Temperature profile in the lowermost mantle from seismological and mineral physics joint modeling

Kenji Kawai^{a,b,1} and Taku Tsuchiya^c

^aDepartment of Earth and Planetary Sciences, Tokyo Institute of Technology, Ookayama 2-12-1, Meguro, Tokyo 152-8551, Japan; ^bInstitut de Physique du Globe de Paris, 4 Place Jussieu-75252, Paris Cedex 05, France; and ^cGeodynamics Research Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama, Ehime 790-8577, Japan

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The internal structure of the core-mantle boundary (CMB) region of the Earth plays a crucial role in controlling the dynamics and evolution of our planet. We have developed a comprehensive model based on the radial variations of shear velocity in the D'' layer (the base of the lower mantle) and the high- P,T elastic properties of major candidate minerals, including the effects of post-perovskite phase changes. This modeling shows a temperature profile in the lowermost mantle with a CMB temperature of $3,800 \pm 200$ K, which suggests that lateral temperature variations of 200–300 K can explain much of the large velocity heterogeneity observed in D''. A single-crossing phase transition model was found to be more favorable in reproducing the observed seismic wave velocity structure than a double-crossing phase transition model.

lowermost mantle | phase transition | seismic velocity | thermal structure

Temperature is one of the most important physical quantities controlling the thermal and dynamical evolution of planets. Many studies have considered the Earth's thermal structure (1). Seismic discontinuities can be used to infer the P,T conditions in the Earth, as they can be associated with phase transitions in the component minerals. The results of such studies (2, 3) suggest that the temperature near the core-mantle boundary (CMB) is strongly depth-dependent and forms a thermal boundary layer (TBL). The geotherm in the deep Earth has often been evaluated based on the P,T conditions of major phase transitions expected in the mantle and core such as the olivine-spinel and spinel-perovskite transitions and the melting of iron alloy. The pv to ppv phase transition (4) can similarly be used to infer the P,T conditions at the top of the D'' layer (5). However, it is difficult to constrain the temperature at the CMB based only on phase transition data, which has been inferred to be from approximately 3,300–4,500 K with a significant variation (1–3).

The perovskite (pv) to post-perovskite (ppv) transition is thought to coincide with the top of D'', a positive seismic velocity discontinuity, at a depth of 200–300 km above the CMB (4, 5) (Fig. 1A). This transition may be a good indicator of the temperature in the deep mantle. A large Clapeyron slope (CS) for this phase change (5) has been invoked in support of a double-crossing (6). This hypothetical second (ppv to pv reverse) transition would correspond to a negative velocity change within D'' which, if it exists, would provide information on the temperature near the CMB (7, 8). There have been many studies of the radial variations of shear velocity in the lowermost mantle. Trial-and-error forward modeling studies and studies using travel times (9) have yielded important information on the D'' discontinuity using triplications in seismic wave fields due to sharp velocity increases (Fig. 1B), which constrain the depth and magnitude of the D'' discontinuity. Recent installation of broadband seismic arrays has provided waveform data that sample D'' in a particular region, thereby allowing the study of the fine structure of the lowermost mantle. One possible approach for analyzing such data are stacking, which was used to obtain a model of the vertical dependence of shear wave velocity beneath the Pacific (7) (Fig. 1C). Another promising approach is the

simultaneous inversion of a large number of waveforms (10–13) (Fig. 1D), which allows direct determination of the detailed shear wave velocity structure within D''.

Mineral physics studies have demonstrated that the P,T conditions at the D'' discontinuity are comparable to the ppv phase boundary in pure MgSiO_3 (4, 5). Recently it has been further reported that the phase transition loop remains relatively sharp even in multicomponent systems, and that a discontinuity would thus still be seismologically detectable (14). Fundamental thermoelastic properties of these lower mantle constituents are important for mineralogical and petrological interpretations of geophysical information. Precise experimental determination of seismic wave speeds at ultrahigh- P,T conditions is still not practical, but theoretical simulations, particularly those based on ab initio quantum mechanical theory, can facilitate quantitative modeling that can be directly compared to geophysical data (15, 16). Wookey et al. (17) carried out such modeling, but considered only the case of pure MgSiO_3 with the CMB temperature fixed to a relatively high value of approximately 4,400 K. Further investigations that consider the effects of major impurity elements, in particular iron and aluminium, on the thermoelasticity of pure phases (18, 19) supply additional information on the effect of compositional variations. These results allow us to perform more realistic modeling of the CMB region.

