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On the likelihood of post-perovskite near the core–mantle boundary: A statistical interpretation of seismic observations

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ABSTRACT

Recent experimental studies indicate that perovskite, the dominant lower mantle mineral, undergoes a phase change to post-perovskite at high pressures. However, it has been unclear whether this transition occurs within the Earth's mantle, due to uncertainties in both the thermochemical state of the lowermost mantle and the pressure–temperature conditions of the phase boundary. In this study we compare the relative fit to global seismic data of mantle models which do and do not contain post-perovskite, following a statistical approach. Our data comprise more than 10,000 P_{diff} and S_{diff} travel-times, global in coverage, from which we extract the global distributions of $d\ln V_S$ and $d\ln V_P$ near the core–mantle boundary (CMB). These distributions are sensitive to the underlying lateral variations in mineralogy and temperature even after seismic uncertainties are taken into account, and are ideally suited for investigating the likelihood of the presence of post-perovskite. A post-perovskite-bearing CMB region provides a significantly closer fit to the seismic data than a post-perovskite-free CMB region on both a global and regional scale. These results complement previous local seismic reflection studies, which have shown a consistency between seismic observations and the physical properties of post-perovskite inside the deep Earth.

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1. Introduction

The lowermost 150–300 km of the mantle (i.e. the D″ region) is one of the most enigmatic and seismically complex regions of the Earth. Postulated as the source region for mantle plumes (Williams et al., 1998), a graveyard for subducted slabs (Van der Voo et al., 1999), and potentially a primitive, melt-bearing layer (Fiquet et al., 2010), it represents a zone in which strong thermal, chemical and structural heterogeneity may be expected. Nonetheless, the 2004 discovery of a phase transition in $(Mg,Fe)SiO_3$ perovskite (Pv) to post-perovskite (pPv) at pressures approaching the Earth's lowermost mantle (Murakami et al., 2004; Oganov and Ono, 2004; Shim et al., 2004) opened up the possibility to explain much of the region's observed seismic behaviour in terms of this transition.

Theoretical calculations indicate that pPv is seismically distinct from Pv: it has a ~1.5–2% higher *S*-wave velocity (Stackhouse and Brodholt, 2007; Wentzcovitch et al., 2006) but a reduced bulk sound velocity (Nishio-Hamane and Yagi, 2009; Hustoft et al., 2008), which may be manifested as little or no change (±0.5%) in *P*-wave velocity. Thus, the Pv to pPv phase transition may be responsible for the so-called D″ discontinuity observed about 150–300 km above the core–mantle boundary (CMB) (Lay et al., 2005), in which a 2–3% increase in *S*-velocity is accompanied by a generally smaller or absent increase in *P*-velocity (Wysession et al., 1998). Lateral variations in post-perovskite content may further explain the intermittent anti-correlation in bulk sound and *S*-wave velocities at the CMB (Wookey et al., 2005). However, the depth and width of the Pv to pPv phase transition is strongly temperature- and composition-dependent (Grocholski et al., 2012; Catalli et al., 2009; Wookey et al., 2005). Given the likely thermochemical heterogeneity in D″ and the large experimental uncertainties on the position of the phase boundary (Hirose, 2007), it is still uncertain if, or where, pPv exists within the mantle. A number of studies (e.g., Chaloner et al., 2009; Hutko et al., 2008; Kito et al., 2007; van der Hilst et al., 2007; Lay et al., 2006; Wookey et al., 2005) have presented recordings of seismic waveforms in the lowermost mantle that are consistent with the presence of a Pv-to-pPv transition. This consistency is primarily based on agreement between the observed structure of the D″ discontinuity and the predicted seismic structure of the perovskite to post-perovskite phase transition. Yet, it is possible that the intermittent deep mantle reflections with variable amplitudes (Wysession et al., 1998) are due to structural complexity associated with subducted slabs,

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changes in bulk chemistry, or anisotropic effects (Lay and Garnero, 2007; Thomas et al., 2004a,b) in a pPv-free mantle.

To complement existing local studies, we will present a robust statistical study of the fit of different mantle models (Table 1) to seismic wave speed variations on a global to regional scale, considering both pPv-free and pPv-bearing mineral assemblages. Our approach resembles a hypothesis test: is post-perovskite present, or absent, at the core–mantle boundary? Rather than focussing on the structure of the Pv-to-pPv transitions and attendant seismic discontinuities, as in previous studies, we focus on the large-scale *S* and *P* wave speed structure of the lowermost mantle using both seismic and mineral physics constraints, and a fitting procedure based on the Metropolis algorithm (Mosegaard and Tarantola, 1995).

Lateral seismic wave speed variations are usually expressed as relative perturbations of *P*-wave velocity (V_P) and *S*-wave velocity (V_S) with respect to a 1D reference model, and referred to as $d\ln V_P$ and $d\ln V_S$, respectively. They are normally calculated via a tomographic inversion (e.g., Masters et al., 2000). However, the inverse problem is ill-posed, and the required regularisation makes it very difficult to assess the corresponding resolution and uncertainty of the wave speed variations. In order to make a quantitative and self-consistent interpretation of the seismic models in terms of thermochemical parameters, and hence pPv content, it is essential that the mineral physics parameters are averaged over the resolving length prescribed by the seismic models and that uncertainties are treated rigorously. Thus, in this work, we use a simplified wave propagation theory, the path-average approximation (Mosca and Trampert, 2009), which fixes the resolution, and converts seismic travel-time measurements directly into $d\ln V_S$ and $d\ln V_P$. This approximation has already been validated on seismic data (Mosca and Trampert, 2009) and has the advantage of allowing a precise quantification of all uncertainties without the need for a regularised inversion. Our approach is reminiscent of a Backus–Gilbert hypothesis test (e.g., Trampert and van Heijst, 2002), which solves an inference problem by fixing the desired resolution *a priori*.

