

New insights into core–mantle boundary region and implications for Earth's internal processes

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The core–mantle boundary (CMB) region, a 200–300 km thick zone in the lowermost mantle bounded between the D'' discontinuity and CMB, plays a significant role in controlling the dynamical processes in the Earth's interior, both in the mantle and in the core as well as their interaction. Earlier, this region was considered as a thermal boundary layer and/or a compositionally distinct layer. High resolution seismological studies of this region over the past one decade coupled with new mineral physics experiments on perovskite at pressure and temperature regimes representing the lowermost mantle conditions have revealed that (i) the D'' discontinuity is a phase transition boundary between perovskite and a new post-perovskite phase, (ii) large lateral and vertical variations in shear velocity and density exist within this region, (iii) large anisotropy in the shear velocity exists indicating lateral flow within the CMB zone and vertical flow in the regions of plume upwellings, and (iv) it is possible to estimate the temperature gradients within the zone from identified paired seismic discontinuities, mainly in the regions of Mesozoic subduction. These results have important implications for estimation of the energy budget of the Earth, heat flow out of the core, and radiogenic heat contribution of the mantle leading to improved understanding of the energy available for mantle convection, core cooling and growth of the inner core, geomagnetic field generation, and core–mantle coupling.

Keywords: CMB region, core heat flux, mantle dynamics, phase transition, seismic structure.

Introduction

ON a broad scale, the Earth's internal structure is considered to be consisting of a number of layers, each having distinct compositional and mechanical properties. One of the most prominent ones is the core–mantle boundary (CMB) that separates the silicate lower mantle from the underlying iron alloy core at the depth of about 2,891 km from the Earth's surface. In early classification of the Earth's layered structure proposed by Bullen¹, the lower mantle between the 660-km phase transition boundary and the CMB was assumed to be having fairly uniform

structure and composition. However, he subsequently reclassified the lower mantle layer (D-layer) and designated the approximately 200-km-thick layer of the lower mantle just above CMB as the *D'' layer* based on the observations that the P- and S-wave velocity gradients decrease in the lowermost region of the lower mantle¹.

Over the past 60 years the understanding about the structure of the D'' layer has considerably improved owing to numerous seismological studies which have shown that this layer is highly heterogeneous in terms of thermal and compositional structure, mechanical properties, anisotropy, etc. Therefore, the region has emerged as much more complex than a simple layered structure and is referred as the CMB region² or the lowermost mantle (LMM). This zone is significant for various geodynamical studies aiming at understanding convection in the mantle and core as it forms the lower thermal boundary layer of the convecting mantle³, akin to the near-surface lithosphere acting as the upper thermal boundary layer, and controls the amount of heat entering into the mantle from the outer core. The nature of the CMB region also has significant implications for studies related to the geomagnetism, nutation of the earth and electromagnetic core–mantle coupling. Recent mineral physics experiments and advanced seismological studies have revealed many new aspects of LMM. In the present article, some of these results are briefly discussed.

Global seismological models of the lower mantle

Early global seismic tomography models based on inversion of P-wave travel time data revealed large-scale structural heterogeneities in the lower mantle correlating with the patterns of the geoid⁴. Ever since the resolution of global seismic tomography models has increased considerably due to the increase in the volume and coverage of data, usage of both P- and S-wave data, and improvements in acquisition and interpretation techniques leading to refined models of the mantle^{5–7}. The high seismic velocity zones in the lower mantle in these tomographic images showed a strong correlation with the locations of palaeo-subduction zones in the Mesozoic⁸. Further refined seismic tomography models^{9,10} revealed subduction of lithosphere, seen as dipping high seismic velocity zones, across the 660 km boundary and accumulation

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of slab material at CMB correlating with the locales of convergent margins in the Mesozoic. These results demonstrated the ability of subducting slabs to penetrate the upper mantle/lower mantle boundary, thus supporting a view that the mantle convects as a whole mantle. Another important feature observed in tomography models was that of the presence of seismically slow regions beneath the Pacific and the African hotspots related to mantle plumes^{5,10–12}. These images have significant implications for mantle dynamics.