Results and Discussion

By using thermoelastic data (15, 18), we calculated shear velocity models for nine different temperature profiles and for two different CS values: a mineral-physically acceptable value of 8 MPa/K (5) and an exaggerated value of 16 MPa/K (see *SI Text* and *Fig. S1 a and b* for details). Both of the CSs were set to pass through the point with a temperature of 2440 K and a pressure corresponding to a depth of 2,675 km to produce the pv to ppv transition at a depth comparable to that of the seismic D'' discontinuity. This point is fixed throughout the present study, since, in contrast to earlier suggestions, recent studies have consistently reported that the pv to ppv transition pressure is relatively unaffected by major impurities such as iron and aluminum (14, 20). For the case of the mineral-physically based CS, a CMB temperature of 3,500 K is too low to produce a double-crossing transition (blue dash-dotted lines in A–D of *Fig. S1b*), but for the case of the exaggerated CS, a double-crossing occurs if the CMB temperature is $>3,220$ K (dash-dotted lines in E–H of *Fig. S1b*).

The following four characteristic features in the velocity models are evident (see *Fig. S1b*). (i) The velocity at the CMB

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¹To whom correspondence should be addressed at: Institut de Physique du Globe de Paris, 4 Place Jussieu-75252, Paris Cedex 05, France. E-mail: kenji@geo.titech.ac.jp.

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Fig. 1. (A) Cross-section of the Earth. The lower mantle extends from a depth of 660 km to a depth of 2,890 km. The D'' region is the lowermost 200–300 km of the lower mantle, directly above the outer core. (B–D) Radial variations of seismic shear velocity in the lowermost mantle, obtained using several different methods. (B) An example of variations of shear velocity models at the base of the mantle in several different regions (central America, Pacific, Alaska, etc.) obtained using forward modeling of seismic waveforms (from Refs. 32–38, figure modified after ref. 9). These models are all roughly similar in that they have about a 2.5–3.0% discontinuous velocity increase at the top of D''. [Reprinted with permission from Wyssession et al. (1998) (Copyright 1998, AGU).] (C) Models obtained by double array stacking beneath the Pacific (7). The models of BIN1–3 are obtained from the data binned according to the bounce point of S_c phases at the CMB at intervals of $\approx 4^\circ$. [Reprinted with permission from Lay et al. (2006) (Copyright 2006, AAAS).] (D) Models obtained using waveform inversion which allows quantitative and objective inference of the shear velocity structure within D''. The velocity models are for Central America (10), the Arctic (11), the western Pacific (12), and Northern Asia (13). [Reprinted with permissions from: Konishi et al. (2009) (Copyright 2009, EPSL); Kawai et al. (2007) (Copyright 2007a, GRL); Kawai et al. (2007) (Copyright 2007b, GRL); and Kawai et al. (2009) (Copyright 2009, GRL).] (E–F) Crystal structures of orthorhombic pv (space group, *Pbnm*) (E) and ppv (space group, *Cmcm*) (F) (5). Here, orange spheres and blue polyhedra indicate Mg atoms and SiO₆ octahedra, respectively. While the SiO₆ octahedra share all their corners with adjacent octahedra in pv, they share the corners along the c direction but share edges along the a direction in ppv.

always becomes significantly slow if a reverse transition occurs. When the CMB temperature is $>4,000$ K, the shear wave velocity is <6.9 km/s below the double-crossing phase transition. (ii) Some velocity decreases can always be seen below the first transition even without a reverse transition. This is due to the superadiabatic temperature increase near the CMB. Thus, even without a reverse transition, a superadiabatic temperature increase produces a continuous but rapid velocity decrease whose magnitude is comparable to or even larger than the 1–2% velocity increases associated with the phase transition from pv to ppv at the top of D''. (iii) As the Fe and Al impurity content increases, the average velocity in the lowermost mantle decreases by ≈ 0.2 km/s for $\delta X = 10$ mol %, and the magnitude of the discontinuities becomes smaller, as has already been reported (17). (iv) The exaggerated CS value tends to yield a double crossing phase transition even with smaller temperature gradients.

The relative difference between T_{int} , the temperature at which the transition intersects the CMB, and T_{cmb} , the temperature at the CMB along the geotherm, is a significant parameter in controlling whether or not a double-crossing transition occurs. A double-crossing will occur if $T_{\text{int}} < T_{\text{cmb}}$ (for example, the dash-dotted red line in B of Fig. S1b), although it will not occur

if $T_{\text{cmb}} < T_{\text{int}}$ (for example, the green and blue lines in B of Fig. S1b). Hence, we consider both the cases of $T_{\text{int}} < T_{\text{cmb}}$ and $T_{\text{cmb}} < T_{\text{int}}$ by varying T_{cmb} . Also, T_{int} will vary depending on which of the two different values of CS is used. In contrast, Lay et al. (7) assumed the existence of a double-crossing phase transition and considered only the case of $T_{\text{int}} < T_{\text{cmb}}$.

