

Tenth anniversary: New insights in deep mantle structure and dynamics

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The post-perovskite phase transition

In 2004 two major breakthroughs impacted the fields of deep Earth mineralogy, structure and dynamics. On May 7, Science published the first report that the Earth's most abundant mineral, Mg-perovskite (pv) undergoes a pressure-induced phase transition to post-perovskite (ppv) at the pressure-temperature conditions of the D'' region of the lowermost mantle (Murakami et al. 2004, Science). The discovery was long overdue, since seismologists had recorded discontinuities within the D'' more than twenty years earlier (e.g. Lay and Helmberger 1983, Geophys. J. Roy. Astron. Soc.) and predicted a phase transition with a large positive Clapeyron slope (dp/dT -slope, Sidorin et al. 1999, Science 286, 1326). The large Clapeyron slope is due to a minor decreases in volume and a large decrease in entropy across the pv- to ppv-transition. The simplified crystal structures are shown in Fig. 1. Deep Earth mineralogists had missed the opportunity to discover the pv-ppv transition earlier by largely ignoring the seismic evidence. We had the capability to discover and investigate the pv-ppv transition at low to moderate pressure, using analogue systems, even in the 1980s and 1990s. Although the 2004-discovery was accidental and unplanned, it greatly stimulated cross-disciplinary research in mineralogy and mineral physics, seismology and geodynamics. The articles by Murakami et al. (2004) and Ono et al. (2004, Nature) have accumulated 820 and 630 citations during the last ten years.

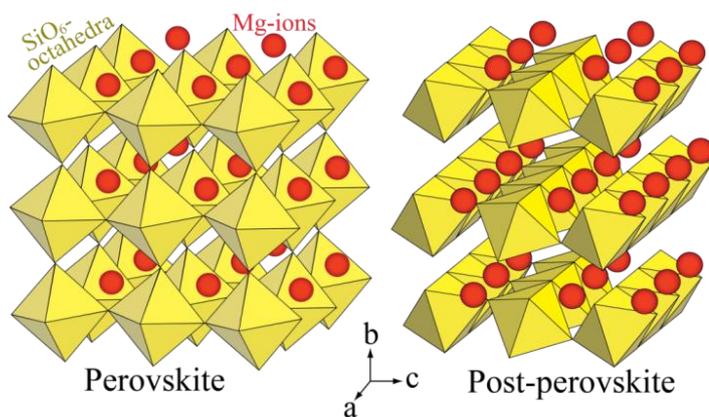


Figure 1. Schematic representation of the crystal structures. The SiO_6 -octahedra are corner-linked in all three crystallographic directions in pv. In ppv they are edge-linked along the a-direction and form a rigid sheet-like structure in the ac-plane. These contrasting features result in thermo-physical properties that are important for the dynamics and structure of the lowermost mantle. The seismic anisotropy in the D''-zone may also be related to the crystal structure of ppv.

Lowermost mantle structure, large igneous provinces and kimberlites

Another leap in our perception of the dynamics of the lowermost mantle was brought about by an article published in late 2004. Burke and Torsvik (2004, Earth Planet. Sci. Lett.) restored the eruption sites of Mesozoic and Neogene Large Igneous Provinces (LIPs) in a paleogeographic reference frame and discovered that they are overwhelmingly close to the surface projections of the margins of two present-day antipodal Large Low Shear-wave Velocity Provinces (LLSVPs, Fig. 2). This was the first in a series of articles documenting the long-term stability of the African and Pacific LLSVPs in the D'' zone and the development of large buoyant plume heads at their margins. In the subsequent articles, Torsvik and collaborators refined and corroborated the pattern of plume generation zones, which are also the locations of maximum lateral S-wave gradients within the D'' zone. This would imply that the LLSVPs must have been relatively stable through the last 300 Ma, and possibly much longer (also Dziewonski et al. 2011, Earth Planet. Sci. Lett.). As demonstrated by Steinberger and Torsvik (2010, Geochim. Geophys. Geosyst.) the configuration of two antipodal LLSVPs at near-equatorial positions with hot ascending mantle and residual geoid highs above will be stabilized by the Earth's rotation. The other important mass contribution to Earth's rotational balance is the dense subducted slab material in the upper mantle and transition zone.

