Physics of the Earth and Planetary Interiors 180 (2010) 222–234

Contents lists available at ScienceDirect

Physics of the Earth and Planetary Interiors

journal homepage: www.elsevier.com/locate/pepi

On the interaction of the geotherm with a post-perovskite phase transition in the deep mantle

John W. Hernlund*

Department of Earth and Ocean Sciences, The University of British Columbia, 6339 Stores Road, Vancouver, BC V6T 1Z4, Canada

ARTICLE INFO

Article history:
Received 2 June 2009
Received in revised form 21 January 2010
Accepted 1 February 2010

Guest Editors
Kei Hirose
Thorne Lay
David Yuen

Editor
G. Helffrich

Keywords:
Post-perovskite
Core-mantle heat flow
Mantle convection
Mantle phase transitions
D”

ABSTRACT

The energy balance in the presence of a perovskite (Pv) to post-perovskite (pPv) transition within Earth's D” layer is examined in order to explore the relationship between changes in seismic velocity associated with this phase change, the extent of the two-phase Pv–pPv coexistence region, and the thermal structure of the deep mantle. This is motivated in part by the fact that discontinuities attributed to the Pv–pPv transition are inferred to be seismically sharper than permitted by some recent estimates of the pressure increment across the two-phase co-existence region. Here it is shown that sharp gradients in phase abundance may arise even when the two-phase loop is very broad, and therefore the pressure increment determined from thermodynamic stability alone is a poor proxy for predicting the sharpness of Pv–pPv related seismic discontinuities. The change in pPv fraction over the steepest gradients in phase can also be highly variable, which would lead to potentially complex variations in the total strength of seismic discontinuities. Latent heat plays an important role in the structure of the pPv phase change and its influence upon the geotherm. For the double-crossing scenario – in which a deeper reverse transformation from pPv to Pv occurs in a steep thermal boundary layer – latent heat release from the shallower Pv–pPv transition moderates the effects of latent heat absorption at the deeper reverse transition.

1. Introduction

It is widely recognized that a better determination of the D” layer geotherm would permit an enhanced understanding of the driving forces responsible for convection in the outer core that produces Earth's magnetic field (Braginsky and Roberts, 1995), provide constraints upon lateral temperature variations in the deep mantle that are intimately related to the extent of deep circulation of subducted lithosphere (Schubert et al., 2001), and elicit insights into the nature of any buoyant instabilities in the deep mantle that may give rise to upwelling thermal plumes which rise upward and trace out volcanic hotspot tracks at Earth's surface (Morgan, 1971). Only recently has the discovery of a post-perovskite (pPv) transition in the dominant lower mantle phase $MgSiO_3$ perovskite (Pv) (Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004a) opened up the possibility of making direct temperature inferences in the D” layer by comparing observations of seismic discontinuities attributed to the Pv–pPv phase change with experimental and ab initio constraints on the position of the phase boundary (Hernlund et al., 2005; Ono and Oganov, 2005; Lay et al., 2006; van der Hilst et al., 2007). These temperature inferences might potentially be used to infer quantities such as CMB heat flux that are central to many of the outstanding questions regarding the evolution of Earth's deep interior (see Lay et al., 2008 for a recent review).

A thermal boundary layer (TBL) exists above the base of Earth's core-mantle boundary (CMB) because conduction down a thermal gradient is the only mechanism capable of accommodating significant radial heat transport out of the surface of the core into the mantle. The surface of the core itself is essentially isothermal, exhibiting lateral temperature variations less than about 10^{-4} K (Braginsky and Roberts, 1995). Variations in temperature and heat flux in the deepest mantle therefore arise exclusively as a consequence of mantle circulation patterns that cool Earth's deep interior, and the core itself plays a strictly passive role by behaving as a sort of heat reservoir with a large thermal inertia. The appearance of pPv-bearing rocks is therefore exclusively controlled by processes operating in the mantle, and its seismic detection and interpretation may lead to important insights into the dynamics of the Earth's deep interior. Additionally, the Pv–pPv phase change has a positive Clapeyron slope, and pPv is stabilized at lower temperatures. Thus pPv-bearing rocks will tend to form in greater abundance within cooler regions of the deep mantle, such as the locations where cool downwellings (e.g., subducted slabs) sink and

* Correspondence address: Department of Earth and Planetary Science, University of California, Berkeley, 307 McCone Hall, Berkeley, CA 94720-4767, USA.
E-mail address: hernlund@gmail.com.

