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# 1 **First-principles calculations of the lattice thermal conductivity of the lower mantle**

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## 12 **Abstract**

13 The temperature variations on top of the core-mantle boundary are governed by the  
14 thermal conductivity of the minerals that comprise the overlying mantle. Estimates of the  
15 thermal conductivity of the most abundant phase, MgSiO<sub>3</sub> perovskite, at core-mantle  
16 boundary conditions vary by a factor of ten. We performed ab initio simulations to  
17 determine the lattice thermal conductivity of MgSiO<sub>3</sub> perovskite, finding a value of  $6.8 \pm 0.9$   
18  $\text{W m}^{-1} \text{K}^{-1}$  at core-mantle boundary conditions (136 GPa and 4000 K), consistent with  
19 geophysical constraints for the thermal state at the base of the mantle. Thermal  
20 conductivity depends strongly on pressure, explaining the dynamical stability of super-  
21 plumes. The dependence on temperature and composition is weak in the deep mantle: our  
22 results exhibit saturation as the phonon mean free path approaches the interatomic  
23 spacing. Combining our results with seismic tomography, we find large lateral variations in  
24 the heat-flux from the core that have important implications for core dynamics.

## 25 **Keywords**

26 MgSiO<sub>3</sub> perovskite; thermal conductivity; mantle dynamics

27

## 28 **1. Introduction**

29 Heat-flux at the core-mantle boundary has important implications for the thermal evolution  
30 of the core and mantle (Lay et al., 2008), the size and stability of plumes (Dubuffet et al.,  
31 1999), and generation of the magnetic field (Gubbins et al., 2011). Despite this, there is a  
32 wide range of estimates of the thermal conductivity of the lower mantle (Osako and Ito,  
33 1991; Hofmeister, 2008; Goncharov et al., 2010; de Koker, 2010; Manthilake et al., 2011;  
34 Haigis et al., 2012; Ohta et al., 2012; Dekura et al., 2013; Tang et al., 2014; Ammann et  
35 al., 2014; Ohta et al., 2014). As insulators and semi-conductors, the major lower mantle  
36 phases: (Mg,Fe)SiO<sub>3</sub> perovskite, CaSiO<sub>3</sub> perovskite, and (Mg,Fe)O ferropericlase are  
37 expected to conduct heat via phonons (lattice vibrations), but experimental and theoretical  
38 studies of their lattice thermal conductivity have suffered significant limitations.

39 Technical constraints mean that experimental measurements are limited to temperature  
40 much lower than those in the deep Earth, and thus long extrapolations must be made to  
41 estimate values in the lowermost mantle. In addition, while the results of ambient  
42 temperature studies of MgSiO<sub>3</sub> perovskite (Osako and Ito, 1991; Ohta et al., 2012) are in  
43 reasonable agreement, measurements at elevated temperature (500-1100 K) and 26 GPa  
44 (Manthilake et al., 2011), suggests a 300 K lattice thermal conductivity almost twice as  
45 large. This suggests that there are discrepancies even at low temperature and pressure.

46 Classical simulations, where simple functional forms define interactions between atoms,  
47 also have considerable uncertainties. Haigis et al. (2012) used a classical potential to  
48 compute lattice thermal conductivity via equilibrium molecular dynamics and Green-Kubo  
49 relations, while Ammann et al. (2014) used a classical potential to calculate lattice thermal  
50 conductivity via non-equilibrium molecular dynamics simulations. The difference of up to a  
51 factor of two between the studies, for the lattice thermal conductivity of MgSiO<sub>3</sub> perovskite,  
52 illustrates the uncertainty due to the choice of classical potential. This source of

53 uncertainty has been highlighted in other studies (Chen et al., 2012; Howell, 2012) and  
54 shows the importance of performing ab initio calculations, where forces are calculated  
55 from first-principles.

56 Previous ab initio calculations of the lattice thermal conductivity of MgSiO<sub>3</sub> perovskite  
57 have also suffered important limitations. Dekura et al. (2013) and Tang et al. (2014)  
58 performed lattice dynamics calculations, which are limited by the assumption that  
59 anharmonic terms are truncated at third-order. The truncation is significant, because it  
60 requires the lattice thermal conductivity to vary as the inverse of the temperature ( $T^{-1}$ ),  
61 more rapidly than observed in silicates and oxide perovskites at temperatures greater than  
62 the Debye temperature (Marquardt et al., 2009a; Hofmeister, 2010), and leads to  
63 underestimation of the conductivity at high temperature.

64 Here, we take a different approach, calculating the lattice thermal conductivity of MgSiO<sub>3</sub>  
65 perovskite using the ‘direct’ non-equilibrium molecular dynamics method (NEMD), with  
66 forces calculated directly from density functional theory. The direct method, which we have  
67 used previously to compute the lattice thermal conductivity of MgO periclase (Stackhouse  
68 et al., 2010), has the advantage that anharmonicity is fully included with no truncation. The  
69 method is conceptually straightforward: lattice thermal conductivity is calculated from  
70 Fourier’s law by computing the temperature gradient induced by an imposed heat-flux.

## 71 **2. Theory**

### 72 **2.1 Non-Equilibrium Molecular Dynamics Simulations**

73 The lattice thermal conductivity of MgSiO<sub>3</sub> perovskite was calculated using ab initio non-  
74 equilibrium molecular dynamics (Stackhouse and Stixrude, 2010). The method is intuitive,  
75 following the design of experimental techniques. The simulation cell is divided up into  
76 sections (Fig. 1(a)). One section is designated the ‘hot section’ and another the ‘cold  
77 section’. These are separated by a distance of half the length of the simulation cell. At

78 regular intervals heat is transferred from the cold section to the hot section, generating a  
79 heat-flux. Over time, a temperature gradient develops between the hot and cold sections  
80 (Fig. 1(b)). Once steady state is reached thermal conductivity is calculated from Fourier's  
81 law:

$$82 \quad k = - \frac{\langle J(t) \rangle}{\langle dT/dx \rangle} \quad (1)$$

83 where  $k$  is the thermal conductivity, and  $\langle J(t) \rangle$  and  $\langle dT/dx \rangle$  are the time average of the heat-  
84 flux and the temperature gradient.