Currently, the Torsvik group explores the potential of LLSVPs as a reference frame for plate tectonic reconstructions beyond 300 Ma. The premise is that the majority of LIPs and kimberlites (Torsvik et al. 2010, Nature) are initiated at the LLSVP margins. Paleomagnetically determined latitudes (in the low- to mid-latitude

range) for such rocks can be matched with one of up to four alternative longitudinal positions, corresponding to the east and west margins of the two LLSVPs. Based on reasonable upper limits for plate velocities, combined with geographic and geologic constraints, i.e. a consistent evolution of the "plate mosaic", only one of the alternative longitude positions will generally be an acceptable choice. Multiple iterations and re-fitting can then improve the plate reconstructions,

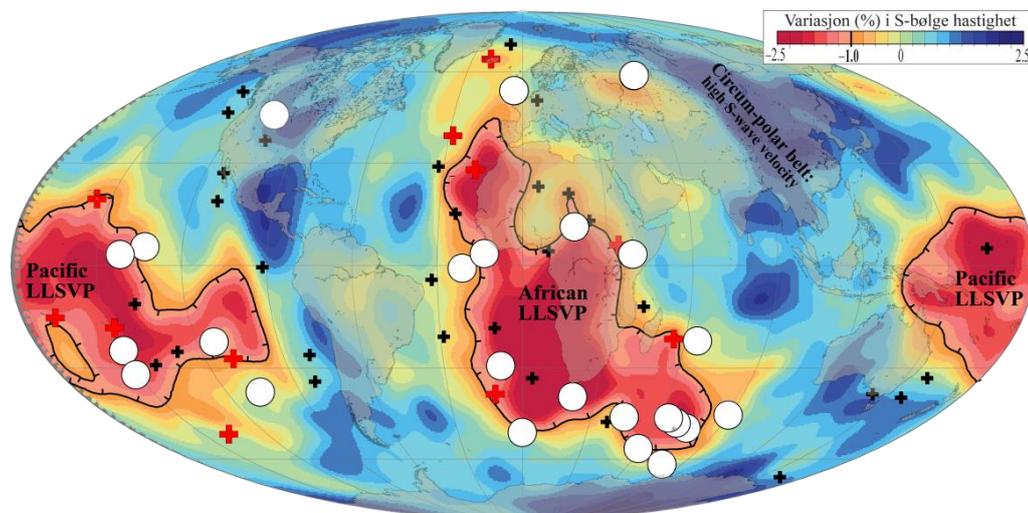


Figure 2. S-wave velocity map of the lowermost mantle (the SMEAN model). Black solid line with cross-bars represent the -1% contour. Reconstructed positions (eruption sites) of large igneous provinces covering the 16-297 Ma time span (white circles) and present-day plumes that have been imaged seismically through the lower mantle (red crosses, Montelli et al. 2006, GGG) lie close to the surface projections of the LLSVPs. Other plumes (black crosses) are also shown. The circumpolar belt with high S-wave velocities is positioned between the two antipodal LLSVP (adapted from Trønnes and Torsvik, 2011, Nature).

