1   Revision #1

Lorenz number and transport properties of Fe: Implications to the thermal conductivity at Earth's core-mantle boundary

Yuan Yin[1,2], Lin Wang[3†], Shuangmeng Zhai[2*], Yun Liu[1,4*]

[1]State Key Laboratory of Ore Deposit Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550081, China

[2]Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550081, China

[3]Earth and Planets Laboratory, Carnegie Institution for Science, Washington, DC 20015, USA

[4]Research Center for Planetary Science, College of Earth Sciences, Chengdu University of Technology, Chengdu 610059, China

[*]Corresponding authors: Shuangmeng Zhai (zhaishuangmeng@mail.gyig.ac.cn) and Yun Liu (liuyun@vip.gyig.ac.cn)

[†]Present address: Bayerisches Geoinstitut, University of Bayreuth, Bayreuth 95440, Germany.

Highlights:

- Four-wire van der Pauw method is applied in the multi-anvil press to measure the electrical resistivity of solid iron at 300 K and pressures to 26 GPa.

- The thermal conductivity of solid hcp iron is calculated as 129±9 W/m/K at 136 GPa and 300 K conditions by the first-principles molecular dynamics method.

- Electrical resistivity and thermal conductivity of solid hcp iron at Earth's CMB are estimated as ~76-83 μΩ·cm and 114 ± 6 W/m/K, respectively.

26   **Abstract**

27   The electrical resistivity (ρ) and thermal conductivity (κ) of the Earth's core compositions

28   are essential parameters for constraining the core's thermal state, the inner core age, and

29   the evolutionary history of the geodynamo. However, controversies persist between

30   experimental and computational results regarding the electronic transport properties (ρ

31   and κ) of the Earth's core. Iron is the major element in the core, and its transport

32   properties under high pressure and high temperature conditions are crucial for

33   understanding the core's thermal state. We measured the ρ values of solid iron using the

34   four-wire van der Pauw method at 300 K and pressures ranging from 3 to 26 GPa within

35   a multi-anvil press. For comparison, we calculated the ρ and κ values of hexagonal close-

36   packed (hcp) iron at conditions of 300-4100 K and 22-136 GPa using the first-principles

37   molecular dynamics (FPMD) method. Our calculations generally align with prior studies,

38   indicating that the electrical resistivity of solid hcp iron at Earth's core-mantle boundary

39   (CMB) conditions is ~76-83 $\mu\Omega$·cm. The resistivity of hcp iron changes small as it melts

40   from solid to liquid at pressures from 98 to 134 GPa. The impact of temperature and

41   pressure on the Lorenz numbers of solid hcp iron are investigated according to our

42   calculation results and previous studies. Under the CMB's pressure conditions, the κ of

43   hcp iron initially decreases with increasing temperature and subsequently increases. The

44   electron-electron scattering plays a dominant role at low temperatures and causes the

45   decrease in κ. At high temperatures, the increase of electronic specific heat significantly

46   increases the Lorentz number and κ. Overall, we estimate the κ of solid hcp iron at

47   CMB's condition to be 114 ± 6 W/m/K, slightly lower than the room temperature value

48   of 129±9 W/m/K at the same pressure. Our model shows that a 0-525 km thickness of a

49   thermally stratified layer may exist beneath the Earth's CMB depending on the core's

50   heat flow and thermal conductivity.

51

52   **Keywords**: iron, first-principles calculation, thermal conductivity, Earth's core, high

53   pressure experiments

3

54 **INTRODUCTION**

55   The Earth's core consists of Fe, Ni, and light elements like Si, S, O, C, H, and P, as

56   suggested by geochemical and geophysical observations (Li and Fei 2014). The thermal

57   conductivity (κ) of iron, the dominant element in the core, is thus essential to constrain

58   the core's thermal properties, which impact geodynamo models, the age of the inner core,

59   thermal evolution, and the magnetic field over geological time (Davies et al. 2015, 2022;

60   Driscoll and Bercovici 2014; Labrosse 2015; Nimmo 2015). Moreover, since electrons

61   are the primary transport particles in metals, the electrical resistivity (ρ, the reciprocal of

62   electrical conductivity) of iron is related to its electronic thermal conductivity (κ_{el}),

63   described by the Wiedemann-Franz law (WFL), $\kappa_{el} = LT/\rho$, where L is the Lorenz number,

64   and T is the temperature. Though the lattice (ionic) thermal conductivity contributes to

65   the total thermal conductivity of pure iron and iron alloys under the Earth's core-mantle

66   boundary (CMB) conditions, it is approximately 2-5% of the electronic part and is

67   negligible (Pozzo et al. 2012; Yue and Hu 2019). Thus, the resistivity of iron and iron

68   alloys can be used to estimate the thermal properties of the Earth's core, and extensive

69   studies on the resistivity have been conducted through experiments and first-principles

70   calculations based on density functional theory (DFT) (see the reviews of Berrada and

71   Secco 2021; Pommier et al. 2022; Yin et al. 2022a). The DFT method usually calculates

72   electronic part of thermal conductivity through the Chester-Thellung formulation of the

73   Kubo-Greenwood formula (Chester and Thellung 1961; Greenwood 1958; Kubo 1957)

74   and ionic contribution with the Green-Kubo formula (Kubo 1957). Furthermore, due to

75   the significant challenge in the experiment, only a few studies have reported the thermal

76   conductivity of iron and iron alloys measured in-situ at high pressure-temperature (*P-T*)

77   conditions (Hasegawa et al. 2019; Hsieh et al. 2020; Konôpková et al. 2016; Saha et al.

78   2020).

79   The thermal conductivity of the Earth's core remains debated. Resistivity measurements

80   and the first-principles calculations both suggest that the Earth's CMB has a high thermal

81   conductivity (~100 W/m/K) (Gomi et al. 2016; Li et al. 2022; Pozzo et al. 2012; Seagle et

82   al. 2013; Xu et al. 2018; Zhang et al. 2022). Nevertheless, thermal conductivity

83   measurement experiments indicate a low κ value of ~20-30 W/m/K at the CMB (Hsieh et

84   al. 2020; Konôpková et al. 2016). The low thermal conductivity in the core implies a low

85   rate of heat transfer by conduction, which can sustain a long-lived thermal dynamo and

86   extend the onset time of inner core solidification to ~3.4 Ga ago (Gomi et al. 2013; Hsieh

87   et al. 2020; Konôpková et al. 2016). Conversely, high thermal conductivity in the core

88   corresponds to a rapid cooling rate and a high initial temperature at the CMB, implying

89   that the solidification of the inner core started less than 1 Ga ago (Li et al. 2022). Pozzo et

90   al. (2022) attempted to reconcile experimental and computational transport properties of

91   Fe-Si alloys at high *P-T* conditions via the DFT calculation method. Compared to

92   experimental results (Hsieh et al. 2020), their calculated thermal conductivity with

93   electron-electron scattering (EES) correction matches the experiments at 72-106 GPa but

94   exceeds at 121-144 GPa.

95   As the high *P-T* resistivity of iron samples in most experiments (Inoue et al. 2020; Ohta

96   et al. 2023; Zhang et al. 2020) is computed based on room-temperature data, this room-

97   temperature information is a vital benchmark. The resistivity of iron at room temperature

98   varies between studies. Previous measurements indicate that the highest resistivity of

99   hexagonal-close-packed (hcp) iron at ~20 GPa and 300 K was ~24 $\mu\Omega$·cm (Gomi et al.

100   2013; Jaccard et al. 2002; Yong et al. 2019), nearly twice of the results (13 μΩ·cm) from

101   recent measurements (Ezenwa and Yoshino 2021; Zhang et al. 2020). One reason for this

102   discrepancy is the systematic uncertainty in estimating sample thickness under high

103   pressure conditions (Lobanov and Geballe 2022). With the DFT method, Gomi et al.