85 In order to conserve the total kinetic energy and linear momentum of the system, the  
86 transfer of energy from the cold section to the hot section is achieved by assigning the  
87 hottest atom in the cold section and coldest atom in the hot section the velocities that  
88 would arise from a hypothetical elastic collision between them (Müller-Plathe, 1997; Nieto-  
89 Draghi and Avalos, 2003).

90 The temperature gradient is determined from a linear fit to the temperature of the  
91 individual sections. Due to the periodic nature of the simulation, heat enters and leaves  
92 from both sides of the hot and cold sections and two temperature gradients develop,  
93 leading to a temperature profile resembling that shown in Fig. 1(b). Rather than discard  
94 one of them, the temperature of symmetrically equivalent sections is averaged. Due to the  
95 non-Newtonian nature of the energy transfer, the temperature gradient is non-linear  
96 around the hot and cold sections. In view of this, these sections are excluded from the fit  
97 to determine the temperature gradient (Supplementary Material Fig. S1(d)).

## 98 **2.2 Finite-Size Effects**

99 Our analysis of finite-size effects follows that of Schelling et al. (2002) and has been used  
100 widely as a means of obtaining results in the limit of infinite systems (Zhou et al., 2009;

101 Sellan et al., 2010; Howell, 2011a, 2011b, 2012; Hu et al., 2011). Kinetic theory relates  
102 thermal conductivity to phonon mean free path

$$103 \quad k = \frac{1}{3} C_v v l \quad (2)$$

104 where  $C_v$  is the volumetric heat capacity,  $v$  is the mean sound velocity and  $l$  is the phonon  
105 mean free path. Since phonons are scattered within the hot and cold sections, the longest  
106 possible phonon mean free path is equal to the distance between them, i.e. half the length  
107 of the simulation cell. If the true phonon mean free path is much longer than this, the  
108 thermal conductivity calculated will be significantly underestimated.

109 If we assume that the phonon mean free path is dependent on two independent  
110 scattering mechanisms: phonon-phonon scattering and phonon-boundary scattering  
111 occurring at the hot and cold sections, then the effective mean free path for a simulation  
112 cell of length  $L$  is

$$113 \quad l_L^{-1} = l_{ph}^{-1} + l_b^{-1} \quad (3)$$

114 where  $l_{ph}$  is the contribution from phonon-phonon scattering and  $l_b$  the contribution from  
115 phonon-boundary scattering.  $l_b$  is assumed to be  $L/4$ , where  $L$  is the total length of the  
116 simulation cell. The factor of 4 arises because phonons originating between the hot and  
117 cold sections will travel, on average, a quarter of the simulation cell length before  
118 encountering the hot and cold sections. Substituting Eq. (3) into (2) and rearranging leads  
119 to

$$120 \quad k_L^{-1} = k_\infty^{-1} + bL^{-1} \quad (4)$$

121 where  $k_L$  is the thermal conductivity calculated for a simulation cell of length  $L$ ,  $k_\infty$  the  
122 thermal conductivity of a simulation cell of infinite length (i.e. the true value) and  $b$  a  
123 constant equal to

124 
$$b = \frac{12}{C_v v} \quad (5)$$

125 Thus by calculating the thermal conductivity for simulation cells of different length and  
126 plotting against  $L^{-1}$ , one can estimate  $k_{\infty}^{-1}$ .

127 Previous studies (Sellan et al., 2010; Howell, 2012) have shown that the linear  
128 extrapolation (Eq. (4)) may be inaccurate when the phonon mean free path is much longer  
129 than the smallest simulation cell. For example, studies of silicon near room temperature,  
130 which has a long phonon mean free path, require simulation cells on the order of 10 000  
131 atoms. In the case of our calculations, smaller simulation cells are sufficient, since the  
132 temperature is much higher and the phonon mean free path much shorter (Tadano et al.,  
133 2014). In our previous calculations of periclase (Stackhouse et al., 2010), we used  
134 simulation cells of a similar size, and found our results to be in good agreement with other  
135 theoretical methods and experimental results, and the phonon mean free path to be  
136 shorter than the smallest simulation cell.

137 Phonon mean free paths can be estimated from the slope of the linear relationship  
138 between  $k_L^{-1}$  and  $L^{-1}$ , combining Eqs. (2) and (5)

139 
$$l = \frac{bk_{\infty}}{4} \quad (6)$$

140 Estimated values of  $l$  (Supplementary Material Table S1) are shorter than the shortest  
141 simulation cell used at all temperature and pressures studied, indicating that our  
142 simulation cells are large enough to obtain accurate results.

143 Calculations may also be inaccurate if the cross-sectional area of the simulation cell is  
144 too small (Schelling et al., 2002; Zhou et al., 2009; Hu et al., 2011). This is because the  
145 phonon population is then biased towards those propagating in the long direction of the  
146 simulation cell, leading to an overestimate of the thermal conductivity. This is not expected

147 to be a serious issue in our simulations, because the phonon mean free path is  
148 comparable to the cross-sectional dimensions. To test this issue, we have performed  
149 simulations with different cross-sectional areas at 110 GPa and 1000 K and 110 GPa and  
150 3250 K. The results are identical within uncertainty (Supplementary Material Table S1).