The velocity contrast, Δv , between the velocity just above the phase transition from pv to ppv (i.e., just above D'') and that at the CMB is controlled by the effects of both the temperature increase across the TBL and the phase transitions (Fig. S2). The contrast can be represented as:

$$\Delta v = v(D'') - v(\text{CMB}) = \Delta v_t + \Delta v_p, \quad [1]$$

where Δv_t and Δv_p are the velocity variations caused by the temperature increase (ΔT) and the phase transition, respectively. Note that the definition used in Eq. 1 means that positive values of Δv imply slower velocities at the CMB. Note also that Δv_p can be further represented as $\Delta v_p = \Delta v_{\text{pv} \rightarrow \text{ppv}} + \Delta v_{\text{ppv} \rightarrow \text{pv}}$. Δv_p should therefore be nearly zero when a double-crossing occurs, because the positive and negative velocity jumps associated with the transitions nearly sum to zero. However, seismological observations demonstrate that the

Fig. 3. (A) The five shear wave velocity profiles from Fig. 2B. The horizontal axis indicates the thickness of the thermal boundary layer (km). The color contour indicates the average integrated temperature deviation (K) from the adiabatic temperature in the lowermost 400 km mantle (*SI Text*). The brown curve indicates the average velocity deviation (%) from the adiabatic mantle velocity model in the lowermost mantle, as shown by the scale at the right of the figure. (B) The relationship between the thickness of TBL and elapsed years computed based on a semiinfinite half-space heated by a constant CMB temperature (*SI Text*). Nominal values for the parameters are heat capacity $C_p = 1,300 \text{ J/kg/K}$, density $\rho = 5,500 \text{ kg/m}^3$ (26) and thermal conductivity $k = 10.0 \text{ W/K/m}$ (37, 38). We define the thickness of the TBL as the distance from the CMB to the point where $(T - T_{\text{adiabat}})/(T_{\text{CMB}} - T_{\text{adiabat}}) = 0.01$.

(14, 27) in the lowermost 400 km of the mantle range for the five models in Fig. 2 are shown in Fig. 3A. As noted above, the thermal effects produce a large integrated velocity deviation. The integrated velocity deviation of a temperature profile with a 400-km TBL thickness is $>3\%$. In other words, a small average temperature difference in the lowermost 400 km of the mantle can produce a significant difference in average velocity. A difference of only 200 K average integrated deviation in the lowermost mantle, for example, can cause a difference of integrated shear wave velocity deviation of as much as $\approx 2\%$ if the phase transition effects are incorporated into the temperature effect.

Even though the velocities immediately above the CMB are almost the same for the five models in Fig. 2B, there can be significant average velocity differences in D'' , which reach 4%. This indicates that a lateral temperature variation of only 200–300 K could produce considerable velocity heterogeneity in the D'' region, although 800–1,000 K variations are usually assumed to be necessary (7). Such small temperature variations could occur even on small regional scales due to, for example, subducted cold slabs or isolation from mantle convection for several hundred million years, since the thermal diffusion is

estimated to be $\approx 0.04 \text{ cm/year}$, which is much slower than the convective heat transfer inferred from the plate velocities of $\approx 5 \text{ cm/year}$ in the upper mantle (Fig. 3B and *SI Text*). However, the possibility of significant chemical heterogeneities, which might be partially responsible to the reported sharp sided boundaries at the edges of two large low shear velocity anomalies (28, 29), cannot be excluded.

Several tomographic studies (30, 31) have suggested that there are two large-scale low velocity regions in the lowermost mantle beneath the Pacific and Africa. It is controversial whether these are due to temperature variation, chemical heterogeneity or both. We suggest that these can be explained as due to Al- and Fe-rich materials such as subducted basaltic oceanic crust ($X \geq 15 \text{ mol } \%$) (Fig. S1b). Some shear velocity studies using transverse component waveforms reported that there is a 15 km-thick large velocity reduction ($\approx -4\%$) immediately above the CMB beneath the Pacific (7) (BIN1 in Fig. 1C), which is possibly related to an ultra-low velocity zone (ULVZ). A reverse transition plus temperature effects would cause a velocity reduction of $\approx -5\%$ (Fig. S1b). Therefore, the reported large velocity reduction, if substantiated by further observations could be interpreted as a double-crossing phase transition due to a local

temperature increase of a few hundred Kelvin which can be produced by the decay of radioactive elements. This additional heating is consistent with the assumption of existence of basalt in which radioactive elements are concentrated at the base of the mantle.

In conclusion, we have examined shear wave velocity models quantitatively by combining the data from state-of-the-art seismological and mineral physical studies. Although the effects of chemical heterogeneity should also be taken into account, we demonstrated that important seismological properties can be interpreted primarily as due to thermal effects. We neglected the

effects of minor minerals such as Ca-pv and ferropericlase, since no phase changes have been found in these secondary phases at the P,T conditions in D". Their effects would thus not make a significant contribution to the velocity structure in D".

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