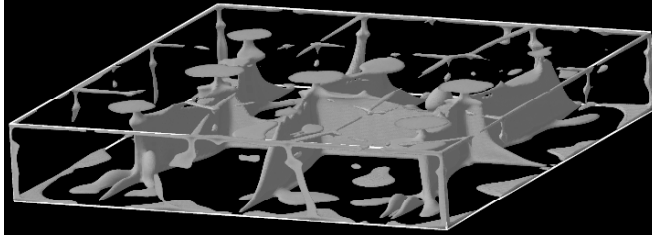
(a) $t = 2.68471441 \times 10^{-4}$



(b) $t = 6.94067556 \times 10^{-4}$



(c) $t = 1.35916630 \times 10^{-3}$



(d) $t = 2.02965442 \times 10^{-3}$

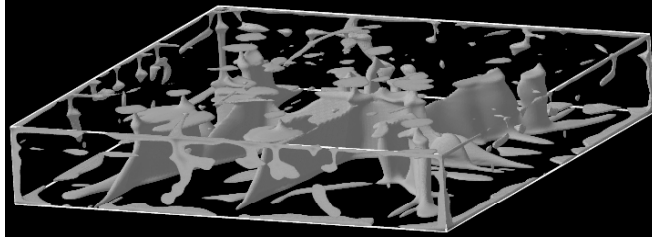
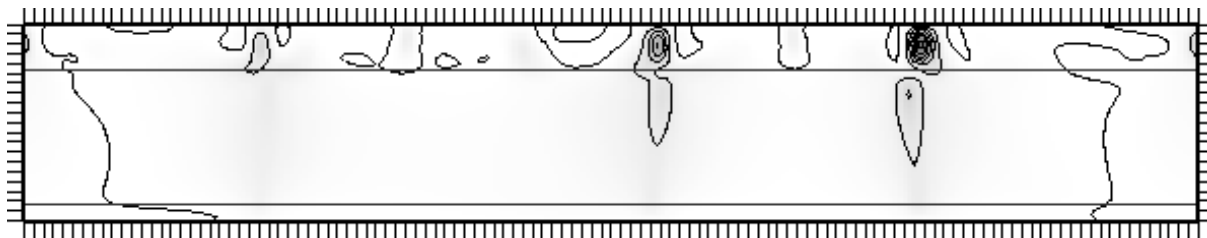


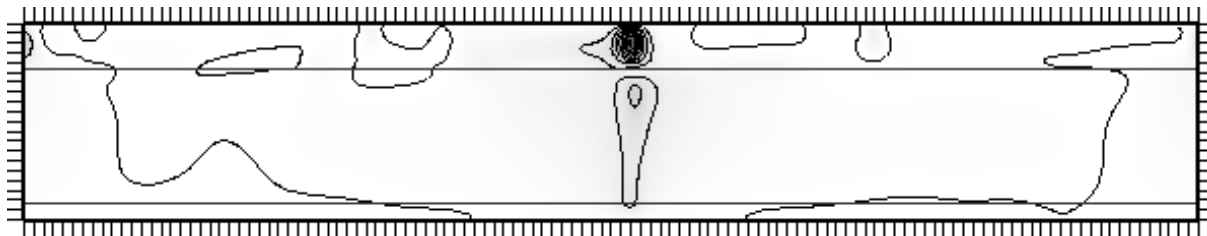
Fig. 8

vertical cross-sections v_z for the snapshot (c)

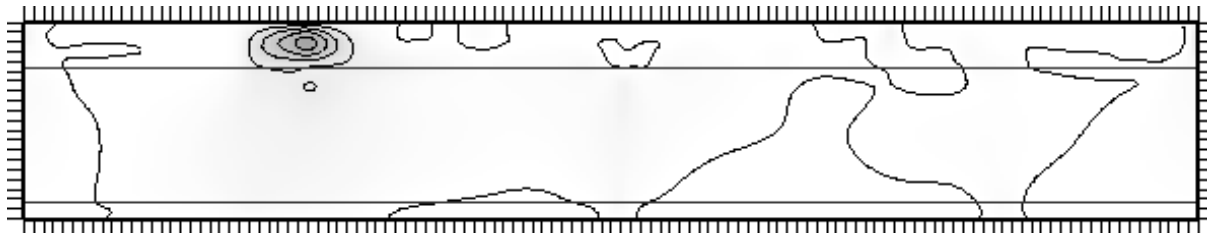
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$y=1.21875000$