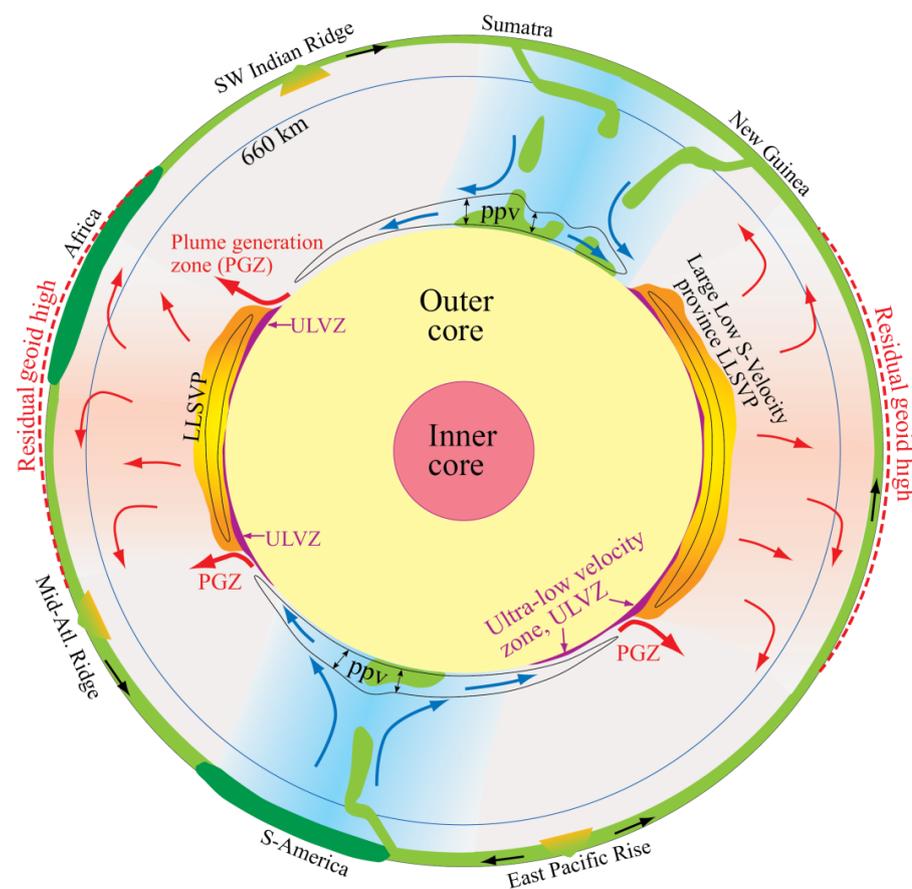


Figure 3. Approximate equatorial section through the Earth with the large-scale mantle flow. The margins of the two antipodal Large Low Shear-Velocity Provinces (LLSVPs) under Africa and the Pacific are favourable locations for the episodic initiation of large thermal upwellings (mantle plumes). The dense and hot LLSVPs with overlying geoid highs are stabilized in an antipodal configuration by the Earth's rotation. Dark and light green lithosphere is continental and oceanic, respectively. The main mantle circulation is shown by sinking regions of Mesozoic to present subduction (a broad circumpolar belt through South- and North America, the North pole, the east Asia, Australia and the and the South pole). Counterflow of hot, ascending mantle occurs above the LLSVPs. Modified from Trønnes (2010, Mineral. Petrol.).

LLSVP structure, materials and origin

The two antipodal LLSVPs are separated by a circumpolar belt of high V_s running beneath east Asia, Australia, Antarctica, South- Central- and North-America and the Arctic, where cool ambient mantle mixed with former slab material sinks (Fig. 2-3). This circumpolar belt with descending cold mantle coincides with a residual geoid low, whereas geoid highs above the two LLSVPs are caused by slow and pervasive ascent of hot and light mantle. To prevent disruption by thermal buoyancy, the LLSVP material must have a density excess of 2-3% relative to the ambient peridotitic mantle. Relatively steep and sharp margins of the LLSVPs might also indicate that the material has elevated bulk modulus (incompressibility).

Basaltic or picritic lithologies, representing subducted oceanic crust, have higher density and bulk modulus than peridotite and might be mechanically separated from slab material and accreted to the LLSVP margins in the plume generation zones. The sinking flow of cold mantle with subducted lithosphere in the circumpolar low- V_s belt must be diverted laterally along core-mantle boundary (CMB) towards the LLSVP margins. The conductive heat flow from the outer core will efficiently heat the material flowing laterally, lowering its viscosity. In the plume generation zones along the LLSVP margins the separation of dense basaltic material from the subducted lithosphere may therefore be more feasible than anywhere else in the mantle (Trønnes, 2010, Mineral. Petrol).

Alternative candidates for dense LLSVP-material are late-stage cumulates and/or solidified melts of Fe-rich peridotitic compositions. Recent studies (Nomura et al. 2011, 2014, Nature; Andraut et al. 2013, Nature) have provided evidence that the Fe/Mg-ratio of peridotitic melts are 2-5 times higher than the coexisting solid residue, even at the pressures of the lower mantle. An experimentally based thermodynamic model of the eutectic melt compositions in the system MgO-SiO₂ predicts that melts in equilibrium with peridotite of bulk silicate Earth (BSE) composition will be slightly more magnesian than BSE (Liebske and Frost, 2012, Earth Planet. Sci. Lett.). This is also supported by a first principles molecular dynamics simulation (Fig. 4).