0031-9201/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.pepi.2010.02.001

pond above the CMB. This makes inferences of temperature using Pv–pPv phase change constraints especially useful because heat transport in the deep mantle is thought to be dominantly controlled by downwellings (e.g., Labrosse, 2002).

Another constraint may be gained from the Pv–pPv phase change because the geotherm may initially pass through the Pv–pPv phase boundary in shallower portions of the D" layer and then revert back to Pv-stability at greater depths inside the TBL if the CMB temperature is greater than the transition temperature at CMB pressure. This has been called the "double-crossing" hypothesis (Hernlund et al., 2005), which offers predictions regarding the seismic velocity structure of the D" layer that can be tested against a variety of seismic data. It was shown more than a decade ago (e.g., Sidorin et al., 1998) that a phase change exhibiting a large Clapeyron slope could best explain the appearance of seismic shear velocity increase discontinuities of up to several percent observed ≈150–300 km above the CMB in some regions (Wysession et al., 1998). If the Pv–pPv phase change (with an estimated Clapeyron slope of order 10 MPa/K) is to account for this velocity increase discontinuity, then a deeper reversion from pPv to Pv will likely be accompanied by a velocity decrease discontinuity (Hernlund et al., 2005). Such a velocity decrease underlying a shallower increase discontinuity has now been reported in numerous studies involving seismic migration beneath Eurasia (Thomas et al., 2004b) and the Cocos-Caribbean region (Thomas et al., 2004a; van der Hilst et al., 2007), waveform modeling beneath the Caribbean (Sun et al., 2006), stacking and inversion of short-period ScS precursors beneath the mid-Pacific (Avants et al., 2006; Lay et al., 2006), and long-period waveform inversion beneath the Cocos-Caribbean region (Kawai et al., 2007a) and Arctic (Kawai et al., 2007b). Furthermore, anti-correlated patterns of P- and S-wave velocity variations that are predicted to occur in pPv elasticity models (e.g., Wookey et al., 2005) have been inferred using seismic data probing D" beneath the Cocos-Caribbean region (Kito et al., 2007; Hutko et al., 2008). Therefore, a variety of seismic techniques thus far support the basic predictions of a Pv–pPv phase change, as well as the occurrence of a double-crossing.

If the Pv–pPv phase change were sensitive to temperature and pressure alone, the double-crossing picture could be expanded to a global scale relatively straightforwardly. For example, because the CMB is isothermal and isobaric, pPv could only occur in lens-like structures above the CMB, and only Pv would be stable at the very base of the mantle (Hernlund et al., 2005). Absence of pPv could then be achieved in some regions as a consequence of a geotherm that is too hot to stabilize pPv. However, large scale variations in bulk composition are almost certainly present in the D" layer, and some of the complex pictures that arise when this is included along with a pPv phase transition have been further explored by Tackley et al. (2007). For example, it has been hypothesized that addition of ferrous iron could have a significant effect, stabilizing pPv inside chemically distinct Fe-rich "piles" that rest at the bottom of the mantle beneath the Pacific and Africa (Lay et al., 2006; Tackley et al., 2007). Spera et al. (2006) studied the form of the pPv double-crossing assuming regular solution in the system $FeSiO_3$–$MgSiO_3$ using early experimental measurements by Mao et al. (2004) and the empirical scaling derived from end-member volume mismatch proposed by Navrotsky (1994). However, the robustness of the pressure standard comparisons of some of these early diamond anvil cell results have since been challenged by Hirose et al. (2006). Indeed, effects involving the system $FeSiO_3$–$MgSiO_3$ that are completely opposite to those reported earlier – with iron destabilizing pPv at lower pressures as opposed to stabilizing it – have since appeared (Tateno et al., 2007). Also, the possibility of a high-spin to low-spin (e.g., Badro et al., 2004) or intermediate-spin (e.g., McCammon et al., 2008) iron transition in perovskite raises further questions about the behavior of Fe at conditions of the deep mantle, and may itself play an unknown but important role in the complex behavior observed in the $FeSiO_3$–$MgSiO_3$ binary system. Additionally, somewhat different perspectives on the partitioning of iron between Pv–pPv and other phases such as ferro-periclase have emerged (e.g., Sinmyo and Ohishi, 2008; Auzende et al., 2008), and this might also have a significant influence on the Pv–pPv phase change. Seismological inferences in support of any of these kinds of scenarios are non-unique, and critically depend upon the mineral physics data and interpretations.