The path-average approximation is accurate for spatial scale lengths of 2000–3000 km laterally, i.e. spherical harmonic degree 8. In this study we use only core diffracted phases, which give rise to a specific path-average sensitivity kernel that fixes the depth resolution to about 50 km near the CMB, with a corresponding known uncertainty. Following this approach allows us to map lateral *P* and *S* wave speed variations with the same spatial resolution, albeit with different – but quantifiable – uncertainties. It is essential to have such coherency between *P*- and *S*-wave structure in order to be able to distinguish thermal from chemical variations (Cobden et al., 2009; Hernlund and Houser, 2008; Deschamps and Trampert, 2003). Moreover, it is imperative to include uncertainties – often neglected or undefinable in tomographic studies – in the analysis to ensure a reliable, quantitative physical interpretation of the seismic data.

Another important difference in our approach is that instead of interpreting geographic maps of $d\ln V_S$ and $d\ln V_P$, or single values of the velocity perturbation at specific locations, we derive histograms of $d\ln V_S$ and $d\ln V_P$, and also the seismic parameter $R = d\ln V_S / d\ln V_P$ near the CMB. The width and shape of the histograms reflect the magnitude, frequency and nature of lateral variations in temperature and composition near the CMB (e.g., Hernlund and Houser, 2008; Deschamps and Trampert, 2003). By compiling histograms, we lose the 3D information on where, geographically, a particular velocity perturbation has come from. However, for our purpose this is not relevant: we wish simply to test whether the morphology of the histograms is better fit by a CMB region where pPv is present, or where it is absent. It is necessary to consider *R* in addition to $d\ln V_S$ and $d\ln V_P$ because globally-compiled histograms of $d\ln V_S$ and $d\ln V_P$ do not fully represent the correlations between V_P and V_S variations, which are important to be able to distinguish between different compositions. *R* is produced by combining two variables ($d\ln V_S$ and $d\ln V_P$) into one, and when used in isolation, can be interpreted non-uniquely (Deschamps and Trampert, 2003). *R* must therefore be analysed in conjunction with the separate $d\ln V_S$ and $d\ln V_P$ distributions. Our seismic approximation is particularly suited to the calculation of *R*, since $d\ln V_S$ and $d\ln V_P$ have the same spatial resolution.

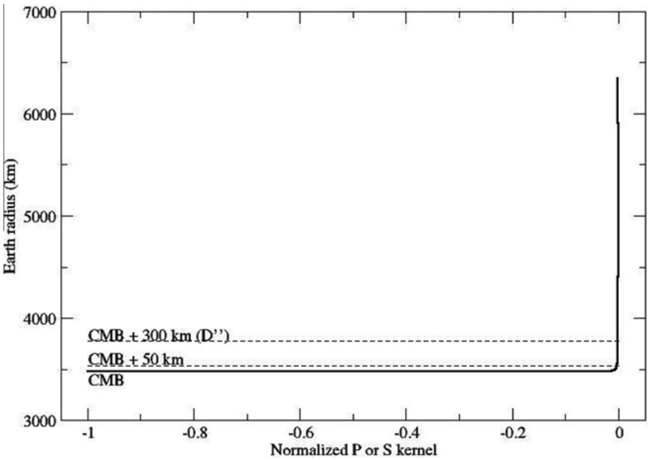

Fig. 1. Sensitivity kernel of the path-average approximation for P_{diff} and S_{diff} waves.

We calculate the seismic properties ($d\ln V_P$, $d\ln V_S$ and *R*) of different hypothetical thermochemical structures at the CMB (Table 1) via thermodynamic computations based on the most recent mineral physics data. For each structure, we make no *a priori* assumptions on the bulk chemical composition or temperature at the CMB. Instead, we create thousands of models in which temperature and composition are allowed to vary freely within extremely broad ranges. From these thousands of models we select the subset whose properties match the seismic data within uncertainties, and perform a statistical analysis of the level of fit to determine the likelihood of a pPv-free, Pv-free and (Pv + pPv)-bearing CMB region.

Table 1
Summary of different thermochemical scenarios tested in this study.

	Name		Description
Case 1	pv + ppv	🟦	Both Pv and pPv are present and lateral velocity variations arise from lateral variations in both temperature (*T*) and composition (*X*)
Case 2	no ppv	🟥	No pPv is present, but there are lateral variations in both *T* and *X*
Case 3	no pv	🟩	No Pv is present, but there are lateral variations in both *T* and *X*
Case 4	ppv:pv = 70:30	🟧	Both Pv and pPv are present in a fixed ratio of 70:30; *T* and *X* vary laterally
Case 5	Fixed *T*[a]	🟨	Both Pv and pPv are present at fixed *T* and variable *X*
Case 6	Fixed *X*[b]	🟪	Both Pv and pPv are present at fixed *X* and variable *T*

[a] Six sets of models, each with different (but fixed) temperature, were calculated, ranging between 3500 and 4000 K.

[b] Hundred sets of models each with different (but fixed) composition were calculated.

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