104   (2013) and Sha and Cohen (2011) calculated the resistivity of hcp iron at room

105   temperature and high pressure conditions using the ordered lattice structures, yielding

106   results deduced at 0 K, coming with lower resistivity values than experiments at 20-80

107   GPa. Moreover, Xu et al. (2018) calculated the electronic transport properties of hcp iron

108   under Earth's core conditions, including the electron-lattice scattering and the EES

109   contribution. However, they omitted the thermal disorder effect and did not address the

110   room temperature situation. Zhang et al. (2020) calculated the resistivity of hcp iron at

111   105 GPa and 2000 K, incorporating the thermal disorder effect and EES effect, aligning

112   with the experimental data. In some studies (Pozzo et al. 2014, 2022; Pozzo and Alfè

113   2016), the thermal disorder effect was included in the calculations for solid hcp iron and

114   iron-silicon alloys, but no discussions on the room temperature conditions.

115   The Wiedemann-Franz law connects electrical resistivity and electronic thermal

116   conductivity through the Lorentz number. Based on the assumption that WFL relies on

117   elastic electron scattering (Klemens and Williams 1986; Uher 2004), Lorentz number has

118   a Sommerfeld theoretical value (L_0) of 2.445×10^{-8} WΩK^{-2}. The inelastic scattering of

119   electrons in thermal conduction makes the Lorentz number deviate from the L_0. A

120   systematic investigation on the Lorenz number for iron and iron-silicon alloys under high

121   *P-T* conditions was conducted by Secco (2017), revealing that the Lorenz number

122   positively deviates from L_0 when the electronic component fails to fully describe the total

123   thermal conductivity. This departure was observed in pure Fe and Fe-Si alloys under

124   ambient pressure and high temperature conditions (Secco 2017). Under high pressures,

125   the inelastic scattering of electrons is enhanced with rising temperature, causing the

126   Lorenz number to fall below L_0 (Secco 2017). As a result, the Lorenz number exhibits

127   variability under high P-T conditions (Pozzo et al. 2022). Experimental results

128   (Konôpková et al. 2016; Zhang et al. 2020) roughly suggest that the Lorentz number of

129   hcp iron at 80-200 GPa and 2000-3000 K is about 0.8-1.0×10^{-8} $W\Omega K^{-2}$ (Yin et al. 2022a),

130   significantly lower than L_0. Even in the case of a Fermi liquid with only inelastic

131   scattering, the L value of hcp iron under Earth's core conditions is 1.59×10^{-8} $W\Omega K^{-2}$,

132   about $0.65L_0$ (Pourovskii et al. 2017), which still exceeds experimental observations.

133   Gomi and Yoshino (2018) calculated the Lorentz number of iron-light elements (Si, Ni, S,

134   C, N, and O) alloys under high P-T conditions, suggesting that the species and

135   concentration of light elements significantly affect the Lorentz number, particularly under

136   high temperature conditions. Liquid Fe-Si-O alloys exhibit smaller Lorentz numbers than

137   pure iron, indicating that light elements can decrease the L values (Pozzo et al. 2013). In

138   addition, Pourovskii et al. (2020) theoretically calculated the L value at Earth's core

139   conditions for the perfect hcp iron lattice at 1.57×10^{-8} $W\Omega K^{-2}$ and for the thermo-

140   disordered one at 2.28×10^{-8} $W\Omega K^{-2}$. However, there are limited reports on the Lorenz

141   number of iron under room temperature conditions.

142   To comprehensively understand the temperature and pressure effects on the electronic

143   transport properties of iron, we applied both experiments and the first-principles

144   calculation method in this study. Though the resistivity of iron has been widely measured

145   and discussed in the multi-anvil press experiments, most previous studies used the

146 conventional four-wire method for resistivity measurement (Ezenwa and Yoshino 2021;

147 Secco and Schloessin 1989; Yong et al. 2019). The four-wire van der Pauw method is

148 broadly employed in diamond-anvil cell experiments to measure the resistivity of iron

149 and iron alloys (Gomi et al. 2013; Seagle et al. 2013; Zhang et al. 2020). For comparison,

150 we used the van der Pauw method to measure the resistivity of iron at room temperature

151 (300 K) and pressures from 3 to 26 GPa in the multi-anvil press. To broaden the pressure

152 and temperature range, we calculated the electrical resistivity of hcp iron at both room

153 temperature and high temperature conditions (300-4100 K and 22-136 GPa). Most

154 previous studies only used ordered lattice structures to calculate the electronic transport

155 properties of solid hcp iron at 300 K (Gomi et al. 2013; Sha and Cohen 2011) and high

156 temperature conditions (Xu et al. 2018). In this study, we applied the first-principles

157 molecular dynamics (FPMD) method and the Kubo-Greenwood formula (Greenwood

158 1958; Kubo 1957). The FPMD method generates disordered lattice structures and

159 naturally includes the thermal disorder effect. Using the Chester-Thellung-Kubo-

160 Greenwood approach (Chester and Thellung 1961), we also estimated the electronic

161 thermal conductivity. Based on the results, we discussed the temperature and pressure

162 effect on the Lorentz number and transport properties of hcp iron at high P-T conditions.

163 These results are also applied to constrain the thermal conductivity in the Earth's core,

164 subsequently used to estimate the adiabatic heat flow in the core, inner core age, and the

165 thermally stratified layer thickness beneath the CMB.

166

167   **METHODS AND CALCULATIONS**

168 **Electrical resistivity measurement of iron**

8

169   All experiments were conducted at room temperature (300 K) and 3-26 GPa in an 800-

170   ton multi-anvil press in the Earth and Planets Laboratory at Carnegie Institute for Science.

171   For high pressure studies, we used an 8/3 assembly, in which the Cr_2O_3-doped MgO

172   octahedron has an 8 mm length edge, and tungsten carbide has a 3 mm length corner-

173   truncated edge. An iron plate sample with a thickness of 0.5 mm and a diameter of 1.6

174   mm was sandwiched by two Al_2O_3 rods and placed at the center of the assembly.

175   Additionally, two MgO bars were placed on top of Al_2O_3 rods to serve as pressure

176   transition materials. The 8/3 assembly sketch is shown in Figure S1 in the supporting

177   information. For the resistivity measurements, we utilized a four-wire van der Pauw

178   method (van der Pauw 1958) and used four tungsten wires (a diameter of 0.1 mm) as

179   leads to measure sample's resistance. The van der Pauw method requires the contact

180   point between the wire and the sample to be as small as possible to minimize errors. Our

181   tungsten wires were much smaller than the sample size, and the contact area at the iron

182   plate's edge was also small. It is crucial to ensure that the sample had a flat shape with

183   uniform thickness and was homogeneous and isotropic. Our sample, a pure iron plate,

184   meets these requirements. Controlling sample deformation and thickness during the

185   experiment presented challenges, but we used two Al_2O_3 rods to minimize the impact of

186   deformation. Figure S1 shows no significant deformation was observed in the recovered

187   samples.

188   The measurement strategy is similar to our previous study (Yin et al. 2022b). We first

189   press the sample to the target pressure, hold the pressure, and then start resistance

190   measurement. All resistance data are acquired during the compression process. However,

191   due to experimental challenges, only two runs yielded reasonable data. The U1419 run

192   reached a maximum pressure of 22.3 GPa before the tungsten leads broke at higher

193   pressures. In the U1423 run, no data was recorded below 13 GPa due to lead

194   disconnection. The pressure uncertainty is 0.5 GPa in our experiments. After experiments,

195   the recovered samples were mounted in epoxy resin and subsequently ground and

196   polished to measure the sample's thickness. The iron plate sample had a thickness of 0.5

197   mm before the experiment and 0.39-0.43 mm after the experiment (Figure S1). With

198   these post-compression dimensions (sample thickness) and measured resistances at 300 K,

199   we calculated the resistivity at different pressure conditions. As the Al_2O_3 rods are much

200   harder than pure iron, we neglected the volume change during decompression. The

201   change in thickness of the iron plates during compression was estimated using an

202   equation of the state for pure iron (Zhang and Guyot, 1999). The total estimation of

203   resistivity error is from the geometry uncertainty and is less than 4% in our experiments.