Another emerging issue is that some kinds of compositional effects on the Pv–pPv phase change have been proposed that might substantially broaden the two-phase co-existence region between Pv and pPv, such as the addition of Al_2O_3 (e.g., Akber-Knutston et al., 2005; Catalli et al., 2009). This might complicate the interpretation of discontinuities attributed to the Pv–pPv transition, which exhibit an observed "gradient thickness" of up to around 75 km, corresponding to about 4 GPa in pressure change (e.g., Wysession et al., 1998). The "gradient thickness" is the apparent depth interval over which the majority of the seismic velocity change occurs, and is often assumed to be distributed over the entire two-phase co-existence loop (e.g., Helffrich and Bina, 1994). This viewpoint suggests that any findings of two-phase co-existence with a pressure increment larger than 4 GPa could mean that the Pv–pPv transition cannot not produce discontinuities that are sharp enough to explain the seismic observations. However, the assumption that gradients are always distributed uniformly over the entire two-phase co-existence loop has been shown to be false in the context of shallower mantle phase transitions, because self-consistently calculated phase abundance profiles can be highly non-linear inside the two-phase region, particularly when the two-phase loop is broad (Stixrude, 1997). However, this effect has never been investigated in the context of the Pv–pPv transition, which is significantly different from the shallower phase changes in that it exhibits a relatively large Clapeyron slope, occurs inside a thermal boundary layer, and is potentially influenced by latent heat to a greater extent.

There are also issues related to energy balances for the pPv double-crossing and its implications for heat flux that have not been resolved. One issue is latent heat, which can deflect the geotherm near the phase transition (Verhoogen, 1965). Using a simple heat balance, Buffett (2007) recently showed that latent heat absorption causes a steepening of the geotherm beneath a pPv double-crossing. Essentially, steady production of the higher entropy Pv phase from a lower entropy pPv phase upon downwelling through the lower crossing requires a net input of heat at the phase boundary to balance the absorption of latent heat, which can only be realized by differences in heat conduction (i.e., changes in the thermal gradient) above and below the transition. The implication is a geothermal gradient beneath the pPv lense which is even steeper than that given by a phase boundary gradient lower bound alone. The effect would be enhanced when a two-phase region is present (Buffett, 2007), because the change in conduction needs to additionally balance the difference in advection at the top and bottom owing to the large temperature gradient. This phenomenon possibly provides more leverage on the thermal gradient at the very deepest levels of the mantle, however, it can only be confidently applied if one can rigorously connect kinematic factors such as downwelling velocity with thermodynamic factors such as latent heat and transport properties like thermal conductivity, all of which exhibit a large range of uncertainty.

The relationship between the appearance of pPv-bearing rock and various kinematic or dynamic factors is also an active area of research. Lay et al. (2006) presented simple fits of an error function-like geotherm to observations of discontinuities beneath the central Pacific in an attempt to bracket how uncertainties in the parameters would trade off with the inferred heat flux beneath what was interpreted to be a pPv double-crossing. More ambitious attempts