### 151 **3 Calculation Details**

152 Calculations were performed using a version of the density functional theory based VASP  
153 code (Kresse and Furthmuller, 1996a, 1996b) modified to perform NEMD. The local  
154 density approximation (Perdew and Zunger, 1981) was used for the exchange-correlation  
155 functional. Ultrasoft pseudopotentials were employed, with valence electron  
156 configurations:  $3s^2$  for Mg,  $3s^23p^2$  for Si and  $2s^22p^4$  for O. The kinetic-energy cut-off for the  
157 plane-wave basis set was set to 400 eV and Brillouin zone sampling was restricted to the  
158  $\Gamma$ -point. Fermi-smearing was applied in all calculations, with a broadening-width equal to  
159 the simulation temperature. The convergence criteria for the self-consistency loop was  $10^{-4}$   
160 eV. The time-step was set to 1 fs and the Nosé thermostat was employed to maintain a  
161 constant temperature (Nosé, 1984). By calculating the forces from first-principles, we  
162 avoid issues associated with empirical pair potentials (Chen et al., 2012; Howell, 2012).

163 The dimensions of all simulation cells used in the current work are listed in  
164 Supplementary Material Table S2. The cell parameters at each pressure and temperature  
165 ( $P$ - $T$ ) point, were determined from equilibrium molecular dynamics simulations using 80  
166 atom  $\text{MgSiO}_3$  models.

167 Before each NEMD calculation, the simulation cell was equilibrated by performing 1 ps  
168 of equilibrium molecular dynamics, after which energy exchange was initiated. The energy  
169 exchange periods used are listed in Supplementary Materials Table S2. These were  
170 chosen to produce a temperature difference of 500-1000 K between the hot and cold  
171 sections and took values of between 40-80 fs. Simulations using longer exchange periods

172 converged more slowly, and led to values with larger associated uncertainties, because  
173 the error in the temperature gradient increased. Initial tests showed that, within a certain  
174 range, using different exchange periods had little effect on the results (Supplementary  
175 Materials Fig. S2).

176 Most NEMD calculations were run for a minimum of about 50 ps (Supplementary  
177 Material Table S2), at least 10 ps of which was allowed for steady state to be reached.  
178 Thermal conductivity was calculated using the remaining portion. In general, this led to  
179 converged values for the heat-flux, temperature gradient and thermal conductivity  
180 (Supplementary Material Fig. S1). When a simulation was judged not to have converged  
181 fully i.e. the time average of the thermal conductivity had not have flattened out,  
182 simulations were run longer.

183 The uncertainty in the time average of the heat-flux was determined using the  
184 appropriate statistics (Flyvbjerg and Petersen, 1989), taking into account correlation. The  
185 same method was also used to compute the uncertainty in the time average of the  
186 temperature of individual sections. To calculate the temperature gradient the temperatures  
187 of symmetrically equivalent sections were averaged and fit using weighted least square  
188 regression, but excluding the values for the hot and cold sections and those either side of  
189 them (Fig. S1(d)). The thermal conductivity for a simulation cell of infinite length was  
190 determined from a weighted least squares fit to a plot of inverse thermal conductivity  
191 against inverse simulation cell length (Supplementary Material Figs. S3 and S4). The  
192 extrapolated values are listed in Supplementary Material Table S1.

#### 193 **4. Results**

194 At lower mantle conditions, we find that the temperature dependence of the thermal  
195 conductivity is weak: at 75 GPa, lattice thermal conductivity decreases from  $5.3 \pm 0.7 \text{ Wm}^{-1}\text{K}^{-1}$   
196 at 2500 K to  $4.7 \pm 0.8$  at 4000 K (Fig. 2). Note that, our results indicate that the lattice

197 thermal conductivity of MgSiO<sub>3</sub> perovskite is isotropic at 75 GPa and 2500 K to within the  
198 uncertainty of our results (Fig. S3 and Table S1), and this is presumed to be the case at all  
199 other conditions. All values shown in Figs. 2 and 3 are for the [100] direction. Both here  
200 and throughout the manuscript the uncertainties indicate the standard error. This variation  
201 is weaker than the often-assumed  $T^{-1}$  dependence, and even weaker than the  $T^{-2/5}$   
202 dependence recently suggested for MgSiO<sub>3</sub> perovskite, based on experimental results at  
203 lower pressures and temperatures (Manthilake et al., 2011). Such weak temperature  
204 dependence indicates saturation (Roufosse and Klemens, 1974; Marquardt et al., 2009a;  
205 Hofmeister, 2010), where the phonon mean free path approaches the inter-atomic  
206 spacing. This means that pressure (or density) dependence dominates throughout most of  
207 the lower mantle: at 4000 K, lattice thermal conductivity increases from  $5.3 \pm 0.7 \text{ Wm}^{-1}\text{K}^{-1}$   
208 at 75 GPa to  $9 \pm 2 \text{ Wm}^{-1}\text{K}^{-1}$  at 145 GPa (Fig. 2).

209 Our results agree well with room temperature experimental data (Osako and Ito, 1991;  
210 Ohta et al., 2012; Ohta et al. 2014), showing comparable pressure dependence. The  
211 measurements of Manthilake et al. (2011), show similar temperature dependence, but are  
212 higher by about  $5 \text{ Wm}^{-1}\text{K}^{-1}$  (Fig. 2 (main)). We note that their results also disagree with the  
213 ambient temperature values of Ohta et al. (2012). Lattice dynamics calculations of Dekura  
214 et al. (2013) agree with our results at low temperature, as expected, but predict a value  
215 half that of our study at core-mantle boundary conditions. We attribute this difference to  
216 the truncation of anharmonic terms at third order in the lattice dynamics calculation, which  
217 assumes  $T^{-1}$  behavior and does not capture the saturation (Roufosse and Klemens, 1974)  
218 that we find at high temperature. The values of Tang et al. (2014), which also suffer from  
219 truncation of anharmonic terms, are much lower than all other studies. It has been  
220 proposed that finite-size effects in NEMD simulations lead to erroneous values (Haigis et  
221 al., 2012), but this issue is expected to be minimal for MgSiO<sub>3</sub> perovskite at lower mantle  
222 conditions, where the phonon mean free path is short and lattice thermal conductivity is

223 low (Supplementary Material Fig. S4 and Table S1) (Tadano et al., 2014). Indeed,  
224 previous simulations based on classical potentials and much larger systems show  
225 remarkably similar values of the thermal conductivity at the core-mantle boundary  
226 (Ammann et al., 2014).

## 227 **5. Discussion**

228 Our results serve as a test of approximate theories of the density and temperature  
229 dependence of the thermal conductivity. Our results disagree with the commonly assumed  
230  $T^{-1}$  or  $T^{-1/2}$  temperature dependence. Instead, we find that our results are reproduced well  
231 by a model (Supplementary Material Section S1) that combines the Leibfried-Schlömann  
232 equation with temperature dependence that includes the effects of saturation (Roufosse  
233 and Klemens, 1974)

$$234 \quad k \propto \frac{M\Omega^{1/3}\theta^3}{\gamma^2 T} \left\{ \frac{2}{3} \left[ \frac{T_S(\Omega)}{T} \right]^{1/2} + \frac{1}{3} \left[ \frac{T}{T_S(\Omega)} \right] \right\} C \quad (7)$$

235 where  $M$  is the mean atomic mass,  $\Omega$  mean atomic volume,  $\theta$  Debye temperature,  $\gamma$   
236 Grüneisen parameter,  $T$  temperature, and  $T_S \propto M\Omega^{2/3}\theta^2/\gamma^2$  is the temperature at which  
237 saturation becomes significant. The term in the brackets accounts for saturation and  
238 causes  $k$  to vary more weakly than  $T^{-1/2}$  at high temperature, in excellent agreement with  
239 our results. The heat capacity  $C$ , accounts for phonon population effects at low  
240 temperature. All quantities are computed from a thermodynamic model (Stixrude and  
241 Lithgow-Bertelloni, 2011). The two constants of proportionality are chosen by fitting to our  
242 NEMD results.

243 We estimate the lattice thermal conductivity across the lower mantle, arriving at a value  
244 of  $8.1 \pm 1.1 \text{ Wm}^{-1}\text{K}^{-1}$  at the core-mantle boundary (Fig. 3), by combining the results of the  
245 present work, with our earlier ab initio predictions for periclase (Stackhouse et al., 2010),

246 and scaling laws for minor phases and impurities (Supplementary Material Sections S2 to  
247 S4). We approximate the lower mantle as pyrolite: (Mg,Fe)SiO<sub>3</sub> perovskite (75 percent),  
248 CaSiO<sub>3</sub> perovskite (6 percent) and (Mg,Fe)O ferropericlasite (19 percent) (Stixrude and  
249 Lithgow-Bertelloni, 2011). Recent experimental results show that iron impurities greatly  
250 reduce lattice thermal conductivity (Manthilake et al., 2011), at least at the low  
251 temperatures at which the measurements were made. By assuming this same large  
252 reduction, previous studies (Manthilake et al., 2011; Haigis et al., 2012) arrived at values  
253 for the lattice thermal conductivity of the lower mantle similar to ours. However, we expect  
254 the impact of impurities to be reduced at lower mantle temperatures. Based on the theory  
255 of Klemens (1960), we estimate the fractional lowering of the lattice thermal conductivity of  
256 the lower mantle due to iron impurities to be 8 percent at the core-mantle boundary, i.e.  
257 our value at the core-mantle boundary in the iron-free limit is very similar:  $8.8 \pm 1.2 \text{ Wm}^{-1}\text{K}^{-1}$ .  
258 The influence of aluminum is expected to be less than that of iron (Ohta et al., 2014).  
259 Our value for an iron-free lower mantle is substantially smaller than that estimated in a  
260 recent experimental study (Manthilake et al., 2011) which we attribute to the long  
261 extrapolation from the experimental results to lower mantle conditions. Our value is a  
262 factor of 2 larger than the estimate based on the lattice dynamics calculations of Dekura et  
263 al. (2013) and a factor of 6 larger than that based on the lattice dynamics calculations of  
264 Tang et al. (2014), which we attribute to the truncation of anharmonic terms in these  
265 studies.

266 The thermal conductivity of iron-bearing phases may be influenced by electronic  
267 transitions at lower mantle conditions. The influence of the high-spin to low-spin transition  
268 on thermal conductivity is unknown. If we assume that the primary effect of the transition is  
269 to decrease the atomic spacing, and take the volume decrease of Tsuchiya et al. (2006),  
270 based on scaling relations (Supplementary Material Section S2), the lattice thermal  
271 conductivity of ferropericlasite may be 3 percent higher in the low-spin state than in the

272 high-spin state. Within the transition region, in which high-spin and low-spin iron coexists  
273 in variable amounts, the mean acoustic wave velocity is reduced. If we assume that bulk  
274 sound velocity is reduced by the amount reported by Wentzcovitch et al. (2009) and that  
275 the shear velocities are unaffected (Marquardt et al., 2009b), based on scaling relations  
276 (Supplementary Material Section S2), the lattice thermal conductivity may be 15 percent  
277 smaller than the high-spin phase. The influence of the spin transition of the lattice thermal  
278 conductivity of perovskite will be much less than in ferropericlase, because of the lower  
279 iron content and the smaller fraction of ferrous iron. The spin transition appears to  
280 decrease phonon thermal conductivity and reduce the electrical conductivity (Goncharov et  
281 al., 2010). Although pure FeO becomes metallic at high pressures and temperatures  
282 (Fischer et al., 2011), thermal transport by electrons is unlikely to contribute significantly to  
283 thermal conductivity for plausible mantle iron concentrations. Extreme enrichment in iron,  
284 i.e. Fe/Si  $\sim 1$ , may produce much greater thermal conductivity by stabilizing new phases in  
285 which heat transport by electrons becomes important (Manga and Jeanloz, 1996), but  
286 seismic evidence rules out such extreme enrichments, even in ultra-low velocity zones  
287 (Rost et al., 2005).

288 In addition to scattering from impurities, scattering from interactions with electrons and  
289 grain boundaries can also influence lattice thermal conductivity. In the lower mantle,  
290 (Mg,Fe)SiO<sub>3</sub> perovskite, CaSiO<sub>3</sub> perovskite and (Mg,Fe)O ferropericlase are insulators  
291 and semiconductors. Older studies of semiconductors (e.g. Boghosian and Dubey, 1978)  
292 suggest that phonon-electron scattering is only important at low temperature (< 5 K), but a  
293 more recent first-principles investigation (Liao et al., 2015) shows that, for silicon with high  
294 carrier concentrations (> 10<sup>19</sup> cm<sup>-3</sup>), it has a marked effect at room temperature. There are  
295 no studies of the effect of phonon-electron scattering at lower mantle conditions, but we  
296 note that the analysis of Liao et al. (2015) indicates that phonon-electron scattering is most

297 significant for phonons with a mean free path greater than 100 nm. This is much longer  
298 than that expected for phonons in MgSiO<sub>3</sub> perovskite (Supplementary Material Table S1)  
299 and MgO periclase (Stackhouse et al. 2010), at lower mantle conditions. Inclusion of  
300 impurities will reduce the phonon mean free paths of the phases further. In view of this,  
301 we conclude that the effect of phonon-electron scattering is negligible in the lower mantle.

302 The effect of phonon-boundary scattering on lattice thermal conductivity becomes  
303 important when the mean free path is comparable to the grain size. Imada et al. (2014)  
304 showed that, at 300 K, there is a significant difference between single- and poly-crystal  
305 lattice thermal conductivity measurements for MgO periclase, in particular, at high  
306 pressure where the phonon mean free path is long in the single-crystal. Their analysis  
307 suggests that at core-mantle boundary conditions the lattice thermal conductivity of the  
308 phase will be independent of grain size, because of the much shorter mean free path.  
309 Since the mean free path of phonons in MgSiO<sub>3</sub> perovskite and iron-bearing phases is  
310 expected to be even shorter than that of MgO periclase, the lattice thermal conductivity  
311 of the lower mantle should be independent of grain size.

312 In some regions of the lower few hundred kilometers of the mantle, it is expected that  
313 perovskite transforms to post-perovskite (Wookey et al., 2005). Some studies indicate that  
314 the lattice thermal conductivity of post-perovskite is a factor of two greater than that of  
315 perovskite (Ohta et al., 2012; Ammann et al., 2014), but others suggest that this is only  
316 true at the low temperatures at which the experiments were conducted and at high  
317 temperature the difference is much smaller (Haigis et al., 2012). In view of this, we ignore  
318 differences in the lattice thermal conductivities of the two phases. We also neglect  
319 possible radiative contributions to the thermal conductivity, because measurements show  
320 that these are less than 0.5 Wm<sup>-1</sup>K<sup>-1</sup> (Goncharov et al., 2008). However, we note that a

321 consensus has not yet been reached: another experimental study concludes that the  
322 radiative contribution could be up to  $5 \text{ Wm}^{-1}\text{K}^{-1}$  (Keppler et al., 2008).

323 Our predicted value of the thermal conductivity at the core-mantle boundary is consistent  
324 with a variety of geophysical constraints (Lay et al., 2008). A boundary layer analysis  
325 (Supplementary Material Section S4) shows that for a thermal boundary layer thickness  $\delta$   
326  $\sim 100$  km (Fig. 4), our results satisfy independent constraints on the temperature across  
327 the thermal boundary layer from extrapolation of the mantle geotherm and inner-core  
328 freezing; the location of the seismic discontinuities caused by the perovskite to post-  
329 perovskite phase transition; and bounds on the heat-flow from intra-plate volcanism and  
330 heat conducted down the core adiabat.

331 The increase in thermal conductivity with increasing depth (Fig. 3) that we find – nearly a  
332 factor of two across the lower mantle – is dynamically significant. Greater thermal  
333 conductivity at depth is essential for stabilizing so-called superplumes: large-scale  
334 structures in the bottom-most 1000 km of the mantle beneath Africa and the Pacific, with  
335 very low shear wave velocity indicating higher than average temperature (Dziewonski et  
336 al., 2010). Dynamical simulations (Dubuffet et al., 1999) show that the buoyant instability  
337 of hot superplumes can be counter-acted and their long-term stability explained if the  
338 thermal conductivity of the lower mantle is higher than the rest of the mantle, just as we  
339 find.

340 While the physical model outlined in the previous sections completely specifies the  
341 calculation of the lattice thermal conductivity at all pressure and temperature conditions,  
342 we recognize that it may be useful to have a simpler, approximate form that captures the  
343 essence of these results. We present a simple approximation to the variation of the lattice  
344 thermal conductivity of pyrolite with pressure and temperature that is valid across the  
345 lower mantle regime

346 
$$k = (4.9 \text{ GPa} + 0.105P)f\left(\frac{T}{1200\text{K}}\right)\left(\frac{1200\text{K}}{T}\right) \quad (8)$$

347 where  $k$  is thermal conductivity ( $\text{Wm}^{-1}\text{K}^{-1}$ ),  $P$  is pressure (GPa),  $T$  is temperature (K) and  $f$   
348 is a function based on the theory of Roufosse and Klemens (1974), which accounts for  
349 saturation (Supplementary Material Section S1). This equation reproduces our results for  
350 pyrolite to within 10 percent along mantle geotherms with potential temperatures between  
351 1000 K and 2000 K and with or without a bottom thermal boundary layer and over the  
352 entire lower mantle pressure regime.

353 According to our results the thermal conductivity in the lower mantle is nearly  
354 homogeneous laterally, because of the weak dependence that we find on temperature and  
355 impurities. For example, varying the temperature by  $\pm 500$  K, changes the thermal  
356 conductivity at the core-mantle boundary by only 5 percent. Superplumes may also be  
357 stabilized by chemical heterogeneity; indeed seismic evidence of sharp sides indicates  
358 that they have a different chemical composition from normal mantle (Ni et al., 2002). We  
359 find that, in the lower mantle, the influence of chemical heterogeneity on thermal  
360 conductivity is minor (e.g. doubling the Fe/Mg ratio decreases the conductivity by only 5  
361 percent). This idea was also suggested by Manthilake et al. (2011), who showed that iron  
362 concentration has little effect on the lattice thermal conductivity of (Mg,Fe)O ferropericlase,  
363 although we note that they estimate a much larger difference between an iron-free and  
364 iron-bearing lower mantle (50 percent) than that found in this study (8 percent). It was  
365 suggested by Ohta et al. (2012), that the difference between iron-free and iron-bearing  
366 phases observed in lower pressure measurements ( $< 26$  GPa) by Manthilake et al. (2011)  
367 should be diminished at lower mantle pressures where iron will exist in a low-spin state.  
368 Enrichment in aluminum is expected to have a smaller effect, because of the similarity in  
369 atomic mass of aluminum to magnesium and silicon. This assumption is supported by  
370 the results of Ohta et al. (2014), but conflicts with those of Manthilake et al. (2011).

371 Lateral homogeneity in thermal conductivity at the core-mantle boundary is significant,  
372 because it implies a direct relationship between the temperature in the lower-most mantle,  
373 which can be inferred from seismology (Kustowski et al., 2008), and lateral variations in  
374 the heat-flux across the core-mantle boundary, via Fourier's law (Nakagawa and Tackley,  
375 2008). Combining Fourier's law for the heat-flux  $q = k\partial T/\partial z$ , with a linear temperature  
376 profile near the core-mantle boundary  $T = T_{CMB} - h\partial T/\partial z$ , and scaling of shear-wave velocity  
377 to temperature  $\xi = (\partial \ln V_S/\partial T)_z$  we find lateral variations in the heat-flux  $dq = -k/h d \ln V_S/\xi$ ,  
378 where  $T$  is temperature,  $z$  is depth,  $T_{CMB}$  is the temperature at the core-mantle boundary,  $h$   
379 is height above the core-mantle boundary, and  $V_S$  is shear-wave velocity. To compute  $dq$   
380 we use our value of  $k$  for pyrolite at the core-mantle boundary,  $d \ln V_S$  from seismic  
381 tomography at 2800 km depth, giving  $h = 90$  km, and the scaling  $\xi$  from a thermodynamic  
382 model (Stixrude and Lithgow-Bertelloni, 2011). We do not include the influence of the  
383 perovskite to post-perovskite transition on  $\xi$  because the pressure at which the transition  
384 occurs is uncertain. We find substantial lateral variation in heat-flux, comparable in  
385 magnitude to the mean value (Fig. 5). The heat-flux varies from zero (i.e. no heat escaping  
386 the core) to nearly twice the mean value. Such large lateral variations in heat-flux have  
387 important implications for our understanding of the origin of Earth's magnetic field (Olson  
388 and Christensen, 2002), its behaviour during reversals (Glatzmaier et al., 1999), and the  
389 structure of the inner core (Gubbins et al., 2011). Geodynamo simulations (Gubbins et al.,  
390 2011) indicate that even for much smaller lateral variation in heat flow than we estimate,  
391 localized melting of the inner core may occur, which may help to explain anomalies in the  
392 structure of the inner core including its radial structure, anisotropy, and hemispherical  
393 dichotomy. We note that our estimates of the lateral variation of heat flux are based on the  
394 assumption that lateral variations in seismic wave velocity are purely thermal in origin. An

395 understanding of the contributions of lateral variations in chemistry to the tomographic  
396 signal will be important for understanding the pattern of heat flow.

## 397 **6. Conclusions**

398 In conclusion, our calculations suggest that the lattice thermal conductivity of  $\text{MgSiO}_3$   
399 perovskite depends strongly on pressure, but that temperature and compositional  
400 dependence is weak in the deep mantle. Combining our results with seismic tomography,  
401 we find large lateral variations in the heat-flux from the core that have important  
402 implications for core dynamics. Our predictions of the thermal conductivity provide a firm  
403 basis from which further to explore the influence of mantle chemical heterogeneity on the  
404 coupled thermal evolution of core and mantle.

405

406

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420

421 **Appendix A. Supplementary Material**

422 Supplementary material related to this article can be found online.

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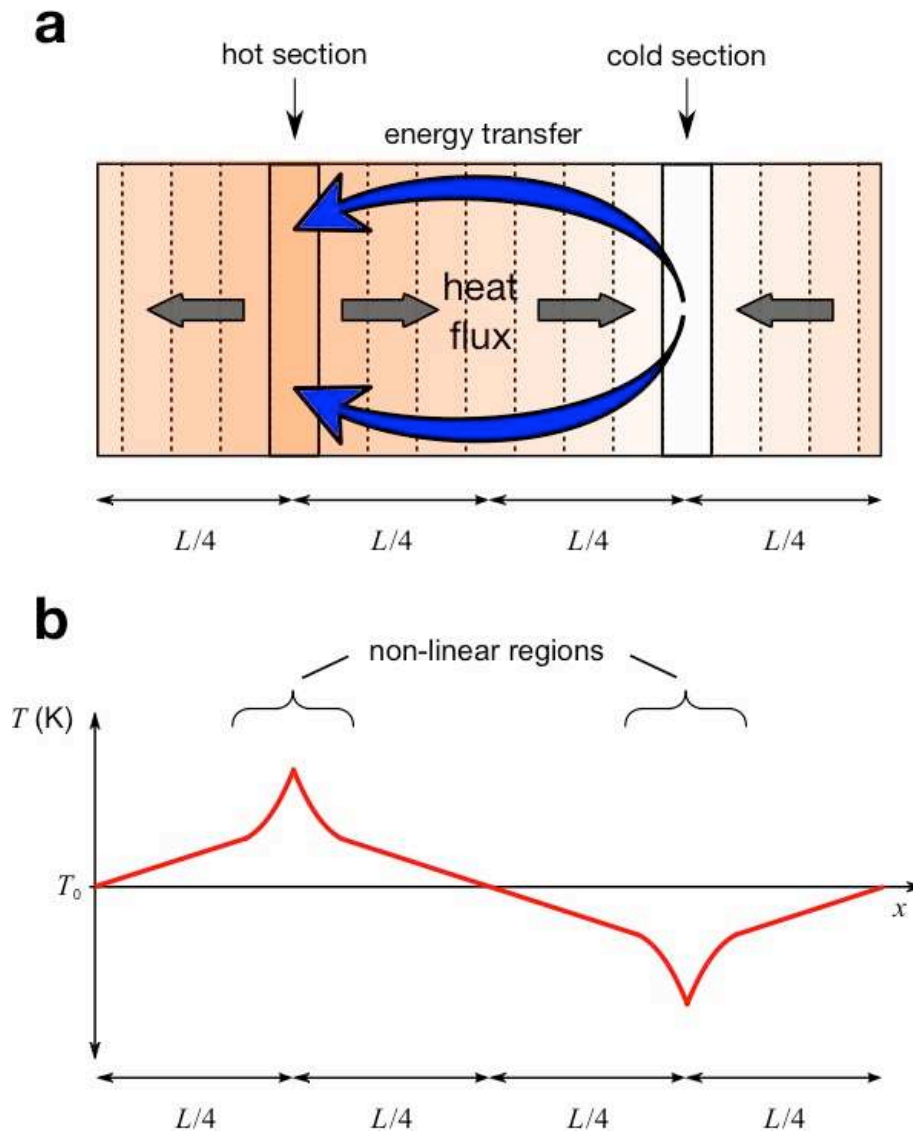
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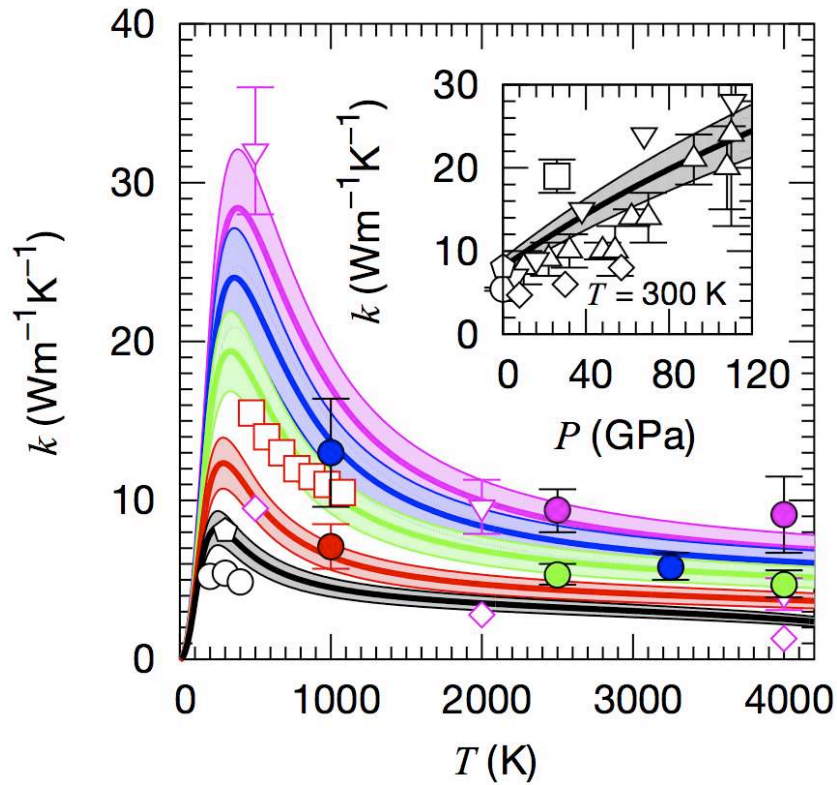


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**Fig. 1.** The non-equilibrium molecular dynamics method for calculating lattice thermal conductivity. The simulation cell is split into sections of equal width. At regular intervals energy is transferred from the 'cold section' to the 'hot section', by means of a virtual elastic collision between the hottest atom in the cold section and coldest atom in the hot section. Due to the periodic nature of the simulation, two temperature gradients form. The non-Newtonian nature of the virtual elastic collision means that the temperature gradient is non-linear around the hot and cold sections. Figure after Stackhouse and Stixrude (2010).

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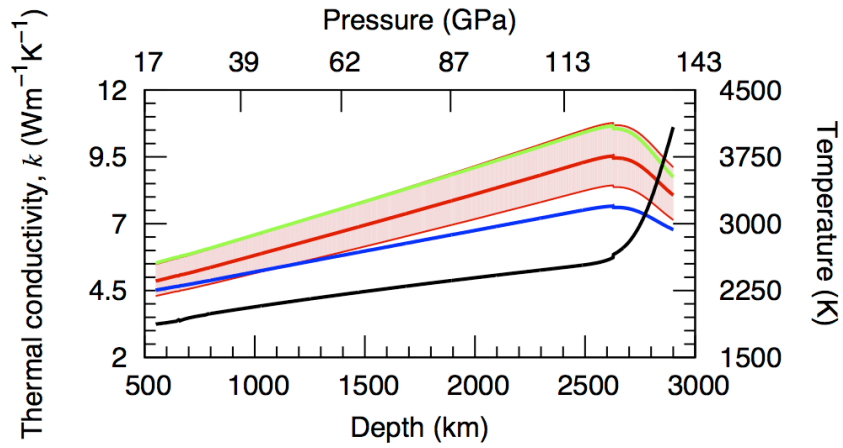
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587 **Fig. 2.** Lattice thermal conductivity of  $\text{MgSiO}_3$  perovskite as a function of temperature at  
 588 various pressures (main) and a function of pressure at 300 K (inset). Filled circles are the  
 589 results of our NEMD simulations and lines are the values predicted by our model  
 590 (described in the main text), with shading and error bars indicating standard error. Empty  
 591 symbols are measured ( $\circ$  Osako and Ito (1991),  $\square$  Manthilake et al. (2011),  $\triangle$  Ohta et al.  
 592 (2012),  $\pentagon$  Ohta et al. (2014)) and calculated ( $\nabla$  Dekura et al. (2013),  $\diamond$  Tang et al.  
 593 (2014)) values from previous studies. Color code for the main figure: black: 0 GPa, red:26  
 594 GPa, green:75 GPa, blue:110 GPa and pink:145 GPa.

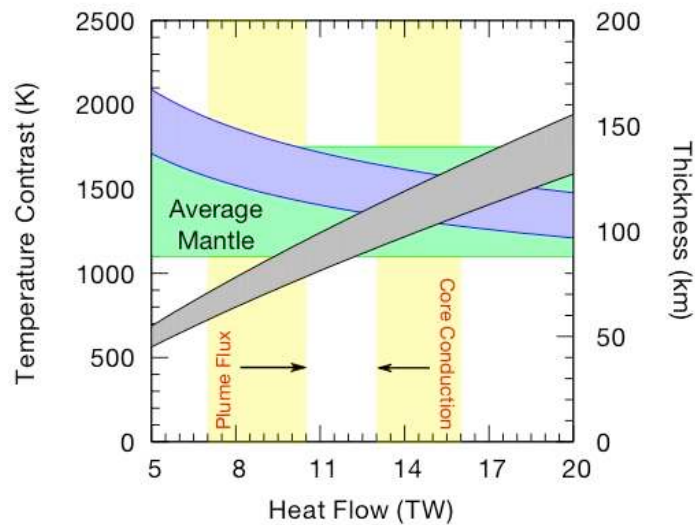
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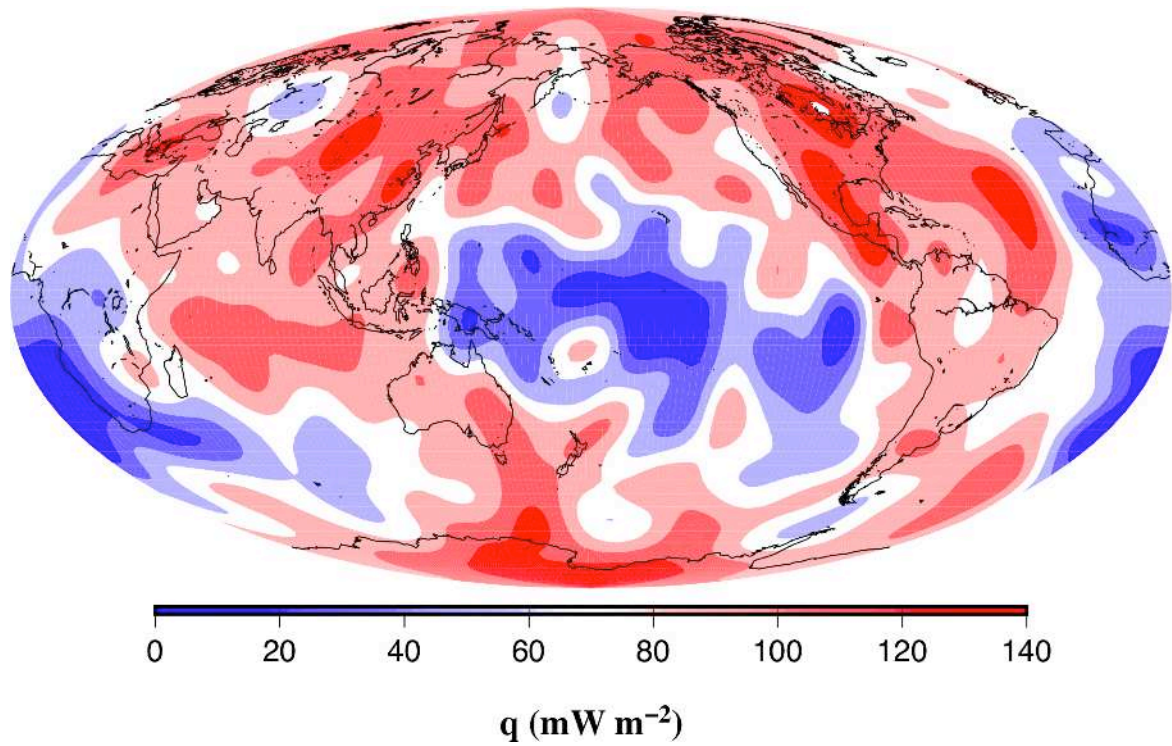
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598 **Fig. 3.** Lattice thermal conductivity of a pyrolite mantle as a function of depth (red line, with  
 599 the shading indicating standard error). Our results for pure MgSiO<sub>3</sub> perovskite (blue line)  
 600 and iron-free pyrolite (green line) are shown for comparison. The geotherm (black line) is  
 601 taken from a thermodynamic model (Stixrude and Lithgow-Bertelloni, 2011).

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603  
 604 **Fig. 4.** Boundary layer analysis of heat flow. Temperature contrast  $\Delta T$  (grey band) and  
 605 thickness  $\delta$  (blue band) of the thermal boundary layer plotted against core-mantle  
 606 boundary heat flow, with the shading indicating the standard error in our determination of  
 607 the thermal conductivity (Supplementary Material Section S4). The green shaded area  
 608 denotes constraints on the temperature contrast across the core-mantle boundary. The  
 609 orange regions highlight constraints on the heat flow at the core-mantle boundary: upper  
 610 bound derived from the heat conducted down the core adiabat and lower bound derived  
 611 from the plume heat-flux and the factor 2-3 increase in the plume thermal anomaly with  
 612 depth (Davies, 2007).  
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616 **Fig. 5.** Heat-flow at the core-mantle boundary. Values calculated from our estimate of  
617 thermal conductivity and the seismic tomographic model of Kustowski et al. (2008) at 2800  
618 km depth.

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