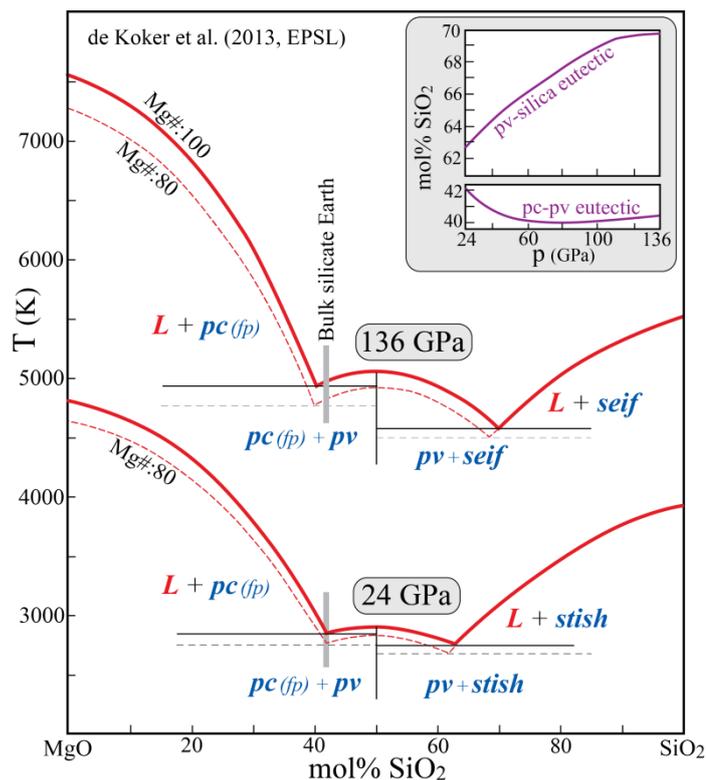


Figure 4. Melting phase relations in the system MS from de Koker et al (2013). The melting curve depression for an Mg# of 80 [= 100Mg/(Mg+Fe)] is derived from experimental partitioning data (Trønnes and Frost, 2002).

During advanced fractional crystallization, the melt, as well as the cumulate minerals Mg-perovskite (pv) and ferropericlasite (fp), become progressively enriched in Fe. Late-stage melts and cumulates have probably also slightly higher (MgO+FeO)/SiO₂ ratios (and higher fp/pv ratios) than BSE. The magma ocean crystallization might have started at some level above the CMB if the cooling melt adiabats are sub-parallel to the liquidus curve (convex towards the melt) at a mid- to deep-mantle level (Stixrude et al. 2009, Earth Planet. Sci. Lett.). Such a scenario with the first intersection of adiabats and the liquidus above the CMB, with a neutral buoyancy level between Mg-perovskite and coexisting melt, would result in an upper magma ocean crystallizing upwards from

the bottom and a lower magma ocean crystallizing downwards from the top. Late-stage dense residual melts and associated Fe-rich pv-fp-cumulates would then form near the CMB and in the upper part of the lower mantle, before the crystallization proceeded to the transition zone (above 700-600 km depth). Even if the magma ocean adiabat initially intersected the peridotite liquidus at the CMB (with the initial crystallization proceeding upwards from the CMB), the scenario with separate lower and upper magma oceans might develop as a result of dense residual melt evolution and downwards melt percolation after the attainment of a significant crystal fraction (e.g. 20-50% of the entire mantle). In either case, the dense pv-fp-cumulate sequence near the top of the lower mantle might become dynamically unstable and start to sink towards the CMB, even before the solidification of the transition zone (TZ) and upper mantle (UM) is complete.

Because the dT/dp -slopes of the peridotite liquidus and solidus steepen markedly in the p -range of the uppermost lower mantle (24-40 GPa, Fig. 5), the TZ and UM will remain mostly molten until the lower mantle is completely solidified. Neutral buoyancy levels for olivine-melt and garnet-melt at about 300 km (10 GPa) and 580 km (20 GPa), respectively, would affect the solidification and fractionation in the UM and TZ depth range (Agee and Walker, 1993, *Earth Planet. Sci. Lett*; Agee, 1998, *Phys. Earth Planet. Int.*; Elkins-Tanton, 2003, *Meteor. Planet. Sci.*). Initial olivine and garnet crystallization and accumulation in the 200-400 km and 500-600 km depth ranges are likely, followed by final accumulation of residual melts within the 400-450 km range (the melt accumulation zone, Lee et al. 2010, *Nature*). The late-stage crystallization products in the latter region could also have sunk to CMB after some cooling and thermal equilibration.