$y=2.85937500$



$y=4.59375000$

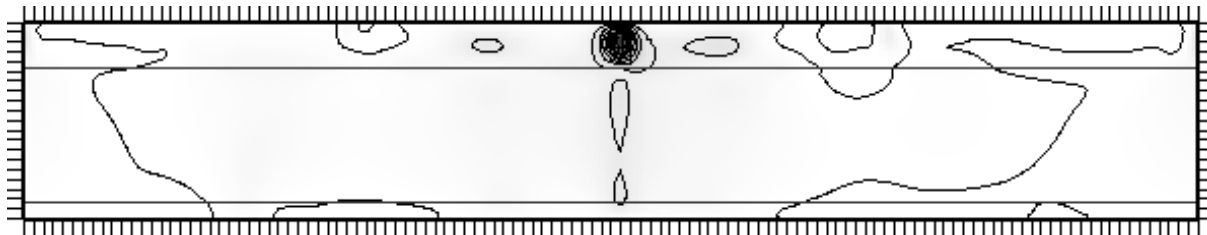
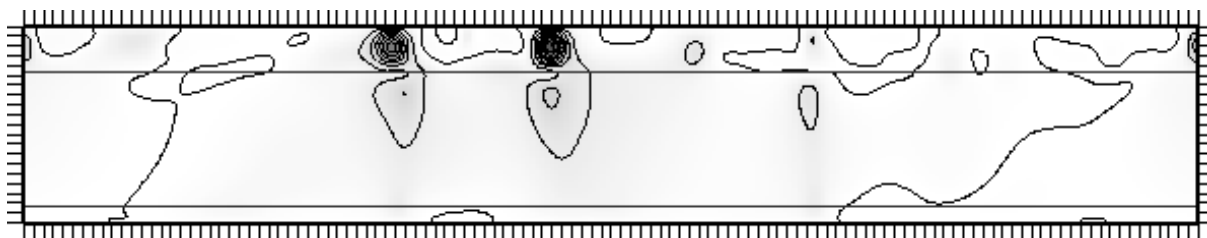


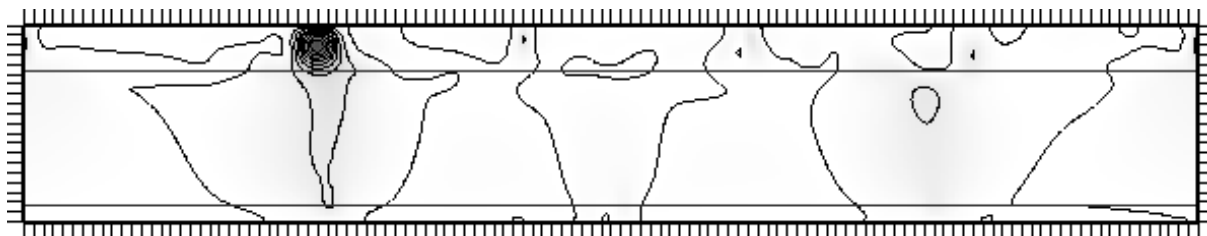
Fig. 9

vertical cross-sections v_z for the snapshot (d)

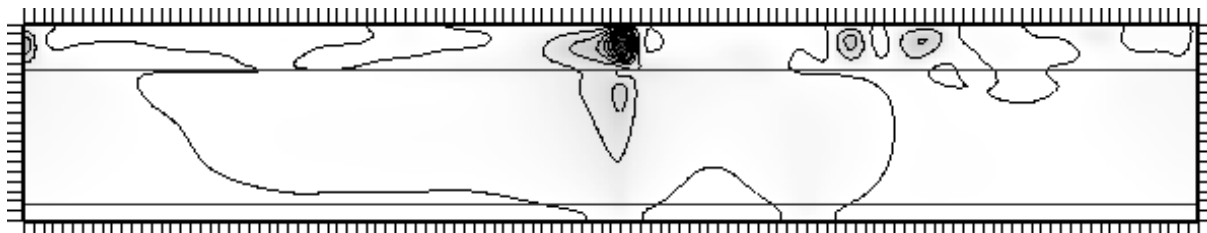
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$y=1.07812500$



$y=2.69531250$



$y=4.87500000$

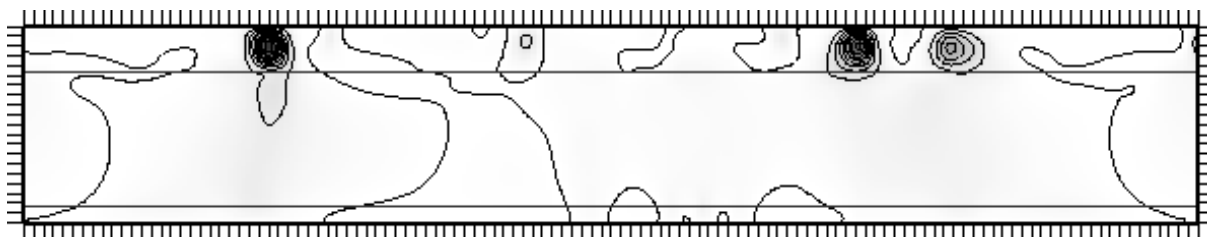


Fig. 10

a) OBSERVED GEOID

b) PREDICTED GEOID

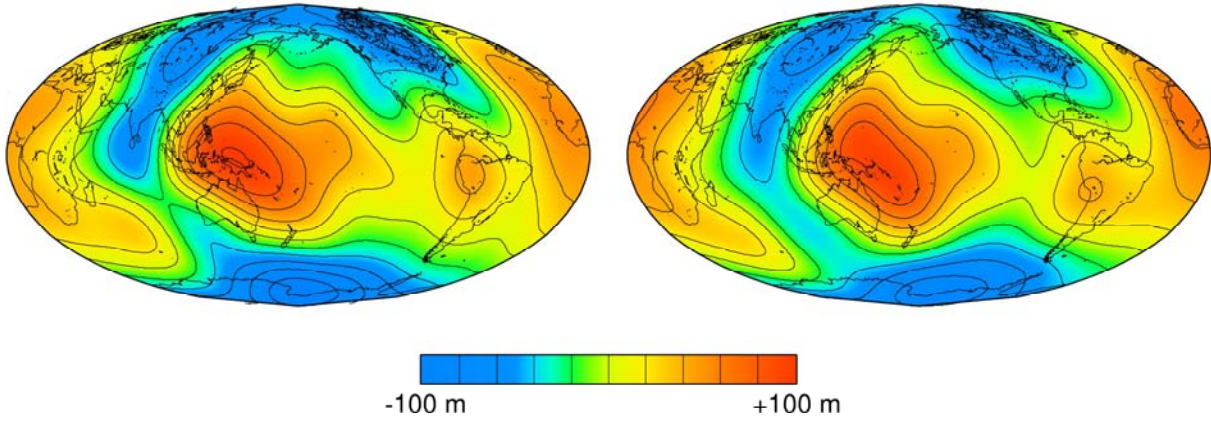


Plate 5

VISCOSITY IN CORE-MANTLE BOUNDARY REGION

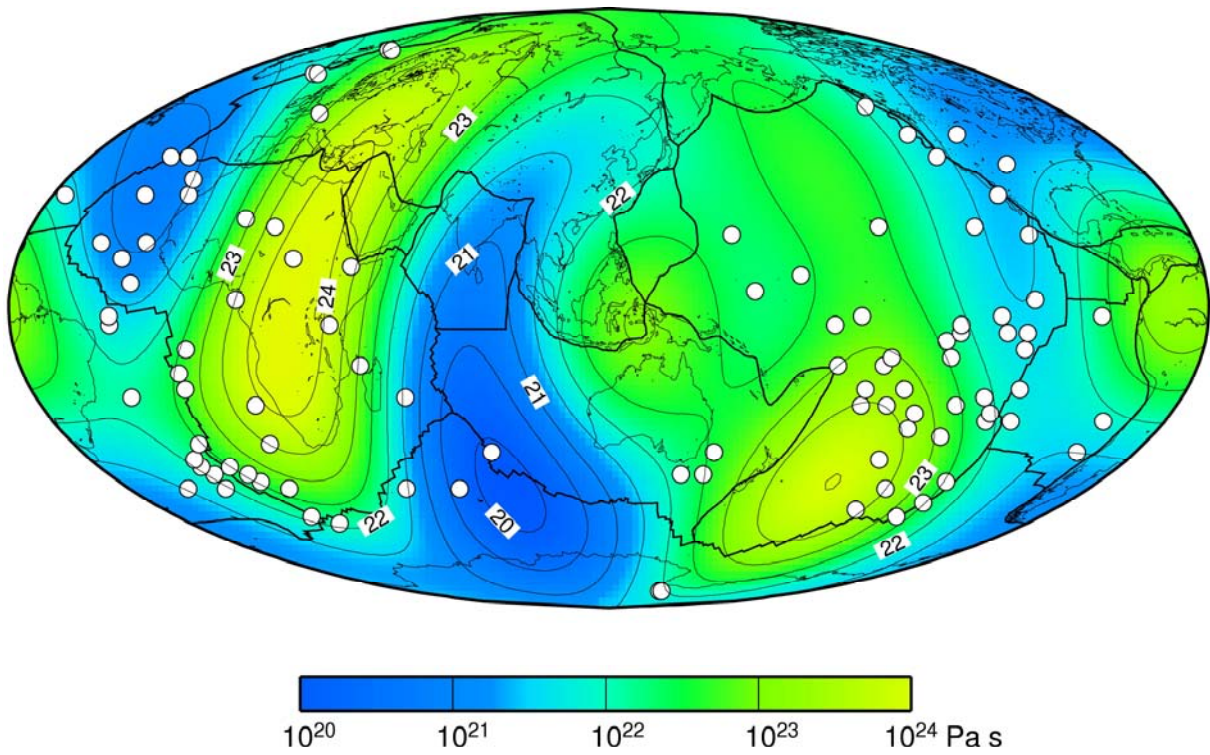


Plate 6

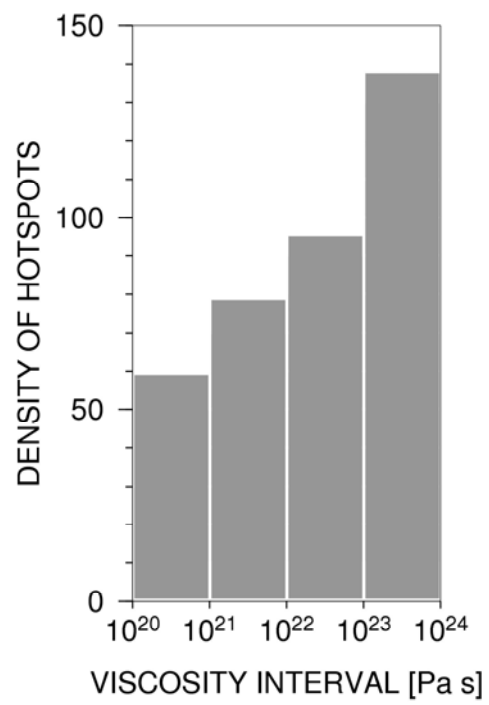


Fig. 11

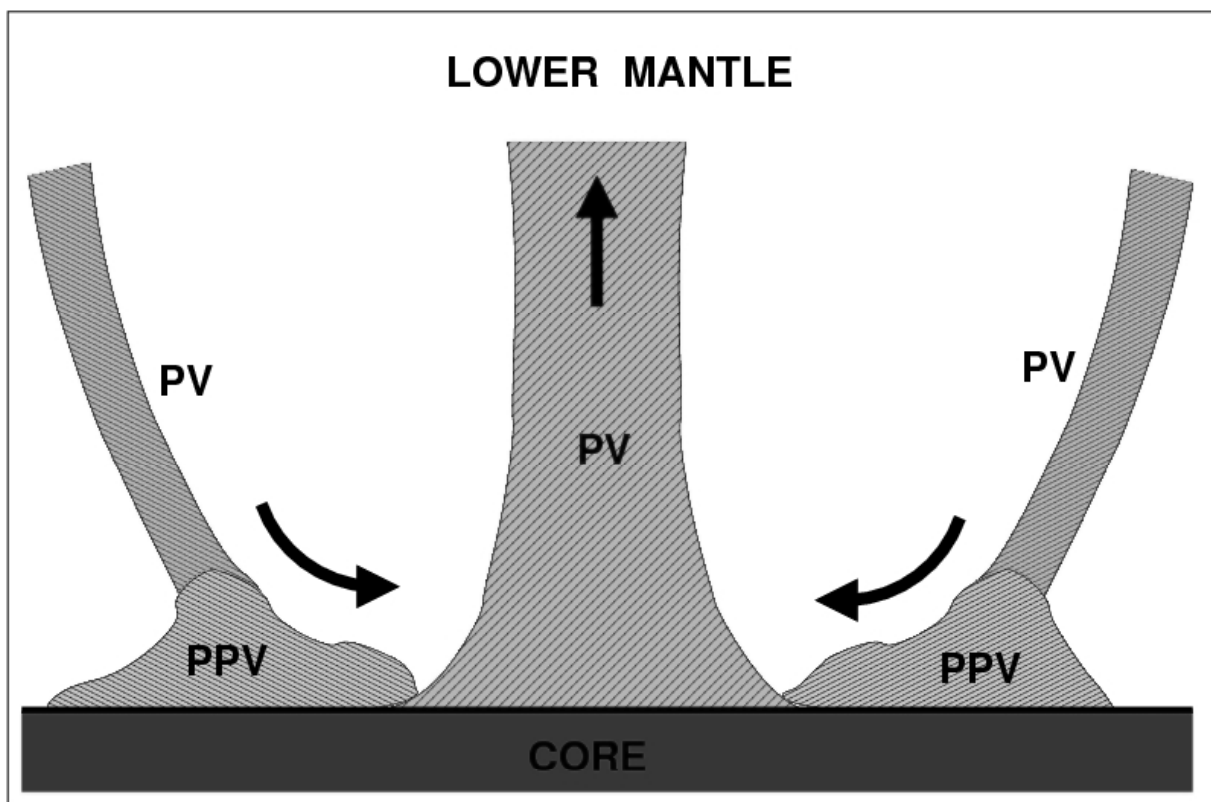


Fig. 12