204

205   **First-principles calculations**

206   The electronic transport properties of iron at 300-4100 K and 22-136 GPa were

207   calculated using FPMD and the Kubo-Greenwood formula in the Computational

208   Geochemistry Lab at the Institute of Geochemistry, Chinese Academy of Sciences.

209   Calculations were carried out using the Vienna Ab initio Simulation Packages (VASP), a

210   plane wave density functional code developed by Kresse and Furthmüller (1996), and

211   incorporated the projector augmented wave (PAW) method (Blöchl 1994; Kresse and

212   Jouber, 1999) to represent ion-electron interaction. The potential file is the Perdew,

213   Burke, and Ernzerhof (Perdew et al. 1996) type ($3p^6 4s^1 3d^7$ valence configuration,

214   labelled PAW_PBE Fe_pv), and the plane-wave cutoff energy is 400 eV (similar to Li et

215   al. 2022 and Wagle et al. 2018). The supercells of the hcp Fe have 150 atoms,

216   comparable to the literature (Li et al. 2022; Pourovskii et al. 2020; Wagle et al. 2018).

217   The unit cell's lattice parameters were derived from high pressure X-ray diffraction

218   experiments in the literature (Anzellini et al. 2013; Dewaele et al. 2006; Fei et al. 2016)

219   (Table S1). For comparison, additional calculations for hcp iron were conducted using the

220   calculated lattice parameters at 0 K, which displayed comparable c/a ratios to previous

221   theoretical studies (Kleinschmidt et al. 2023; Pourovskii et al. 2014). Figure S2 shows

222   that the c/a ratios calculated by the DFT method at 0 K are smaller than the experimental

223   results at 300 K. Kleinschmidt et al. (2023) suggested that the electronic transport

224   properties of hcp iron are insensitive to the c/a ratios under high temperature conditions.

225   However, the impact of c/a ratios under room temperature conditions remains unclear.

226   Volume is a significant parameter in the Kubo-Greenwood formula, and thermal

227   expansion influences the volume under high temperatures. Thus, we exclusively used the

228   experimental lattice parameter to construct supercells at high temperatures ranging from

229   1500 to 4100 K. Then, we employed FPMD with the canonical ensemble (NVT: number

230   of atoms, volume, and temperatures are constant) to update the atomic coordinates of the

231   supercell at a time step of 1 fs. Temperature is controlled by the Nosé-Hoover thermostat

232   (Hoover 1985; Nosé 1984). The FPMD simulation ran for 11 ps, with the first ps

233   discarded for equilibration, and one snapshot of nuclear positions was extracted every

234   500 molecular dynamic steps from the final 5 ps. The electronic states were occupied

235   according to Fermi-Dirac statistics at the thermostat's temperature, and only the gamma

236   point was used to sample the Brillouin zone during molecular dynamics simulations.

237 Using a VASP post-processing tool, KG4VASP (Di Paola et al. 2020), we calculated the

238 electrical resistivity through the Kubo-Greenwood formula (Greenwood 1958; Kubo

239 1957) and electronic thermal conductivity with the Chester-Thellung-Kubo-Greenwood

240 formula (Chester and Thellung 1961). The electrical and thermal conductivities are

241 derived as the frequency in Onsager coefficients in the above formulas approach zero (Di

242 Paola et al. 2020). Like Korell et al. (2019), we employed a linear extrapolation method

243 when the frequency equals zero as the results usually unphysically decrease at very small

244 frequencies. For every snapshot, we used a dense grid of 4x4x4 k-points in the Gamma

245 centered scheme, which ensured convergence in calculations. The Dirac delta functions

246 were approximated with one Gaussian function with a spreading of 10 meV, minimizing

247 its value to remove the small oscillations in the optical conductivity arising from the

248 discretization of the band structure. After calculation, we averaged ρ and κ_{el} over the

249 snapshots and considered one standard deviation as the uncertainty. In this study, the

250 electronic transport properties were calculated at the DFT level, including electron-lattice

251 scattering, while the EES was disregarded. Given the computational cost and its slight

252 impact on results at pressures above 50 GPa (Korell et al. 2019), the spin polarization

253 effect was also neglected. The Lorenz number ($L=k_{el}*\rho/T$) was determined through the

254 WFL based on our electrical and thermal conductivity results.

255

RESULTS AND DISCUSSIONS

257 **Electrical resistivity of hcp Fe**

258   In Figure 1a, we present the results of our experimental measurements of iron's electrical

259   resistivity under conditions of 3-26 GPa and 300 K, alongside our theoretical calculation

260   results at 22-136 GPa and 300 K. Figure 1a also includes the previous experimental

261   results (Ezenwa and Yoshino 2021; Gomi et al. 2013; Jaccard et al. 2002; Seagle et al.

262   2013; Ohta et al. 2023; Zhang et al. 2018, 2020) and theoretical calculation results (Gomi

263   et al. 2013; Sha and Cohen 2011). When the pressure increases from 3 to 11 GPa, the

264   iron's resistivity decreases, followed by a rapid increase from 11 to 19 GPa. Then,

265   resistivity decreases once again as the pressure rises from 19 to 26 GPa (Figure 1a). The

266   inflection point in resistivity at 11 GPa is due to the phase transition of iron from bcc to

267   hcp phase, ending at 19 GPa. Within the 11-19 GPa range, the sample is a mixture of bcc

268   and hcp phases. Our results are roughly consistent with those of Ezenwa and Yoshino

269   (2021), who measured the bcc to hcp phase transition pressure range between 12-20 GPa.

270   Our results align with Seagle et al. (2013) and Zhang et al. (2020) within the range of

271   uncertainties. However, it is worth noting that, below 5 GPa, the results from Ezenwa and

272   Yoshino (2021) were significantly larger than those of this study and Zhang et al. (2020).

273   In the study by Ezenwa and Yoshino (2021), iron probes were used for resistivity

274   measurements, while we used tungsten probes, which are also used and discussed in other

275   studies (Silber et al. 2018; Berrada et al. 2021). The diffusion of probe material into the

276   sample impacts resistivity measurements under high temperature conditions. Given that

277   our experiments were conducted at room temperature, such influence is negligible. The

278   sample deformation and measurement approach may contribute to the variations between

279   the results of Ezenwa and Yoshino (2021) and this study. The highest resistivity of hcp

280   iron measured in this study is about 14.1-15.3 $\mu\Omega$·cm at 300 K, consistent with certain

13

281   literature results (Ezenwa and Yoshino 2021; Zhang et al. 2020), but lower than others

282   (Gomi et al. 2013; Jaccard et al. 2002; Zhang et al. 2018). Therefore, the electrical

283   resistivity of hcp iron at 300 K and pressures below 60 GPa may not be as high as some

284   previous estimations (Figure 1a).

285   In comparison with the results by Sha and Cohen (2011) and Gomi et al. (2013), our

286   calculated ρ values for hcp iron at 22-136 GPa and 300 K are generally consistent with

287   experiments (Figure 1a). Notably, in Figure 1a, the R2 simulation (solid down triangle)

288   employed experimental lattice parameters at 300 K from the literature, while the R1

289   simulation (solid up triangle) used the optimized lattice parameters to the lowest energy

290   at 0 K, based on DFT calculations. Though these runs exhibit rough consistency below 80

291   GPa, discrepancies emerge at 80-136 GPa. This is probably due to the different c/a ratios

292   of hcp structure between the experimental data and calculations (Figure S2). Korell et al.

293   (2019) found that spin-polarization impacts the electronic transport properties of liquid

294   iron at 20-50 GPa, which may also impact the solid hcp iron. Pourovskii et al. (2014)

295   indicated that the contribution of EES to the resistivity of hcp iron is ~5% of the total

296   resistivity at 20 GPa and 294 K, and the contribution decreases with increasing pressures.

297   In this study, our calculated results at 20-60 GPa have slightly lower resistivity and much

298   higher thermal conductivity values than experiments (Figure 1). It is possibly due to the

299   omission of spin-polarization and EES effects, both of which tend to increase resistivity

300   and decrease thermal conductivity under high P-T conditions (Korell et al. 2019;

301   Pourovskii et al. 2020).

302   Moreover, we conducted resistivity calculations for hcp iron at high P-T conditions,

303   including 98 GPa (1562 K and 3521 K), 132 GPa (2725 K), and 134 GPa (4114 K). The

304   results are shown in Figure 2a and Table 1. Generally, our results agree with both the

305   experimental data (Zhang et al. 2020) and calculation results (Korell et al. 2019; Xu et al.

306   2018; Zhang et al. 2020). Xu et al. (2018) used ordered lattice structures for simulation,

307   applied a parallel resistor correction for resistivity saturation, and included the EES effect.

308   In Figure 2a, the resistivity calculated by Xu et al. (2018) is slightly higher than ours,

309   likely due to the inclusion of the EES effect. No remarkable resistivity saturation is

310   observed in hcp iron below 134 GPa and 4114 K (Figure 2a). The electrical resistivity of

311   hcp iron shows a quasi-linear temperature dependence in both computational and

312   experimental configurations, suggesting conformability with the Bloch-Grüneisen

313   formula. Our results are also consistent with the calculation results from Korell et al.

314   (2019) under conditions of 135 GPa and 3700 K, indicating a negligible impact from the

315   spin-polarization effect in such conditions. In a recent experimental study, resistivity

316   measurements were conducted for liquid iron at pressures up to 140 GPa (Ohta et al.

317   2023). Figure 2a illustrates that liquid iron at 105 and 135 GPa has slightly higher

318   resistivities than solid hcp iron at 98 and 134 GPa. This implies that the transition from

319   solid hcp iron to a liquid state may not significantly increase the resistivity at

320   pressures >105 GPa. According to previous DFT calculations, the resistivity of hcp iron

321   only experiences a minor increase of 6-10 % upon melting under Earth's core conditions

322   (Pozzo et al. 2014, 2012; Xu et al. 2018).

323

324   **Thermal conductivity of hcp Fe**

325   Figure 1b shows our computed thermal conductivity of hcp Fe with previous

326   experimental (Hsieh et al. 2020; Ohta et al. 2018) and computational results

15

327   (Kleinschmidt et al. 2023). Hsieh et al. (2020) measured the thermal conductivity of bcc

328   and hcp iron at 1-120 GPa and 300 K using the time-domain thermoreflectance (TDTR)

329   technique, a well-established ultrafast metrology method that accurately measures the

330   thermal conductivity of materials under high pressure conditions. The thermal

331   conductivity of iron first increases from 76 to 88 W/m/K as pressure increases from 1 to

332   13 GPa, then rapidly decreases to ~55 W/m/K at 22 GPa. This value remains nearly

333   constant between 22 and 45 GPa, subsequently increasing to 120 ± 30 W/m/K as pressure

334   rises from 45 to 120 GPa (Figure 1b). Compared to the results from Hsieh et al. (2020),

335   Ohta et al. (2018) reported similar κ values at 40-45 GPa but markedly lower values at

336   16-24 GPa. They employed thermal diffusivity, density, and isobaric heat capacity to

337   calculate thermal conductivity (Ohta et al. 2018), and the observed discrepancies in κ

338   values at ~20 GPa may be attributed to uncertainties arising from heat capacity. The

339   markable change in the thermal conductivity at 13 GPa is a consequence of the phase

340   transition from bcc to hcp Fe (Figure 1b). The low and nearly constant experimental

341   thermal conductivity at 22-45 GPa is possibly due to the electronic topological transition

342   of pure Fe (Glazyrin et al. 2013).

343   Compared to the experimental data, our calculated κ values for hcp iron are higher at 22-

344   80 GPa but consistent at 80-105 GPa and 300 K (Figure 1b). In Figure 1b, the electronic

345   thermal conductivity in the R1 simulation decreases from 134 to 86 W/m/K as the

346   pressure increases from 60 to 136 GPa, while that of the R2 simulation increases from

347   116 to 129 W/m/K as the pressure increases from 50 to 136 GPa (Table 1). However, at

348   room temperature, the total thermal conductivity of hcp iron increases with increasing

349   pressure from 80 to 136 GPa (Hsieh et al. 2020). The unexpected decrease of thermal

16

350   conductivity in R1 simulation is due to its lattice parameter that was derived at 0 K by

351   DFT calculations. The increase of resistivity between 80-136 GPa in R1 simulation, as

352   shown in Figure 1a, makes it expected in the decrease of thermal conductivity. Therefore,

353   the experimental lattice structures (R2) are more suitable than those (R1) derived from

354   DFT calculations at 0 K for estimating the electronic transport properties of iron under

355   room temperature conditions. At 22-60 GPa, we observe that the calculated resistivity is

356   slightly lower than that in experiments, but the calculated thermal conductivity is much

357   higher. This difference is likely due to disregarding EES and spin-polarization effects

358   during calculation. At 300 K and pressures higher than 50 GPa, the EES and spin-

359   polarization effects become very small (Korell et al. 2019, Pourovskii 2014). Under high

360   *P-T* conditions, the spin-polarization effect impacts resistivity and thermal conductivity

361   almost equally (Korell et al. 2019), while EES affects thermal conductivity more than

362   resistivity (Pourovskii et al. 2020). Hence, the EES effect may have a dominant impact

363   within the pressure range of 22-60 GPa at 300 K. Above 80 GPa, the pressure

364   dependence of hcp iron's thermal conductivity on the isotherm of 1850 K reported by

365   Kleinschmidt et al. (2023) agrees with our result at 300 K (Figure 1b). Overall, our

366   results estimate the κ for hcp iron as 129 ± 9 W/m/K at 136 GPa and 300 K (Table 1).

367   Konôpková et al. (2016) suggested that the thermal conductivity of hcp iron at the Earth's

368   CMB conditions is as low as 35-55 W/m/K. Figure 2b shows that the electronic thermal

369   conductivity of hcp iron at 2725-4114 K and 132-134 GPa, similar to CMB conditions, is

370   130-158 W/m/K, nearly three times of the experimental results. The EES significantly

371   affects the electronic transport properties of pure Fe and Fe-Si alloys (Pourovskii et al.

372   2014, 2020; Zhang et al. 2022). The EES contribution to the total resistivity of hcp iron

373   increases quasi-linearly from 0 to 28.5% as the temperature increases from 300 to 4000 K

374   at 110-150 GPa (see Figure S7 in the study by Zhang et al. (2022)). Under the Earth's

375   core conditions (360 GPa and 5802 K), including the EES effect, the electrical resistivity

376   of solid hcp iron increased by 9%, and the thermal conductivity decreased by 24%

377   (Pourovskii et al. 2020). Though thermal disorder is the dominant contribution to total

378   scattering, the impact of inelastic scattering from EES cannot be discarded (Pourovskii et

379   al. 2020). Our FPMD calculation method naturally includes the thermal disorder effect

380   but lacks the EES effect. Here we assume that the impact of EES on the electronic

381   thermal conductivity of solid hcp iron at Earth's CMB conditions is temperature-

382   dependent (Xu et al. 2018; Zhang et al. 2022) and increases linearly from 0 to 28.5% as

383   temperature rises from 300 to 4000 K (Figure S3). As mentioned above, EES impacts

384   thermal conductivity more than electrical resistivity. Thus, our assumption may

385   underestimate the EES effect at Earth's CMB condition.

386   With the EES correction, the thermal conductivity of hcp iron in this study at 98-136 GPa

387   and high temperatures is accordingly reduced to somewhere roughly aligns with the

388   results of the DFT study by Xu et al. (2018), who also accounted for the EES effect in

389   their calculations (Figure 2b). Above all, the EES correction is essential in the calculation

390   of solid iron's thermal conductivity, particularly under high temperature conditions.

391   Figure 2b illustrates that, at 105-136 GPa, the electronic thermal conductivity of hcp iron

392   first decreases with increasing temperature from 300 to ~2000-3000 K and then gradually

393   increases as the temperature rises to 4000 K. In contrast, experiments directly measuring

394   the thermal conductivity suggest that the temperature dependence of the pure hcp iron's

395   thermal conductivity follows a $T^{-1/2}$ relationship (Konôpková et al. 2016) at CMB

396   conditions, deviating significantly from the predicted trend from calculations (Figure 2b).

397   To explain such low thermal conductivity of hcp iron in the experiment, apart from the

398   EES effect, stronger inelastic scattering mechanisms are required to reduce electronic

399   thermal conductivity. At 106-134 GPa and ~1800 K, our calculated results match the

400   upper boundary of thermal conductivity of iron measured by Saha et al. (2020) (Figure

401   2b). Overall, solid hcp iron's electronic thermal conductivity (with EES correction) at

402   134 GPa and 4100 K is calculated as 114 ± 6 W/m/K, consistent with previous studies

403   (Xu et al. 2018; Zhang et al. 2020).

404

Lorenz number of hcp Fe

406   We computed the total Lorentz number of iron at room temperature through the electrical

407   resistivity (Seagle et al. 2013; Zhang et al. 2020) and thermal conductivity (Hsieh et al.

408   2020), both directly measured in experiments. We only considered the contribution from

409   thermal conductivity on the uncertainty of the total Lorentz number, as the errors for the

410   experimental resistivity measurement are smaller than those of the thermal conductivity

411   measurement. We have shown that our experimental and calculated results are partly

412   consistent with those measured in the literature (Hsieh et al. 2020; Seagle et al. 2013;

413   Zhang et al. 2020). It remains reasonable to compare the Lorentz number calculated from

414   these literature data with our calculation results, despite large uncertainty arising from

415   different data sources. In Figure 3a, an experimental Lorentz number is as low as ~1.50

416    $\times 10^{-8}$ WΩK^{-2} at 22-55 GPa and 300 K, smaller than the L_0, indicating a significant

417   inelastic scattering effect in this pressure range. The Lorentz number at pressures

418   between 20 and 50 GPa experiences a drop. It is possibly because the resistivity of hcp

419   iron decreases largely in this pressure range, while the thermal conductivity remains

420   consistent and lower than our calculations based on the assumption of elastic electron

421   scattering. Strong inelastic electron scattering processes can cause the L value to

422   negatively depart from L_0 (Secco 2017). The EES effect induces strong inelastic electron

423   scattering in hcp iron at a pressure range of 22-55 GPa and 300 K and causes the

424   remarkably lower Lorentz numbers compared to L_0 and calculated results from this study.

425   Above 50 GPa, the experimental Lorentz number gradually increases to ~2.3×10^{-8} WΩK^{-}

426   ^{2} and remains relatively constant at higher pressures. Pourovskii et al. (2020) calculated

427   the Lorentz number for a perfect lattice structure of solid hcp iron, with $L = 1.57\times10^{-8}$

428   WΩK^{-2}, while for the disordered lattice structure, $L = 2.28\times10^{-8}$ WΩK^{-2}. At 300 K and

429   below 60 GPa, the calculated Lorentz number in this study varies from 2.59 to 2.73×10^{-8}

430   WΩK^{-2}, exceeding both the L_0 and experimental values (Figure 3a; Table 1). At 300 K

431   and 80-136 GPa, the calculated Lorentz number is in the range of 2.1-2.3×10^{-8} WΩK^{-2}

432   (Figure 3a, Table 1), lower than the L_0 value but consistent with experiments.

433   Under 110-190 GPa and 2000-3000 K conditions, Xu et al. (2018) reported the L value of

434   hcp iron as 2.1 $\times10^{-8}$ WΩK^{-2}. As the EES effect on the hcp iron's electrical resistivity is

435   temperature-dependent suggested by Zhang et al. (2022), we accordingly reduce 0-28.5%

436   from the calculated Lorentz number of hcp iron in this study, as shown in Figure 3b,

437   resulting in consistent data with Xu et al. (2018). Pourovskii et al. (2017) indicated that

438   the fraction of EES is enhanced with increasing temperature, and the L value of hcp iron

439   under inner core's pressure conditions decreases from L_0 to ~$0.65L_0$ (1.59×10^{-8} WΩK^{-2},

440   representing the pure Fermi liquid result) as temperatures rise from 300 to 30000 K

441   (Figure 3b, black short dot line). Additionally, Gomi and Yoshino (2018), considering

442 ordered lattice structures (no thermal disorder and EES effect), calculated the Lorentz

443 number of pure iron and iron alloys. Their results indicate a similar positive temperature-

444 dependence of hcp iron's Lorentz number as the temperatures increase from 300 to 4000

445 K at 120 GPa (black short dash line in Figure 3b). The inset graph in Figure 3b

446 demonstrates that the Lorentz number (with EES correction) of hcp iron decreases with

447 increasing temperatures from 300 to 2000-3000 K and then increases with increasing

448 temperatures to 4000 K at 98-140 GPa. Under high *P-T* conditions, the total Lorentz

449 numbers derived from experimental studies by Zhang et al. (2020), Saha et al. (2020),

450 and Konôpková et al. (2016) are as low as $\sim 0.8 \times 10^{-8}$ $W\Omega K^{-2}$, which seems unreasonable

451 because it is much lower than the case of pure Fermi liquid (1.59×10^{-8} $W\Omega K^{-2}$) with only

452 inelastic scattering (Pourovskii et al. 2017) (Figure 3a). It is essential to acknowledge that

453 the total Lorentz numbers derived from non-internal experiments exhibit considerable

454 uncertainty under high-temperature conditions, which could potentially lead to

455 unreasonable interpretations.

456 As shown in Figure 2b, the computed κ of hcp Fe at 105-136 GPa initially decreases with

457 increasing temperature and subsequently increases. The main reason is the total Lorentz

458 number. In the case of a constant Lorentz number for pure metals, $\kappa \propto T/\rho$. The residual

459 resistivity (ρ_0) causes the rapid decrease in κ at temperatures below 1000 K, as $\rho = \rho_0 +$

460 A*T* (Williams, 1998). At high temperatures, $\rho \approx$ A*T*, thus κ approaches to a constant.

461 However, the total Lorentz number, *L(T)* is a function of temperature. When the slope of

462 *L(T)* is positive, the κ will increase with increasing temperature at high temperatures. This

463 is the case in this work and the study of Gomi et al. (2018). Including the EES effect, the

464 *L* values are reduced to below the Sommerfeld value (L_0) (Figure 3b). However, the *L* is

465   proportional to the electronic specific heat, and the high-order terms of the electronic

466   specific heat cause the deviation of L from the L_0 (Gomi et al., 2015). For hcp iron, below

467   ~2000 K, both numerical and Sommerfeld values of the electronic specific heat show

468   similar linear T-dependences (Boness et al., 1986), suggesting a small slope of L. In this

469   temperature range, the EES effect increases faster than the L as rising temperatures,

470   indicating an EES dominant effect and thus a decrease in κ. But above ~2000 K, the

471   numerical values increase more rapidly than the Sommerfeld value (Gomi et al., 2018)

472   (Figure 3b, S4). Thus, the slope of L becomes larger than that of EES, increasing κ. In

473   comparison to Gomi et al. (2018), our L values are smaller due to the thermal disorder

474   effect (Figure. 3b), but the slope of L under high temperatures is indeed large enough to

475   increase the κ. In summary, the thermal disorder effect systematically reduces the L of

476   hcp iron, the EES effect reduces the L with a linear T-dependence, and the increase of

477   electronic specific heat rapidly enlarges the L at high temperatures.

478

479   **IMPLICATIONS**

480   **Thermal conductivity at the Earth's CMB**

481   At 134 GPa and 4100 K, the thermal conductivity of hcp iron without EES correction is

482   about 158 ± 8 W/m/K, much higher than 100 ± 10 W/m/K estimated by Zhang et al.

483   (2020) and ~97 W/m/K computed by Xu et al. (2018). After EES correcting, the thermal

484   conductivity is reduced to 114 ± 6 W/m/K. Pozzo et al. (2022) pointed out that resistivity

485   saturation may occur for hcp iron above 3000 K. However, our data shows no obvious

486   resistivity saturation for hcp iron from 1500 to 4100 K (Figure 2a). Xu et al. (2018)

487   computed the saturation resistivity of hcp-Fe under the conditions of the Earth's outer

488   core (136 GPa) and inner core (360 GPa) to be 155 and 143 $\mu\Omega\cdot$cm, respectively, using

489   the criterion mean free path. At 134 GPa and 4100 K, the computed and experimental

490   resistivity of hcp iron is about 80 $\mu\Omega\cdot$cm, far below the saturation resistivity (Figure 2a).

491   Thus, no apparent resistivity saturation for hcp iron is found in this study. Using the real-

492   time formalism of time-dependent DFT method, Ramakrishna et al. (2023) calculated the

493   electrical resistivity of hcp iron at conditions related to Earth's core. They detected no

494   apparent resistivity saturation, even at temperature as high as 6000 K.

495   With the WFL, we estimated the thermal conductivity of hcp iron at the Earth's CMB

496   conditions according to the Bloch-Grüneisen fit data for the resistivity (Figure 2a) from

497   Zhang et al. (2020) and Lorentz numbers (Figure 3b) from this study. As show in the

498   inset of Figure 3b, the Lorentz number varies around 2.20×10^{-8} WΩK^{-2} (0.9 times of L_0),

499   depending on the temperature and pressure. We set the L value of hcp iron to vary from

500   2.0 to 2.4×10^{-8} WΩK^{-2} at the CMB conditions. The short-dashed lines and grey regions

501   in Figure 2b show the estimation of thermal conductivity at 105 and 136 GPa and

502   temperatures of 300-4100 K. Thus, we estimated the thermal conductivity of solid hcp

503   iron at Earth's CMB conditions as 106-127 W/m/K (136 GPa and 4100 K). The upper

504   boundary of thermal conductivity measured by Saha et al. (2020) falls into the estimated

505   range. After correcting the potential thickness errors of iron samples in the experiments,

506   Lobanov and Geballe (2022) revised the thermal conductivity of hcp iron as 133 W/m/K

507   at Earth's CMB conditions, slightly higher than our estimations. For liquid iron at Earth's

508   CMB conditions, its thermal conductivity could be lower at ~95-114 W/m/K because the

509   electrical resistivity of solid hcp iron may increase ~6-10 % at the onset of melting

23

510   (Figure 2a) (Yin et al. 2022a). Furthermore, the lattice thermal conductivity of an iron-

511   rich liquid outer core is about 2.5-4 W/m/K, which is negligible compared to the

512   electronic thermal conductivity (Pozzo et al., 2012). The light elements, such as silicon

513   and oxygen, in the Earth's liquid outer core can also lower the thermal conductivity of

514   iron. With the EES correction (~24% reduction on the κ) to the calculated thermal

515   conductivity of the Fe-Si (Pozzo et al. 2022) and Fe-Ni-O (Li et al. 2022) system, the

516   thermal conductivity at the Earth's CMB is estimated as ~75-85 W/m/K. Therefore, we

517   suggest that the reasonable thermal conductivity at the Earth's CMB is likely from 70 to

518   90 W/m/K.

519

520   **Stable thermal stratification**

521   The thermal state of Earth's outer core depends on the core compositions, CMB

522   temperature, and thermal conductivity (Nimmo 2015). The adiabatic heat flow (Q_{ad}) in

523   the core can be approximately computed through the formula:

524     $$Q_{ad} = -4\pi r^2 \kappa \frac{T_{ad}}{dr} \tag{1}$$

525   where r is the radius, κ is the thermal conductivity, $\frac{T_{ad}}{dr}$ is the adiabatic temperature

526   gradient. The adiabatic temperature gradient at CMB is about 0.9-1.0 K/km (Davies et al.

527   2015; Labrosse 2015). Here we simply assumed that the total heat flow in the core (Q_T) is

528   also a function of radius, so that:

529     $$Q_T = Q_{cmb} = -4\pi r^2 \kappa \frac{dT}{dr} \tag{2}$$

24

530   which is a good approximation for the heat flow near the CMB (Q_{cmb}). When the

531   uppermost core is subadiabatic, $Q_{cmb} < Q_{ad}$, a thermal stratification layer may exist

532   beneath the CMB (Davies 2015; Nimmo 2015; Zhang et al. 2022). Here, we calculated

533   the adiabatic heat flow across the CMB, ranging from 13.7 TW (with κ = 90 W/m/K) to

534   10.7 TW (with κ = 70 W/m/K), by assuming a 1.0 K/km adiabatic temperature gradient at

535   the topmost of outer core. The present-day total heat flow across the lowermost mantle is

536   estimated at ~10-12 TW according to the thermal conductivity (~10 W/m/K) and

537   temperature gradient data for the lowermost mantle (Okuda et al. 2020). Given the low

538   thermal conductivity of liquid silicate under CMB conditions (~5.3 W/m/K, Deng and

539   Stixrude 2021), the present-day Q_{cmb} may be reduced to 6-7 TW. Davies et al. (2022)

540   employed numerical geodynamo simulations with theoretical scaling laws to propose that

541   a present-day Q_{cmb} in the range of 12-16 TW best aligns with the model for the

542   evolutionary history of Earth's magnetic field strength. However, Frost et al. (2022)

543   suggest a Q_{cmb} of ~15 TW derived from reasonable historic mantle temperatures. In the

544   models from Li et al. (2022), the core's entropy remains positive throughout Earth's

545   history when Q_{cmb} exceeds 7 TW, supporting the existence of the geomagnetic field

546   beginning at 3.5 Ga ago.

547   In the case of high thermal conductivity (111.68-182.33 W/m/K) in the core, Li et al.

548   (2022) calculated the inner core's age in a range from 0.502 to 1.221 Ga (Figure 4).

549   Pozzo et al. (2022), based on a low thermal conductivity of 75-81 W/m/K at Earth's

550   CMB and considering radiogenic heating contribution with 30 ppm ^{40}K in the core,

551   estimated the inner core's age as 0.4-0.8 Ga. Davies et al. (2015) proposed that

552   subadiabatic condition could result in the formation of a thermally stratified layer,

553   potentially hundreds of kilometers thick and stable against thermal convection, beneath

554   the CMB. Using the same approach as Zhang et al. (2022) and assuming the potential

555   thermal conductivity of ~70-90 W/m/K at the CMB, we calculated the thickness of the

556   stratified layer at various Q_{cmb} values (Figure 4). All the parameters used for this

557   calculation are listed in Table S2. When Q_{cmb} is below 13.7 TW, thermal stratification

558   can occur, with its thickness varying from 0 to 1000 km as Q_{cmb} further decreases to 7

559   TW. Notably, thermal stratification is not feasible at the uppermost of the liquid core

560   when Q_{cmb} exceeds ~15 TW. When the Q_{cmb} ranges from 10 to 12 TW, the stratified layer

561   may have a thickness between 0 and 525 km (Figure 4). Similarly, Davies and

562   Greenwood (2023) suggested that the maximum thickness of the thermal stratification

563   layer ranges from 400 to 500 km when the thermal conductivity at the CMB is about 70

564   W/m/K. However, instead of thermal stratification, chemical stratification may play a

565   pivotal role. For instance, a compositional stratification layer may form via chemical

566   interactions between the liquid core and mantle (Buffet and Seagle 2010; Davies et al.

567   2020). Experiments conducted under high *P-T* conditions have revealed the liquid-liquid

568   immiscibility in the Fe-S-H system occurs at pressures up to 118 GPa, providing a

569   scenario of chemical stratification to explain the low-velocity layer beneath the CMB

570   (Yokoo et al. 2022).

571

CONCLUSIONS

573   We investigated the electrical resistivity of hcp iron at high pressures and room

574   temperature conditions, using both the experimental and first-principles calculation

575   methods. At 136 GPa and 300 K, the electrical resistivity and thermal conductivity of hcp

576   iron are calculated at 5.72 ± 0.65 μΩ·cm and 129 ± 9 W/m/K, respectively. At 134 GPa

577   and 4100 K, they are 79.58 ± 3.59 μΩ·cm and 114 ± 6 W/m/K, respectively. At 98-136

578   GPa and 300-4100 K, the Lorentz number of hcp iron varies with pressure and

579   temperature. Based on the resistivity results and Lorentz number, we estimated the

580   thermal conductivity of solid hcp iron at 105 and 136 GPa via the Wiedemann-Franz law.

581   Thus, solid hcp iron at Earth's CMB conditions (136 GPa and 4100 K) has an electronic

582   thermal conductivity of 106-127 W/m/K. Considering the impact of light elements and

583   melting, the corresponding thermal conductivity at CMB decreases to ~70-90 W/m/K.

584   Therefore, a potential subadiabatic condition in the outer core could form a thermally

585   stratified layer with a thickness of 0-525 km beneath the CMB, depending on the current

586   total heat flow across the CMB.

587   Most of our data reconcile the experimental and computational results for the resistivity

588   and thermal conductivity of solid hcp iron at high pressure and room temperature

589   conditions. However, to explain the abnormally low thermal conductivity of hcp iron at

590   20-60 GPa and 300 K, further calculations involving the EES and spin-polarization

591   effects are necessary, though these calculations are expensive. Additionally, it's essential

592   to note that the experimental Lorentz number of pure iron in this study was not derived

593   from internal measurement studies. Consequently, future works should focus on

594   generating internally consistent experimental datasets, encompassing electrical resistivity

595   and thermal conductivity, to gain a comprehensive understanding of the Lorentz number

596   for iron and iron alloys under high P-T conditions. The overall picture of the transport

597   properties of iron from room to high temperature conditions suggests that the liquid outer

598   core has possible low thermal conductivity only if there are a large number of light

599   elements in the outer core.

600

601   **ACKNOWLEDGEMENTS**

608

609   **FUNDING**

References cited

615

616   Anzellini, S., Dewaele, A., Mezouar, M., Loubeyre, P., and Morard, G. (2013) Melting of

617   iron at Earth's inner core boundary based on fast x-ray diffraction. Science, 340,

618   464–466, https://doi.org/10.1126/science.1233514.

619   Berrada, M., and Secco, R.A. (2021) Review of electrical resistivity measurements and

620   calculations of Fe and Fe-alloys relating to planetary cores. Frontiers in Earth

621   Science, 9, 1–21, https://doi.org/10.3389/feart.2021.732289.

622   Berrada, M., Secco, R.A., and Yong, W. (2021) Adiabatic heat flow in Mercury's core

623   from electrical resistivity measurements of liquid Fe-8.5 wt%Si to 24 GPa. Earth

624   and Planetary Science Letters, 568, 117053–117053,

625   https://doi.org/10.1016/j.epsl.2021.117053.

626   Blöchl, P.E. (1994) Projector augmented-wave method. Physical Review B, 50, 17953–

627   17979, https://doi.org/10.1103/PhysRevB.50.17953.

628   Boness, D.A., Brown, J.M., and McMahan, A.K. (1986) The electronic thermodynamics

629   of iron under Earth core conditions. Physics of the Earth and Planetary Interiors,

630   42, 227–240, https://doi.org/10.1016/0031-9201(86)90025-7.

631   Buffett, B.A., and Seagle, C.T. (2010) Stratification of the top of the core due to chemical

632   interactions with the mantle. Journal of Geophysical Research: Solid Earth, 115,

633   2009JB006751, https://doi.org/10.1029/2009JB006751.

634   Chester, G.V., and Thellung, A. (1961) The Law of Wiedemann and Franz. Proceedings

635   of the Physical Society, 77, 1005–1013, https://doi.org/10.1088/0370-

636   1328/77/5/309.

637 Davies, C.J. (2015) Cooling history of Earth's core with high thermal conductivity.

638   Physics of the Earth and Planetary Interiors, 247, 65–79,

639   https://doi.org/10.1016/j.pepi.2015.03.007.

640 Davies, C.J., and Greenwood, S. (2023) Dynamics in Earth's core arising from thermo-

641   chemical interactions with the mantle. In T. Nakagawa, T. Tsuchiya, M. Satish-

642   Kumar and G. Helffrich, Ed., Core-Mantle Co-Evolution: An Interdisciplinary

643   Approach, p. 219-258. American Geophysical Union, U.S.

644   https://doi.org/10.1002/9781119526919.ch12.

645 Davies, C.J., Pozzo, M., Gubbins, D., and Alfè, D. (2015) Constraints from material

646   properties on the dynamics and evolution of Earth's core. Nature Geoscience, 8,

647   678–685, https://doi.org/10.1038/ngeo2492.

648 Davies, C.J., Pozzo, M., Gubbins, D., and Alfè, D. (2020) Transfer of oxygen to Earth's

649   core from a long-lived magma ocean. Earth and Planetary Science Letters, 538,

650   116208, https://doi.org/10.1016/j.epsl.2020.116208.

651 Davies, C.J., Bono, R.K., Meduri, D.G., Aubert, J., Greenwood, S., and Biggin, A.J.

652   (2022) Dynamo constraints on the long-term evolution of Earth's magnetic field

653   strength. Geophysical Journal International, 228, 316–336,

654   https://doi.org/10.1093/gji/ggab342.

655 Deng, J., and Stixrude, L. (2021) Thermal conductivity of silicate liquid determined by

656   machine learning potentials. Geophysical Research Letters, 48, e2021GL093806,

657   https://doi.org/10.1029/2021GL093806.

658   Dewaele, A., Loubeyre, P., Occelli, F., Mezouar, M., Dorogokupets, P.I., and Torrent, M.

659   (2006) Quasihydrostatic equation of state of Iron above 2 Mbar. Physical Review

660   Letters, 97, 29–32, https://doi.org/10.1103/PhysRevLett.97.215504.

661   Di Paola, C., Macheda, F., Laricchia, S., Weber, C., and Bonini, N. (2020) First-

662   principles study of electronic transport and structural properties of $Cu_{12}Sb_4S_{13}$ in

663   its high-t. Physical Review Research, 2, 033055–033055,

664   https://doi.org/10.1103/PhysRevResearch.2.033055.

665   Driscoll, P., and Bercovici, D. (2014) On the thermal and magnetic histories of Earth and

666   Venus: Influences of melting, radioactivity, and conductivity. Physics of the Earth

667   and Planetary Interiors, 236, 36–51, https://doi.org/10.1016/j.pepi.2014.08.004.

668   Ezenwa, I.C., and Yoshino, T. (2021) Martian core heat flux: Electrical resistivity and

669   thermal conductivity of liquid Fe at Martian core P-T conditions. Icarus, 360,

670   114367, https://doi.org/10.1016/j.icarus.2021.114367.

671   Fei, Y., Murphy, C., Shibazaki, Y., Shahar, A., and Huang, H. (2016) Thermal equation

672   of state of hcp-iron: Constraint on the density deficit of Earth's solid inner core.

673   Geophysical Research Letters, 43, 6837–6843,

674   https://doi.org/10.1002/2016GL069456.

675   Frost, D.A., Avery, M.S., Buffett, B.A., Chidester, B.A., Deng, J., Dorfman, S.M., Li, Z.,

676   Liu, L., Lv, M., and Martin, J.F. (2022) Multidisciplinary constraints on the

677   thermal-chemical boundary between Earth's core and mantle. Geochemistry,

678   Geophysics, Geosystems, 23, e2021GC009764,

679   https://doi.org/10.1029/2021gc009764.

680   Glazyrin, K., Pourovskii, L.V., Dubrovinsky, L., Narygina, O., McCammon, C., Hewener,

681   B., Schünemann, V., Wolny, J., Muffler, K., Chumakov, A.I., and others (2013)

682   Importance of correlation effects in hcp iron revealed by a pressure-induced

683   electronic topological transition. Physical Review Letters, 110, 117206–117206,

684   https://doi.org/10.1103/PhysRevLett.110.117206.

685   Gomi, H., and Hirose, K. (2015) Electrical resistivity and thermal conductivity of hcp

686   Fe–Ni alloys under high pressure: Implications for thermal convection in the

687   Earth's core. Physics of the Earth and Planetary Interiors, 247, 2–10,

688   https://doi.org/10.1016/j.pepi.2015.04.003.

689   Gomi, H., and Yoshino, T. (2018) Impurity resistivity of fcc and hcp fe-based alloys:

690   Thermal stratification at the top of the core of super-earths. Frontiers in Earth

691   Science, 6, 1–22, https://doi.org/10.3389/feart.2018.00217.

692   Gomi, H., Hirose, K., Akai, H., and Fei, Y. (2016) Electrical resistivity of substitutionally

693   disordered hcp Fe–Si and Fe–Ni alloys: Chemically-induced resistivity saturation

694   in the Earth's core. Earth and Planetary Science Letters, 451, 51–61,

695   https://doi.org/10.1016/j.epsl.2016.07.011.

696   Gomi, H., Ohta, K., Hirose, K., Labrosse, S., Caracas, R., Verstraete, M.J., and Hernlund,

697   J.W. (2013) The high conductivity of iron and thermal evolution of the Earth's

698   core. Physics of the Earth and Planetary Interiors, 224, 88–103,

699   https://doi.org/10.1016/j.pepi.2013.07.010.

700   Greenwood, D.A. (1958) The Boltzmann equation in the theory of electrical conduction

701   in metals. Proceedings of the Physical Society, 71, 585–596,

702   https://doi.org/10.1088/0370-1328/71/4/306.

703   Hasegawa, A., Yagi, T., and Ohta, K. (2019) Combination of pulsed light heating

704   thermoreflectance and laser-heated diamond anvil cell for in-situ high pressure-

705   temperature thermal diffusivity measurements. Review of Scientific Instruments,

706   90, 074901, https://doi.org/10.1063/1.5093343.

707   Hoover, W.G. (1985) Canonical dynamics: Equilibrium phase-space distributions.

708   Physical Review A, 31, 1695–1697, https://doi.org/10.1103/PhysRevA.31.1695.

709   Hsieh, W.P., Goncharov, A.F., Labrosse, S., Holtgrewe, N., Lobanov, S.S., Chuvashova,

710   I., Deschamps, F., and Lin, J.F. (2020) Low thermal conductivity of iron-silicon

711   alloys at Earth's core conditions with implications for the geodynamo. Nature

712   Communications, 11, 1–7, https://doi.org/10.1038/s41467-020-17106-7.

713   Inoue, H., Suehiro, S., Ohta, K., Hirose, K., and Ohishi, Y. (2020) Resistivity saturation

714   of hcp Fe-Si alloys in an internally heated diamond anvil cell: A key to assessing

715   the Earth's core conductivity. Earth and Planetary Science Letters, 543, 116357–

716   116357, https://doi.org/10.1016/j.epsl.2020.116357.

717   Jaccard, D., Holmes, A.T., Behr, G., Inada, Y., and Onuki, Y. (2002) Superconductivity

718   of ε-Fe: Complete resistive transition. Physics Letters, Section A: General,

719   Atomic and Solid State Physics, 299, 282–286, https://doi.org/10.1016/S0375-

720   9601(02)00725-9.

721   Kleinschmidt, U., French, M., Steinle-Neumann, G., and Redmer, R. (2023) Electrical

722   and thermal conductivity of fcc and hcp iron under conditions of the Earth's core

723   from ab initio simulations. Physical Review B, 107, 085145,

724   https://doi.org/10.1103/PhysRevB.107.085145.

725   Klemens, P.G., and Williams, R.K. (1986) Thermal conductivity of metals and alloys.

726   International Materials Reviews, 31, 197–215,

727   https://doi.org/10.1179/095066086790324294.

728   Konôpková, Z., McWilliams, R.S., Gómez-Pérez, N., and Goncharov, A.F. (2016) Direct

729   measurement of thermal conductivity in solid iron at planetary core conditions.

730   Nature, 534, 99–101, https://doi.org/10.1038/nature18009.

731   Korell, J.-A., French, M., Steinle-Neumann, G., and Redmer, R. (2019) Paramagnetic-to-

732   diamagnetic transition in dense liquid iron and its influence on electronic

733   transport properties. Physical Review Letters, 122, 086601,

734   https://doi.org/10.1103/PhysRevLett.122.086601.

735   Kresse, G., and Furthmüller, J. (1996) Efficient iterative schemes for ab initio total-

736   energy calculations using a plane-wave basis set. Physical Review B, 54, 11169–

737   11186, https://doi.org/10.1103/PhysRevB.54.11169.

738   Kresse, G., and Joubert, D. (1999) From ultrasoft pseudopotentials to the projector

739   augmented-wave method. Physical Review B, 59, 1758–1775,

740   https://doi.org/10.1103/PhysRevB.59.1758.

741   Kubo, R. (1957) Statistical-mechanical theory of irreversible processes. I. General theory

742   and simple applications to magnetic and conduction problems. Journal of the

743   Physical Society of Japan, 12, 570–586, https://doi.org/10.1143/JPSJ.12.570.

744   Labrosse, S. (2015) Thermal evolution of the core with a high thermal conductivity.

745   Physics of the Earth and Planetary Interiors, 247, 36–55,

746   https://doi.org/10.1016/j.pepi.2015.02.002.

747   Li, J., and Fei, Y. (2014) Experimental constraints on core composition. In H.D. Holland

748   and K.K. Turekian, Ed., Treatise on Geochemistry (Second Edition), p. 527–557.

749   Elsevier, Oxford. https://doi.org/10.1016/B0-08-043751-6/02014-4.

750   Li, W.J., Li, Z., He, X.T., Ma, Z., Fu, Z.G., Lu, Y., Wang, C., and Zhang, P. (2022) Ab

751   initio calculations on thermal conductivity of Fe-Ni-O fluid: Constraints on the

752   thermal evolution of Earth's core. Earth and Planetary Science Letters, 589,

753   117581, https://doi.org/10.1016/j.epsl.2022.117581.

754   Lobanov, S.S., and Geballe, Z.M. (2022) Non-isotropic contraction and expansion of

755   samples in diamond anvil cells: Implications for thermal conductivity at the core-

756   mantle boundary. Geophysical Research Letters, 49, e2022GL100379,

757   https://doi.org/10.1029/2022GL100379.

758   Nimmo, F. (2015) Energetics of the Core. In G. Schubert, Ed., Treatise on Geophysics

759   (Second Edition), p. 27–55. Elsevier, Oxford.

760   Nosé, S. (1984) A unified formulation of the constant temperature molecular dynamics

761   methods. The Journal of Chemical Physics, 81, 511–519,

762   https://doi.org/10.1063/1.447334.

763   Ohta, K., Nishihara, Y., Sato, Y., Hirose, K., Yagi, T., Kawaguchi, S.I., Hirao, N., and

764   Ohishi, Y. (2018) An experimental examination of thermal conductivity

765   anisotropy in hcp iron. Frontiers in Earth Science, 6, 176,

766   https://doi.org/10.3389/feart.2018.00176.

767   Ohta, K., Suehiro, S., Kawaguchi, S.I., Okuda, Y., Wakamatsu, T., Hirose, K., Ohishi, Y.,

768   Kodama, M., Hirai, S., and Azuma, S. (2023) Measuring the electrical resistivity

769   of liquid iron to 1.4 Mbar. Physical Review Letters, 130, 266301,

770   https://doi.org/10.1103/PhysRevLett.130.266301.

771   Okuda, Y., Ohta, K., Hasegawa, A., Yagi, T., Hirose, K., Kawaguchi, S.I., and Ohishi, Y.

772   (2020) Thermal conductivity of Fe-bearing post-perovskite in the Earth's

773   lowermost mantle. Earth and Planetary Science Letters, 547, 116466,

774   https://doi.org/10.1016/j.epsl.2020.116466.

775   Perdew, J.P., Burke, K., and Ernzerhof, M. (1996) Generalized gradient approximation

776   made simple. Physical Review Letters, 77, 3865–3868,

777   https://doi.org/10.1103/PhysRevLett.77.3865.

778   Pommier, A., Driscoll, P.E., Fei, Y., and Walter, M.J. (2022) Investigating metallic cores

779   using experiments on the physical properties of liquid iron alloys. Frontiers in

780   Earth Science, 10, 956971, https://doi.org/10.3389/feart.2022.956971.

781   Pourovskii, L.V., Mravlje, J., Ferrero, M., Parcollet, O., and Abrikosov, I.A. (2014)

782   Impact of electronic correlations on the equation of state and transport in ε-Fe.

783   Physical Review B, 90, 1–5, https://doi.org/10.1103/PhysRevB.90.155120.

784   Pourovskii, L.V., Mravlje, J., Georges, A., Simak, S.I., and Abrikosov, I.A. (2017)

785   Electron–electron scattering and thermal conductivity of ϵ-iron at Earth's core

786   conditions. New Journal of Physics, 19, 073022–073022,

787   https://doi.org/10.1088/1367-2630/aa76c9.

788   Pourovskii, L.V., Mravlje, J., Pozzo, M., and Alfè, D. (2020) Electronic correlations and

789   transport in iron at Earth's core conditions. Nature Communications, 11, 5–12,

790   https://doi.org/10.1038/s41467-020-18003-9.

791   Pozzo, M., and Alfè, D. (2016) