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Thermal and compositional anomalies in a detailed xenolith-based lithospheric mantle profile of the Siberian craton and the origin of seismic midlithosphere discontinuities

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ABSTRACT

The fine structure and thermal state of >200-km-thick cratonic lithosphere remain poorly explored because of insufficient sampling and uncertainties in pressure (*P*) and temperature (*T*) estimates. We report exceptionally detailed thermal and compositional profiles of the continental lithospheric mantle (CLM) in the Siberian craton based on petrographic, *in situ* chemical, and *P-T* data for 92 new garnet peridotite xenoliths from the Udachnaya kimberlite, as well as literature data. The thermal profile is complex, with samples indicating model conductive geotherms between 40 and 35 mW/m² at ~55–130 km, colder (35 mW/m² geotherm) mantle from 140 to 190 km, and hotter layers at the CLM base (190–230 km) and at ~135 km. The latter, previously unidentified, anomalous midlithospheric horizon has rocks up to 150 °C hotter than the 35 mW/m² geotherm, that are rich in garnet and clinopyroxene, have low Mg#, and have melt-equilibrated rare earth element patterns. We posit that this horizon formed in a depth range where ascending melts stall (e.g., via loss of volatiles and redox change), heat wall-rock harzburgites, and transform them to lherzolites or wehrlites. This may explain some seismic midlithosphere discontinuities (MLDs) in cratons. By contrast, we found no rocks rich in metasomatic volatile-rich amphibole, phlogopite, or carbonate matching the MLD, nor layers composed of peridotites with distinct melt-extraction degrees. The CLM below 190 km contains both coarse and variably deformed rocks heated and reworked (Mg#$_{Ol}$ down to 0.86) by localized lithosphere-asthenosphere interaction.

INTRODUCTION

Cratons comprise the oldest and thickest sections of the continental lithospheric mantle (CLM). The unique tools used to explore it are seismic data and studies of xenoliths in volcanic rocks (e.g., Carlson et al., 2005). Seismic data define intermittent layering in CLM velocity profiles at 60–160 km depth known as midlithospheric discontinuities (MLDs; Rader et al., 2015; Krueger et al., 2021). Their nature, attributed to various physical or petrologic factors, remains elusive, but it can be better elucidated using more detailed xenolith-based CLM profiles than those reported so far by combining petrographic, chemical, and robust pressure (*P*) and temperature (*T*) data.

Literature *P-T* and compositional data for CLM in the central Siberian craton are contradictory. For instance, Boyd (1984) inferred a 40 mW/m² geotherm (Pollack and Chapman, 1977) without substantial inflections, while Doucet et al. (2013) outlined a colder geotherm, and Goncharov et al. (2012) found scattered *P-T* values for coarse peridotites in the 3.5–5.5 GPa range. Modal and chemical variations with depth inferred from garnet extracted from kimberlites (Griffin et al., 1999) are at odds with xenolith data (Ionov et al., 2010).

We report the petrography, chemical compositions of minerals, and *P-T* estimates for 92 new garnet peridotite xenoliths from the Udachnaya kimberlite and combine this data set with recalculated *P-T* estimates for 73 samples from literature to robustly establish thermal, petrographic, and chemical variations in a Siberian CLM profile.

SAMPLES AND METHODS

The samples are from the ca. 360 Ma Udachnaya-East kimberlite near the center of the Siberian craton (Fig. 1). They were collected together with xenoliths reported in previous publications focused on bulk-rock studies (Doucet et al., 2013; Ionov et al., 2010, 2017, 2020), but they are smaller (5–15 cm). We selected 92 xenoliths (listed in the Supplemental Material[1]) for chemical and *P-T* studies based on low alteration and the presence of garnet. The large number and unbiased selection of garnet peridotites suggest that the suite may contain all essential types of such rocks, and provide robust constraints on their relative proportions in a complete and detailed CLM profile.

Minerals were analyzed in polished grain mounts by electron probe microanalysis (EPMA) and laser-ablation–inductively coupled plasma–mass spectrometry (LA-ICP-MS) at conditions adapted to improve detection limits and accuracy for elements critical for *P-T*

[1]Supplemental Material. Methods, data and supplemental figures. Please visit https://doi.org/10.1130/GEOL.S.19579447 to access the supplemental material, and contact editing@geosociety.org with any questions.

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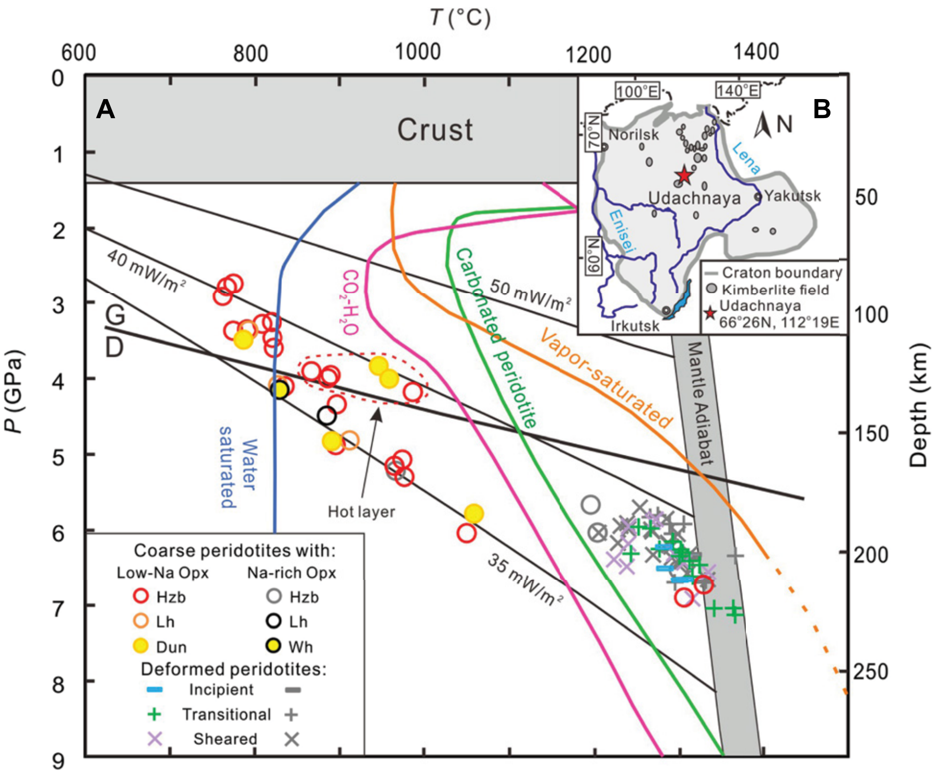

Figure 1. (A) Pressure-temperature (*P-T*) and rock type profile (Hzb—harzburgite; Lh—lherzolite; Dun—dunite; Wh—wehrlite; Opx—orthopyroxene) beneath Udachnaya (Siberia) at 360 Ma. Also shown are model conductive geotherms (Hasterok and Chapman, 2011), graphite-diamond (G/D) transition (Holland and Powell, 1998), mantle adiabats, and solidi of dry (Dasgupta et al., 2013) and hydrous carbonated peridotites (Wallace and Green, 1988; Foley et al., 2009). (B) Udachnaya and kimberlite fields on the Siberian craton.

estimates (see the Supplemental Material for details). Modal compositions were obtained from area proportions of minerals in thin sections (see the Supplemental Material) for 46 samples or estimated visually. *P-T* values for new and literature samples (see the Supplemental Material) were primarily obtained by a combination of the two-pyroxene thermometer of Taylor (1998) (T_{TA98}) and the Al-in-Opx barometer of Nickel and Green (1985) (P_{NG85}). This combination yields robust estimates for common cratonic peridotites containing orthopyroxene (opx) with moderate Na_2O (Nimis and Grütter, 2010). Other methods were used to validate the *P-T* estimates and to identify inconsistent results, which could indicate disequilibrium or excessive contents of minor elements (see the Supplemental Material); in particular, for high-*T* (≥1200 °C) xenoliths with Na-rich opx, which required a pressure correction (Fig. S1 in the Supplemental Material). All data are given in the Supplemental tables.

RESULTS

Our new samples included 76 harzburgites (<5% clinopyroxene [cpx]), 10 lherzolites, 5 dunites, and 1 wehrlite (see the Supplemental Material). In terms of texture (Fig. S2), 58 xenoliths were coarse, 12 showed incipient deformation at olivine grain boundaries, 16 were transitional (minor neoblasts), and 6 were sheared (dominant neoblasts) (Ionov et al., 2010). While our data confirm that the great majority of coarse Udachnaya peridotites are harzburgites or lherzolites, which are low in clinopyroxene (cpx ≤ 6%) and garnet (e.g., Doucet et al., 2013), we also identified a previously unreported group ranging from garnet- and/or cpx-rich lherzolites to wehrlite (Figs. S3A and S4). Six samples contained accessory (<1%–3%) interstitial phlogopite. Similar to previous studies, no peridotites with more significant amounts of mica or amphibole were found.

The EPMA results, including robust data from the literature, and the *P-T* estimates are given in the Supplemental Material. The median olivine Mg# [$Mg\#_{ol} = Mg/(Mg + Fe)_{at}$] was 0.92, but it was lower (0.86–0.90) in a few samples (Fig. S5). Orthopyroxene was mainly low in Na_2O (median 0.06 wt%), but 19 samples had ≥0.2 wt% Na_2O.

DISCUSSION

Temperature Distribution in the CLM Profile

The temperature distribution with depth at the time of kimberlite eruption is shown in Figure 1. At 80–130 km, the samples plot between the 40 and 35 mW/m² geotherms of Hasterok and Chapman (2011) and then follow the 35 mW/m² geotherm down to 190–200 km. Entrapment conditions reported for inclusions in a diamond from Udachnaya (Nestola et al., 2019) fall on the extension of this geotherm.

Six samples at ~4 GPa recorded up to 150 °C higher *T* and outlined a previously unknown hot midlithospheric horizon at ~135 km (Fig. 1). Another anomalously hot zone made up the CLM base at 190–230 km, as is common in cratons (Boyd, 1984; Carlson et al., 2005). A "*T*-gap" of ~140 °C (1050–1190 °C) occurred between the shallowest high-*T* and the deepest low-*T* samples at ~6 GPa (Fig. 1; Fig. S1D; Doucet et al., 2013). We posit that the *P* values for the high-*T* Udachnaya peridotites reported by Goncharov et al. (2012) are too low, and the matching geotherm is too high, because these authors used the P_{NG85}-T_{TA98} pair without corrections for Na-rich opx (Figs. S1A–S1C). Thus, their assertion that both "cold" and "hot" peridotites occur at 145–180 km is unsupported. Our study most accurately, and in detail, defines the *P-T* conditions of the CLM base in central Siberia.

As noted earlier (Agashev et al., 2013; Doucet et al., 2013), the hot zone at the CLM base is composed mainly of sheared rocks, but it also contains ubiquitous coarse or lightly deformed peridotites (Figs. 1 and 2). This suggests that heating and deformation, albeit closely related, may not be concurrent. Like in the high-*T* horizon at ~135 km, *T* values at a given depth at the CLM base range by up to 150 °C, indicating uneven heating likely controlled by local, small-scale processes. The highest *P* values (7.1 GPa) correspond to a depth of ~230 km; i.e., slightly deeper than earlier estimates of Goncharov et al. (2012) and Ionov et al. (2010). They plot on the mantle adiabat (Fig. 1A) and thus define the lithosphere-asthenosphere boundary (LAB).

Rock Type Distribution in the CLM Profile

The distribution of rock types with depth is shown in Figure 1, and data on modal cpx and garnet are shown in Figures 2A and 2B. Three to 33 samples represent each 0.5 GPa (~18 km) segment of the profile at 2.5–7.5 GPa (Fig. S2A) and thus provide a much greater vertical resolution than previous xenolith studies at Udachnaya (Boyd, 1984; Goncharov et al., 2012; Doucet et al., 2013) and in other cratons (Pearson and Wittig, 2014). Garnet harzburgites are dominant above the hot basal zone (<190 km). The proportions of the peridotite types and modal cpx and garnet do not change significantly with depth from ~80 km to 190 km. The only exception is the anomalous horizon at ~135 km, which includes rocks with abundant coarse garnet and cpx, and occasional accessory phlogopite (Fig. S4). The concurrence of the more fertile and hotter rocks at ~135 km is unlikely to be accidental. The distribution of cpx-free harzburgites is

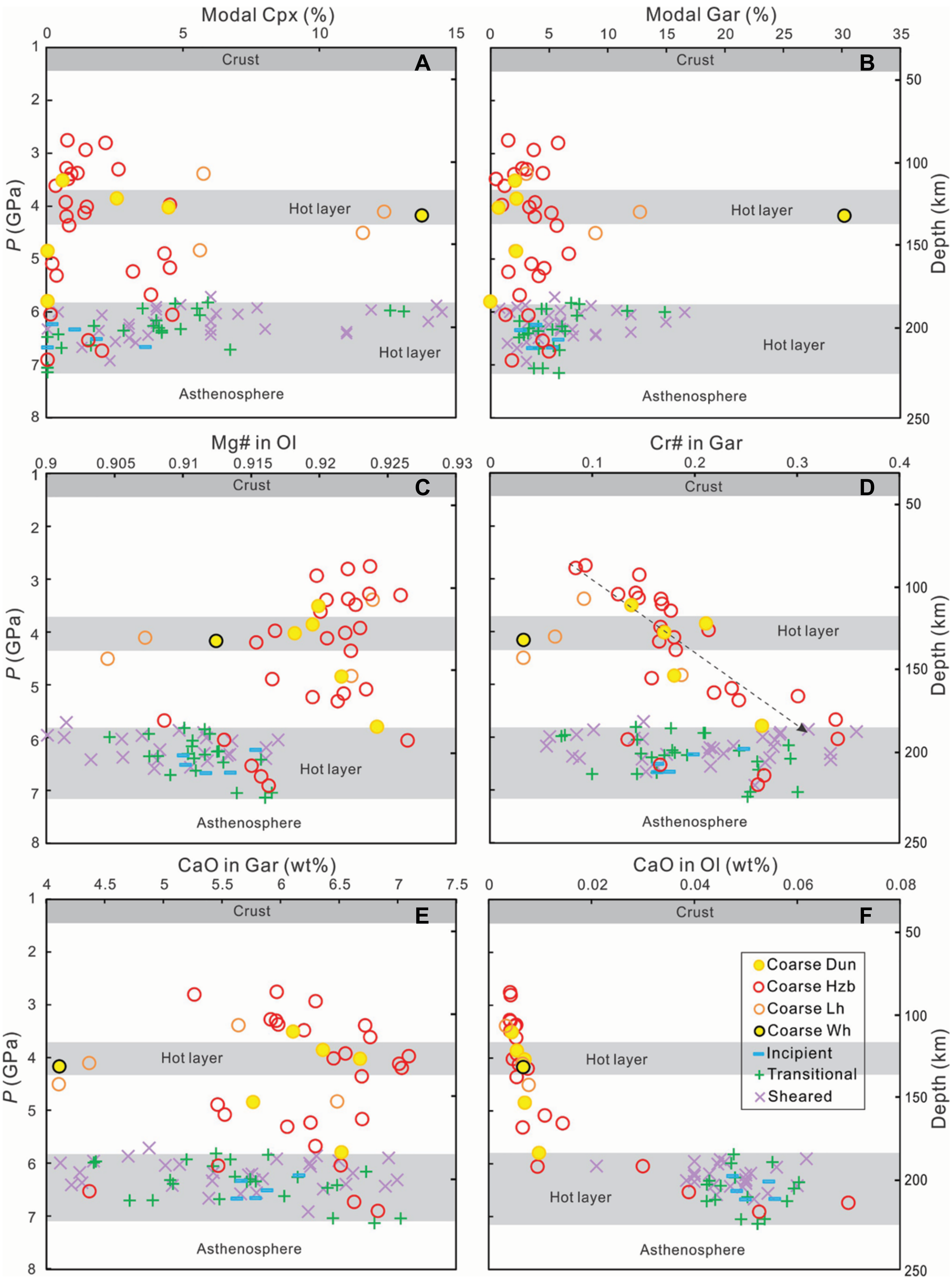

Figure 2. Modal and chemical variations with depth. $Mg\#_{ol} = Mg/(Mg + Fe)_{at}$; $Cr\#_{Gar} = Cr/(Cr + Al)_{at}$. "Hot" layers are as in Figure 1. Cpx—clinopyroxene; Gar—garnet; Ol—olivine; Hzb—harzburgite; Lh—lherzolite; Dun—dunite; Wh—wehrlite.

less well resolved because of the uncertainties of the T_{NG10} method (less reliable than T_{TA98}) used for these rocks, yet our data show no significant variations in their abundance with depth (Fig. S1). Below 190 km, garnet- and cpx-rich lherzolites are more common among strongly deformed peridotites (Figs. 3A and 3B), indicating that deformation was accompanied by input of Ca.

Overall, we found no significant CLM layering above ~190 km (apart from the hot, garnet- and cpx-rich horizon at ~135 km). By contrast, Griffin et al. (1999) asserted, using data on garnet extracted from kimberlites, that the CLM beneath Udachnaya is strongly layered in terms of rock type, with predominantly "lherzolites" down to 150 km and "harzburgites" at 150–180 km. This claim, however, is disputable, because *P* estimates were obtained by projecting inexact *T* estimates onto a single cold geotherm such that thermally perturbed samples may have been placed at too great depth. Also, the source "rock types" of the garnets were assumed from Ca-Cr relations (Fig. S9), which contradict xenolith data (Doucet et al., 2013).

The absence of rocks rich in amphibole and mica in our large collection confirms previous observations (e.g., Doucet et al., 2013; Ionov et al., 2020) and suggests that such rocks cannot be significant components in the CLM of the Siberian craton.

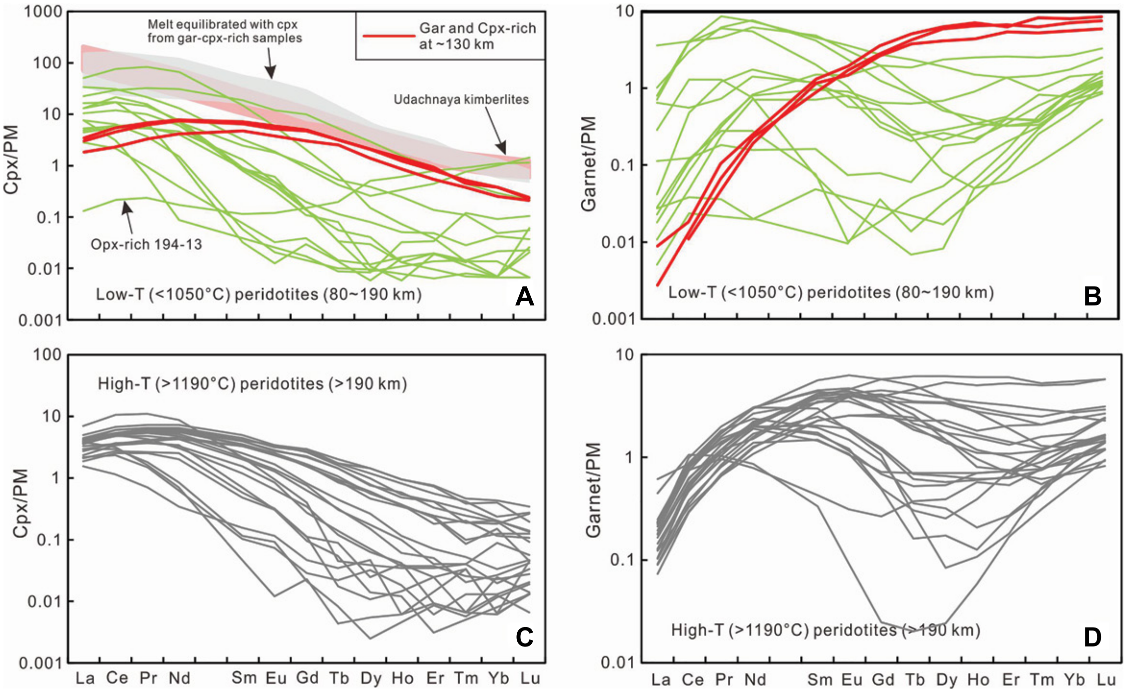

Figure 3. Primitive mantle (PM)–normalized (Hofmann, 1988) rare earth element (REE) patterns in clinopyroxene (Cpx) and garnet (Gar), and fields for Udachnaya (Siberia) kimberlites and liquids equilibrated with cpx from cpx- and garnet-rich xenoliths (Doucet et al., 2013). Opx—orthopyroxene.

Chemical Variations in the CLM Profile

The Mg#$_{Ol}$ in residual cratonic peridotites ranges from 0.92 to 0.93, depending on melting degree and depth during CLM formation, but it is lower in metasomatized rocks (Pearson and Wittig, 2014). The Mg#$_{Ol}$ in the majority of coarse Udachnaya xenoliths above 190 km (0.918–0.927; Fig. 2C) falls in the range of melting residues, but it is lower in two zones of the profile: (1) high-*T*, garnet-rich and cpx-rich samples at ~135 km (0.904–0.917), and (2) high-*T* peridotites at the CLM base (≥190 km) with Mg#$_{Ol}$ of 0.872–0.918 (Fig. S5).

The Cr#$_{Gar}$ [Cr/(Cr + Al)$_{at}$] in coarse peridotites generally increases with *P*, but xenoliths with the highest modal garnet and cpx at ~135 km, as well as most high-*T* xenoliths at >190 km, plot off the Cr#$_{Gar}$ versus *P* correlation to very low Cr#$_{Gar}$ values (Fig. 2D). The high-*T* and garnet- and cpx-rich samples at ~135 km and some rocks at ≥190 km have low (4.0–4.5 wt%) CaO$_{Gar}$ (Fig. 2E). Empirical correlations for coarse Udachnaya peridotites (Ionov et al., 2010) suggest that CaO$_{Gar}$ <4.5 wt% indicates whole-rock Al_2O_3 ≥2.5 wt%, whereas CaO$_{Gar}$ >5.5 wt% generally indicates whole-rock Al_2O_3 ≤1.5 wt%. These values agree with Al_2O_3 estimates from modal and mineral compositions (see the Supplemental Material) and suggest strong melt metasomatism in the CLM at ~135 km and below 190 km.

The concentrations of some minor elements in olivine from mantle peridotites are affected by *T* and *P* (De Hoog et al., 2010), but also by modal and whole-rock chemical composition (Ionov, 2007). Overall, the contents of Ca, Al, and Cr in olivine in our study showed positive exponential covariation versus *T* and/or *P* (Fig. S6). Yet, Ca and Al showed broad variations over narrow *P* and *T* ranges for high-*T* peridotites. The latter, together with Na and Ti variations (Fig. S6), may be linked to metasomatism.

Primitive mantle–normalized rare earth element (REE) patterns of garnet and cpx (Fig. 3) ranged from sinusoidal, typical for coarse peridotites, to bell-shaped or light REE (LREE)–depleted for deformed samples and for garnet- and cpx-rich xenoliths at 135 km. Previous work on Udachnaya peridotites (Ionov et al., 2010; Agashev et al., 2013) showed that the sinusoidal patterns form by entrapment of small-volume, carbonate-rich media in melting residues, whereas the bell-shaped or LREE-depleted patterns suggest equilibration with evolved kimberlite or alkali basaltic liquids. Thus, the REE patterns for xenoliths at 135 km and ≥190 km, as well as their anomalous modal compositions and equilibration temperatures, are ascribed to strong melt metasomatism.

Origin of Temperature, Modal, and Chemical Variations in the CLM

Coarse peridotites on the 35 mW/m^2 geotherm trace steady-state thermal conditions of the CLM (Lee et al., 2011), but anomalously hot and metasomatized layers precede, or are concurrent with, kimberlite volcanism. The "*T*-gap" of 1050–1190 °C at 190 km (Fig. 1) between coarse low-*T* samples and high-*T*, mainly deformed and metasomatized (Figs. 2 and 3) rocks at the CLM base encompasses the solidi of both dry and hydrous carbonated mantle. As asthenosphere-derived, CO_2-rich melts ascend through the CLM base, they cool down, lose volatiles, and finally solidify when they reach their solidus temperatures to form a thermal and petro-geochemical interface at 190 km (Fig. 4). The strong deformation, Fe enrichment, and thermal contrasts at greater depths cannot be long-term features of global CLM and appear to exist only above asthenospheric upwellings that induced kimberlite magmatism (Agashev et al., 2013).

The reworked hot and/or garnet- and cpx-rich rocks at 135 km may represent a level where ascending melts stall, crystallize, and react with a colder CLM sufficiently long to yield texturally equilibrated, coarse hybrid rocks before the eruption of their host kimberlite (e.g., Bussweiler et al., 2018). These processes may be enhanced by loss of volatiles and/or redox change, as suggested by a sharp upward decrease in water content in minerals (Doucet et al., 2014, their figures 4A and 4B) and an increase in oxygen fugacity (Goncharov et al., 2012, their figure 5B) at ~4 GPa reported in earlier work on Udachnaya peridotites (Table S1B). Recent melt or fluid additions heat the horizon and produce intergranular phlogopite and fine-grained cpx.

Xenolith Evidence for the Origin of the MLD

Midlithosphere discontinuities involving intermittent downward shear wave velocity drops of 1%–6% are detected in the CLM mainly at 60–160 km depth (Krueger et al., 2021; Rader et al., 2015), though no S-receiver function data are currently available for the Siberian craton. Layering in melt depletion degrees or physical

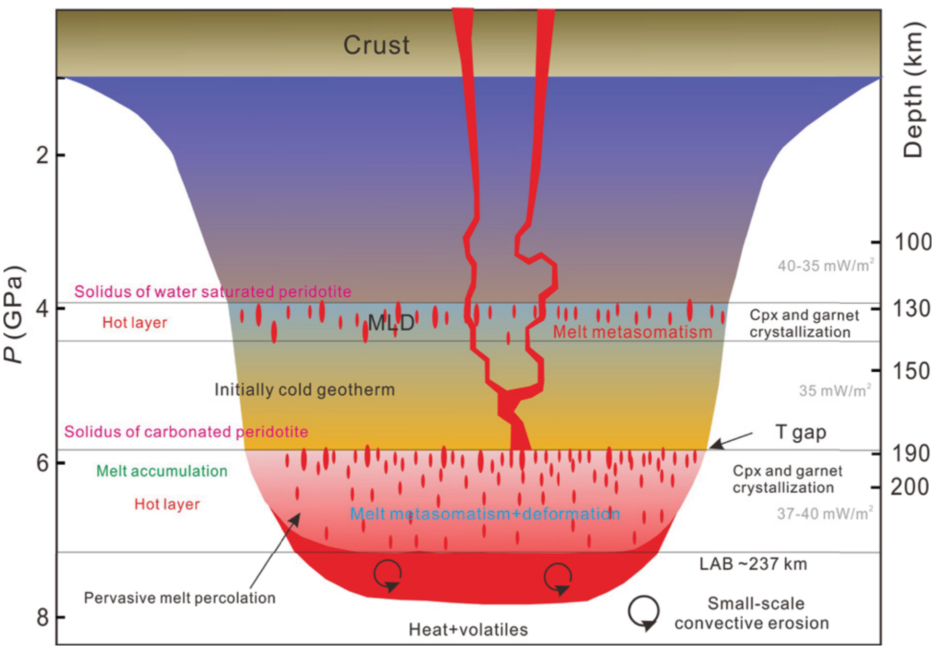

Figure 4. Schematic illustration of the origin of "hot" and metasomatized continental lithospheric mantle (CLM) layers in the central Siberian craton. MLD—midlithospheric discontinuity; LAB—lithosphere-asthenosphere boundary; Cpx—clinopyroxene; T—temperature.

parameters like anisotropy (Bascou et al., 2011; Priestley et al., 2021) may contribute to MLDs but cannot, on their own, cause them (Krueger et al., 2021; Selway et al., 2015). The MLDs are often attributed to the injection of hydrous and/or carbonatitic melt into the CLM to form abundant minerals with low seismic velocities. Estimates suggest that a 2%–7% velocity decrease requires addition of either 5%–15% carbonate, phlogopite, or amphibole or 45%–100% pyroxene to melt-depleted CLM (Rader et al., 2015). While some cratonic peridotites contain carbonates or phlogopite (Ionov et al., 2018), xenoliths rich in volatile-bearing phases mainly occur in areas of recent or ancient rifting (Aulbach et al., 2017; Pearson and Wittig, 2014; Wölbern et al., 2012) and cannot be typical of cratonic CLM in general (Saha et al., 2021).

CONCLUSIONS

The detailed *P-T*, petrographic, and chemical CLM profile in our study can help to identify potential MLD sources in the Siberian craton, and possibly other cratons (Fig. 4). (1) We found no layering in melt depletion degrees from ~80 to 190 km. (2) We found no carbonates or amphibole in the xenoliths, nor phlogopite-rich rocks. (3) We discovered an ~20-km-thick, low-Mg#, garnet- and cpx-rich horizon at ~135 km, where repeated heating and metasomatism by evolved, volatile-bearing liquids occurred. We posit that MLDs could be linked to such horizons.

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