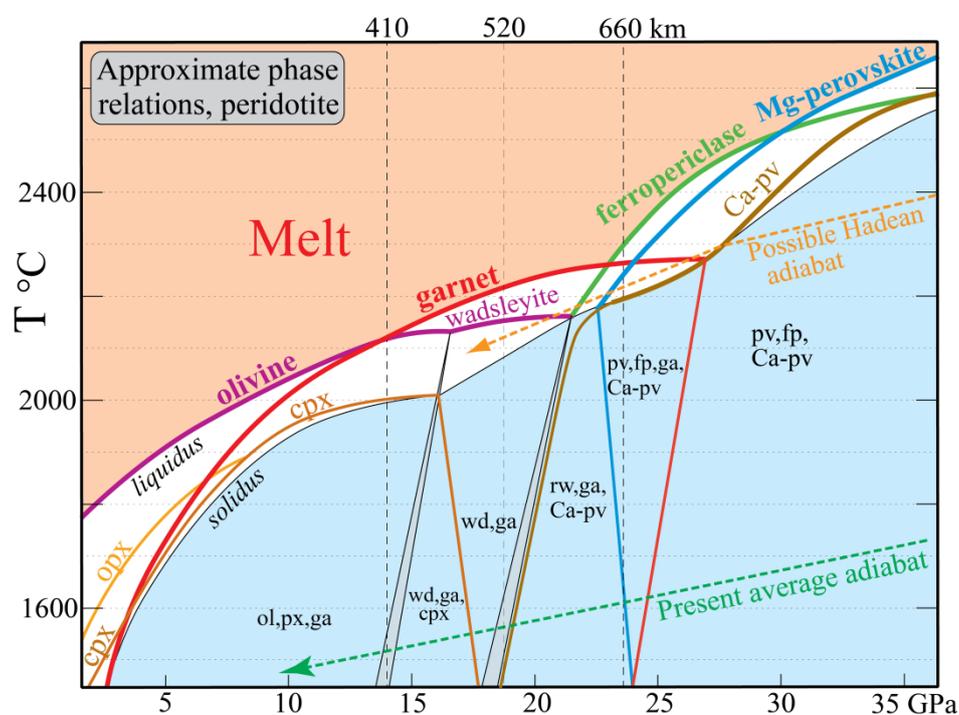


Figure 5. Melting and subsolidus phase relations of peridotite (KLB1 and pyrolite composition), mainly from Zhang and Herzberg (1994, *J. Geophys. Res.*), Trønnes and Frost (2002, *Earth Planet. Sci. Lett.*) and Ito et al. (2004, *Phys. Earth Planet. Int.*).

After the magma ocean solidification strong convective flow, driven by gravitational instabilities, including the sinking of dense cumulates from the TZ, would also lead to deep melting in hot rising plumes. Such melts, formed at a range of depths in the LM, TZ and UM would also accumulate at 400-450 km depth, below the stability range of olivine. After solidification and thermal equilibration, such melt material could sink to the CMB and possibly contribute to the LLSVP-material.

In an ordinary peridotitic mantle with low Fe/Mg-ratio, the stability range of post-perovskite (ppv) in terms of depth (pressure) is widest in the cold regions of the D" zone. The large positive dp/dT -slope of the pv- to ppv-transition, combined with the large thermal gradient from about 4000 K in the outermost core (at the CMB) to 2500 K about 300 km above the CMB, give rise to a scenario with "double-crossing" of the phase boundary with re-stabilization of pv in the lowermost D"-zone (Hernlund et al. 2005, *Nature*). The S-wave model presented by Lay et al. (2006, *Science*) includes a 250 km thick ppv lens in the northeastern region of the Pacific LLSVP (about 1000 km SSE of Hawaii), thinning rapidly towards the LLSVP margin. This seismological interpretation

seemed to be consistent with early experimental results (e.g. Mao et al. 2004, PNAS; Auzende et al. 2006, EPSL), indicating that iron partitions from pv to ppv. More recent experimental studies on Al-bearing compositions, however, have indicated that iron partitions in the opposite direction (Catalli et al. 2009, Nature; Andraut et al. 2010, EPSL; Sinmyo et al. 2011, JGR). Ongoing ab initio molecular dynamics computations on compositions along the MgSiO₃-FeSiO₃ and MgSiO₃-FeAlO₃ joins indicate that the components FeSiO₃ and FeAlO₃ partition in opposite directions toward ppv and pv, respectively (Mohn and Trønnes, 2014, Abstr. ppv@10-mtg, Bristol). These findings resolve the contradictory experimental results and may support the S-wave model of Lay et al. (2006, Science) for the northeastern part of the Pacific LLSVP.

The implications of LLSVP-material composed mostly of Fe-rich peridotites generated from the late stage crystallization of the last Hadean magma ocean or from partial melts formed during deep melting in hot Hadean plumes may be that the present D"-zone structure stabilized by the Earth's rotation might have prevailed for more than 4 Ga. Such an old structure might have controlled or modulated the mantle convection pattern and thereby Earth's evolution. The degree-2 structure of the lowermost mantle that seems to have remained mostly unchanged during the last 300 Ma can possibly be used as a global reference frame for paleogeographic and geological reconstructions for considerably longer periods, e.g. throughout the Phanerozoic. Developing tighter constraints on the LLSVP materials and structure and further evaluation and testing of the LLSVP reference frame are high priority research goals, within CEED and in the international community.