New insights into CMB region

In recent years, a new perovskite (Pv) to post-perovskite (pPv) phase transition has been identified in the lower mantle coinciding with the D'' discontinuity¹³. In an earlier work, Sidorin *et al.*¹⁴ inferred the presence of a solid-solid phase transition with positive Clapeyron slope at the depths of the D'' discontinuity based the identification of a core diffracted phase Scd and analysis of differential travel times between this phase and the direct S phase. They converted shear wave velocity tomography image

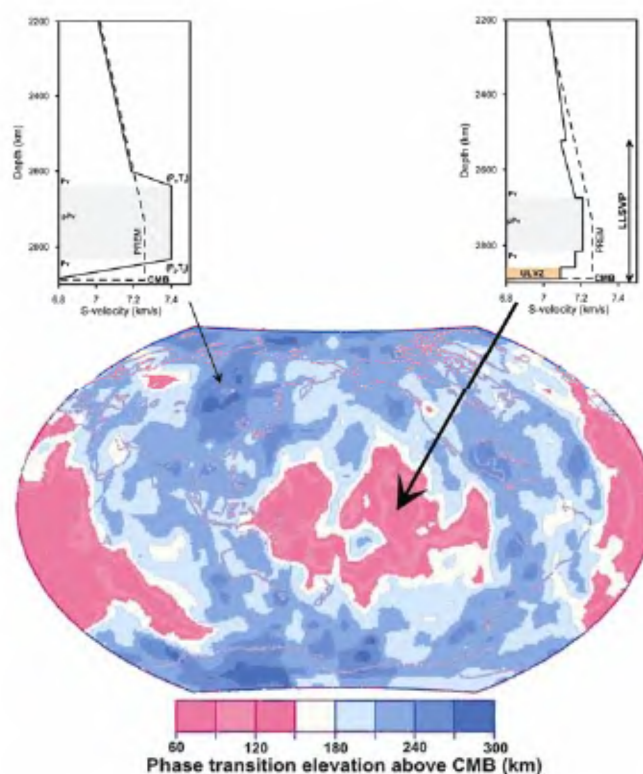


Figure 1. An image showing the elevation of the phase boundary above CMB, derived from the seismic shear wave velocity structure (from ref. 14). The phase boundary is thin in seismically slow regions (pink) of Africa and Pacific and thick in seismically fast regions (blue) of Asia and America. Superimposed are the fine-scale shear velocity structure of the lowermost mantle for two regions, one beneath NW Russia (from ref. 24) representing cold region and the other beneath central Pacific (from ref. 47) representing hot region. PREM (ref. 23) model is also shown in dashed line.

of the lower mantle¹⁰ into a map of the height of the D'' phase boundary above CMB and showed that the CMB zone is thick beneath Asia and shallow beneath Africa and Pacific (Figure 1). Existence of the Pv–pPv phase transition revealed by high pressure mineral physics experiments and identification of fine-scale structures within this layer by improved seismological techniques as well as better geographical coverage has provided necessary impetus towards development of better understanding of the mantle dynamics and core processes. In this article, we briefly describe these new results and their implications for the dynamics of the deep Earth. A recent review on the structure of the CMB region may be found in Lay¹⁵. Earlier work on this topic may be found in refs 2, 16–18.

Experimental results on Pv to pPv transition

The first experimental confirmation of the anticipated phase transition¹⁴ was reported by Murakami *et al.*¹³ who performed *in situ* X-ray diffraction analysis of pure MgSiO₃ composition up to 134 GPa and 2600 K in a diamond anvil cell to cover the P–T conditions in the CMB region. They observed transformation of perovskite to a new post-perovskite phase above 125 GPa pressure and 2500 K temperature. This pressure corresponds to the depth about 200 km above CMB. The phase transition has associated density increase of 1.0–1.2%. The experimental observation of this pPv phase change provides a thermometer indicating the absolute temperature of LMM about 200–300 km above CMB. Subsequent studies put the transition boundary at 119 GPa and 2400 K (ref. 19). A natural outcome of these experiments was an estimate of the Clapeyron slope which is helpful in constraining the temperature at CMB. There are some discrepancies between the estimates obtained by Au and MgO scales, Au scales yielding lower estimates of the Clapeyron slope. These estimates vary between +6.0 and +13.3 MPa/K; +6.0 being by seismological studies¹⁴, +7.5 by theoretical *ab initio* calculations²⁰, and +7.0 (ref. 21) and +11.5 (ref. 19) by experimental studies. Recent studies on Pv to pPv transition in the temperature range 1640–4380 K and pressure range 119–171 GPa show a considerably high Clapeyron slope $+13.3 \pm 1.0$ MPa/K (ref. 22). Figure 2 shows the results of some of these experiments and the Clapeyron slopes.

Seismological characteristics of the CMB region

The top of the CMB region is marked by an increase of P- and S-wave velocities. The increase in the S-wave velocity is about 1.5–3% and in P-wave velocity of about 0.5–1.0% (ref. 15). This boundary is considered to be associated with the Pv to pPv phase transition. Earlier image of large wavelength features, dominated by degree 2 and 3 spherical harmonic components, of high and low

seismic velocity regions in LMM has been greatly refined in the recent years mainly with the use of differential time of seismic phases scanning this region and those that reflect from CMB or graze it. A number of studies carried out to illuminate the CMB region have brought out a highly heterogeneous, both vertically and laterally, and anisotropic nature of LMM^{2,15–18}. Recent studies have delineated the existence of paired seismic discontinuities mainly in the regions of palaeo-subducted slabs, ultra-low seismic velocity zones just above CMB, large low shear velocity provinces having shear velocity lower than PREM²³ values, strong seismic anisotropy, and dense material at CMB in the regions of low seismic velocity (Figure 1).

Paired seismic discontinuities: The heterogeneous nature of the CMB region, akin to the lithospheric heterogeneities, prompted studies to resolve fine-scale structures within this region. Thomas *et al.*²⁴ studied fine structure of the CMB region beneath northwestern Russia, where large-scale high velocity CMB region has been linked to the accumulation of cold subducted slabs, using seismic migration of shear waves. They found a sharp increase in seismic velocity 206–312 km above CMB followed by a sharp velocity decrease 55–85 km above CMB (Figure 1). Seismic migration studies of D'' beneath the Cocos region also indicated the existence of a similar shear wave velocity pair²⁵. These seismic discontinuity pairs have significant implications for constraining the thermal structure of LMM and CMB when analysed along with the experimental results on Pv–pPv transition. A ‘double-crossing’ model was proposed which accounts for transformation of Pv to pPv at D'' discontinuity and then transformation back of pPv to Pv at deeper levels when the thermal gradient were larger than the Clapeyron slope²⁶. The second transformation results in a decrease in the

shear wave velocity. Thus, paired seismic discontinuities in association with the ‘double-crossing’ model can provide two tie points for the temperature (Figure 3) and thus a tight constraint on the thermal gradient in the CMB region. These paired discontinuities are expected to occur in thermally cold regions than in hot regions because of the large temperature gradients in the former region.

Ultra-low velocity zones: Another important inference about the CMB region is the presence of thin, up to 40 km thick, ultra-low velocity zones (ULVZ) just above CMB in which the S-wave velocity drops by about 30% and the P-wave velocity reduces by 10% (refs 27, 28). This layer lies below a zone of large-scale low seismic velocities (Figure 1) referred as large-scale low shear velocity province (LLSVP). A factor of 3 larger decrease in the S-velocity compared to the P-velocity has been attributed to various mechanisms such as partial melting of lower mantle, lateral infiltration of core material, subduction and segregation of late Archaean banded-iron formations, Fe-rich forms of pPv, and the mushy residuum of a fractionally crystallized primordial dense melt layer²⁹. It is inferred that ULVZ in LLSVP may be a MORB-rich dense material³⁰.

Seismic anisotropy: The CMB region is also characterized by the presence of significant anisotropy reflected in the horizontally polarized (SH) and vertically polarized (SV) components of shear waves. The regions of north Pacific, Alaska, Cocos, north-west Asia and northern Indian Ocean show the presence of strong anisotropy whereas weak anisotropy is inferred for the southern Pacific and central Atlantic¹⁵. In most regions, the SH polarized wave travels about 1–3% faster than the SV polarized wave. The observations on shear wave splitting have important implications for the flow in the CMB region, this being a source region for mantle plumes and a repository for subducting slabs. Faster velocity of the SH component coinciding with the horizontal flow at the boundary layer

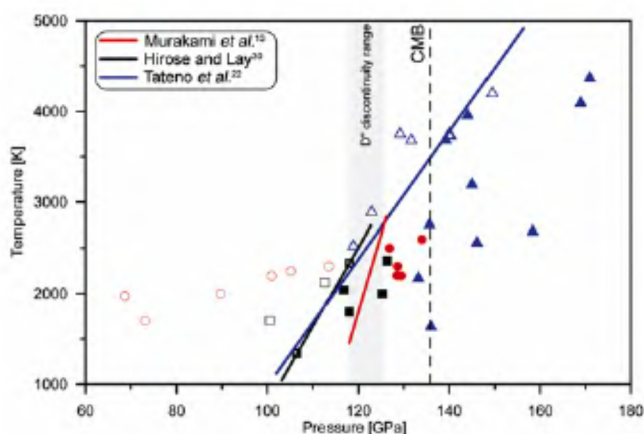


Figure 2. Experimental results by Murakami *et al.*¹³, Hirose and Lay³⁰ and Tateno *et al.*²² on perovskite (Pv) to post-perovskite (pPv) phase transition. Open and filled symbols show Pv and pPv phase respectively. Clapeyron slopes reported in these studies are shown by solid lines. Black line is the Clapeyron slope obtained by Sidorin *et al.*¹⁴ and used by Mukarami *et al.*¹³ in their results.

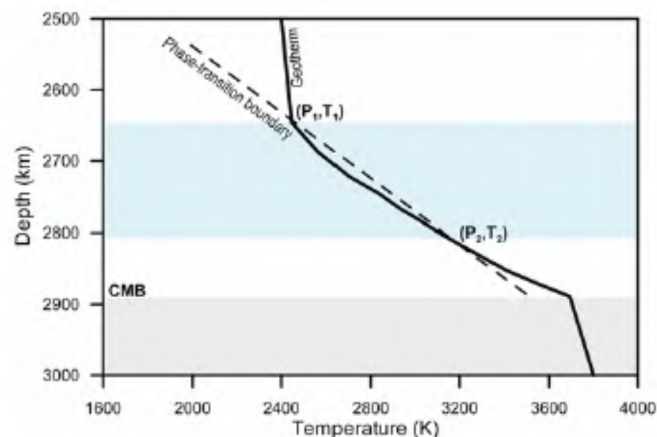


Figure 3. Use of paired seismic discontinuities to estimate geothermal gradient within the CMB region (modified after Tateno *et al.*²²).

provides information on the rheological property of the medium. Experimental studies have also shown formation of platy crystals of post-perovskite¹³, supporting the anisotropic nature of the pPv phase.

Implications for deep earth dynamics

The thermal structure in the CMB region has profound implications for the temperature and dynamics of the core and the lower mantle.

Mantle dynamics

The net rate of heat loss from the surface of the Earth is linked to the heat released by the solidification of the inner core, secular cooling of Earth, heat generated by the radiogenic elements in the mantle and crust, and possibly in the core. However, estimates of the present day surface heat flow are obtained mainly from the temperature gradients measured in shallow boreholes and from the estimates of the convective heat loss at mid-oceanic ridges. In the mantle, the information about the thermal structure becomes uncertain. Two major phase boundaries in the mantle, the olivine to wadsleyite exothermic phase boundary at 410 km depth and the wadsleyite/ringwoodite to perovskite + magnesiowuestite endothermic phase boundary at 660 km depth, provide two reference points for constraining the temperature at these depths as these phase changes occur in a specific pressure–temperature regime. Extrapolation of temperature along the adiabat constrained by these reference points across the lower mantle and up to CMB is expected to yield erroneous values in the CMB region as temperature becomes non-adiabatic in the boundary layer.

The identification of the Pv to nPv phase transition at about 120 GPa pressure and 2400 K (ref. 13) temperature and its correlation with the D'' discontinuity above the CMB has added another reference point for constraining the thermal structure of the mantle. Thus, the seismic images of the D'' discontinuity can provide useful constraints for the heat entering into the lower mantle from the boundary layer. Nevertheless some uncertainty exists about the P–T estimates for the Pv–pPv phase transition depending on the likely mineralogy of the rocks and calibration scales used to analyse data²². Another new insight into the structure of the D'' region gained by seismological experiments^{24,25} is the presence of paired seismic discontinuities in the CMB region. This pattern is mainly observed in cold regions of the LMM and has been associated with transformation of Pv to pPv at the upper surface and back to Pv at the lower surface. Such a scenario is possible when the temperature gradient is larger than the Clapeyron slope of the phase transition such that the temperature crosses the Clapeyron boundary two times. This observation provides two reference points within the

CMB region as the constraints for the thermal structure of this region and it is possible to tightly constrain the temperature gradient within the CMB region and thus the temperature at CMB.

An important consequence of constraining the estimates of the temperature at CMB is an improved estimation of the heat transport from the core into the mantle and thus a better understanding of the energy available to drive mantle convection. Diverse approaches have been pursued to estimate the total heat flux at CMB. Early estimates gave values in the range 3–13 TW based on thermal evolution and mantle convection models^{3,31,32}. The thermal gradients obtained through the correlation of paired seismic discontinuities with the phase transition results yield local heat flux at CMB of 85 ± 25 mW/m² for central Pacific and 35–70 mW/m² under the Caribbean, leading to an estimate of 7–15 TW for the total heat flux from CMB²⁹. The estimate of the CMB heat flux is also useful in estimating the contribution of the radiogenic elements in the mantle to the total heat budget as improved estimates of the surface heat flux are available.

Besides thermal constraints, these seismic studies also yield information about the compositional and rheological changes in the CMB region affecting the nature of the mantle convection. The likely presence of high density material in ULVZ just above CMB in thermally hot regions of central Pacific and Africa would affect the nature of plume upwellings. The difference in the rheological properties of Pv and pPv would also influence the mantle dynamics. There are indications that the pPv deforms by dislocation creep and has lower viscosity than the Pv which most likely deforms by diffusion creep^{33–35}. There are certain indications that the yield strength difference between Pv and pPv may be as high as 2–3 orders of magnitude³⁶ leading to large viscosity contrasts within the CMB region.

Core dynamics

The estimation of heat flux in the LMM by recent seismological and mineral physics studies has implications also for the dynamics and evolution of the core. The fluid outer core convects on a short time scale, of a few thousand years over-turn time, compared to the mantle over-turn time of several million years and is considered as the source region for the generation of the geomagnetic field through a dynamo mechanism. The convection in the fluid core depends on the ability of the mantle to remove heat from CMB. Thus, the mantle heat flow can also be linked to the geomagnetic field. Large lateral variations in the structure of the CMB region impose non-uniform heat flux conditions on the core. For example, the cold regions of the LMM consisting of subducted slabs impose large heat flux and the hot regions related to source regions of mantle plumes have low heat flux. Large-scale

features imaged in the lower mantle by seismic tomography provide quantitative estimates of the large lateral variations in the heat flux at CMB through an empirical relation between seismic velocity and temperature. Recent seismic migration studies give well-constrained heat flux values in these regions. Therefore, better estimates of CMB heat flux and its lateral variation are now available.

Convection in the fluid core is driven by thermal and compositional sources of buoyancy, and the Coriolis force due to the rotation of the planet. The heat is released by secular cooling and growth of the inner core and the compositional buoyancy arises due to the expulsion of light density elements into the fluid core at the solidification front separating the inner core from the outer core^{37,38}. A significant fraction of the released heat is conducted towards CMB along the adiabat as a result of high thermal conductivity of liquid iron alloy³⁹. Therefore, the amount of heat available to drive convection in the liquid core is controlled by the heat flux in the CMB region. For cases where the heat flux in the CMB region is smaller than the conductive heat flux from the core a thermally stably stratified boundary layer may form at the top of the core⁴⁰ in which convection may be driven by compositional buoyancy, strength of which depends on the total CMB heat flux rather than on the super-adiabatic heat flux⁴¹. It is estimated that the total adiabatic heat flux at CMB could be 5–8 TW (ref. 42). However, owing to uncertainties in the thermal conductivity values this estimate remains largely uncertain. Recent estimates of thermal conductivity suggest an adiabatic heat flow closer to 3–4 TW (ref. 43). Comparing these values with the recent estimates of the heat flux in the LMM can help in understanding the nature of the outermost core, e.g. whether the whole of the fluid core is convecting in super-adiabatic state or it has stable thermal and/or compositional layering at the top of the core. A laterally heterogeneous LMM may support a scenario in which some regions of the outermost core below the regions of mantle plumes may have stable stratification and support accumulation of light density elements in these regions whereas the regions falling below subducted slabs may have more vigorous convection.

Another approach to constrain the CMB heat flux could be to delineate the structure of the outermost core near CMB by seismological techniques. Some seismological studies support the presence of a thin anomalous seismic velocity structure in this region but infer low velocity⁴⁴ and high velocity⁴⁵. Geomagnetic constraints suggest that any stratified layer is less than 100 km thick⁴⁶.

Conclusions

The core–mantle boundary region, bounded between the D'' discontinuity and CMB, has emerged as a highly

complex zone consisting of large-scale thermal and compositional heterogeneities. These heterogeneities correlate well with the probable locations of palaeo-subduction and super-plumes. Seismic migration studies have revealed further fine-scale features within this zone such as the presence of ULVZ and paired seismic discontinuities. These observations together with new insights from mineral physics experiments on phase transition of perovskite have shown that the D'' discontinuity may be a phase boundary and that the temperature at the top of the CMB region may be well constrained thus providing the likely estimates of the temperature gradient within the CMB region and the temperature at CMB. These new results are significant in improving our understanding of the dynamics of the mantle and the core, and also of the coupled core–mantle interactions.

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ACKNOWLEDGEMENTS. I am grateful to Dr R. N. Singh for valuable comments on the manuscript and to Dr C. P. Rajendran for his encouragement and support. A part of the article was prepared at the Max-Planck Institute for Solar System Research, Germany. The permission by the Director, NGRI, to publish this work is gratefully acknowledged.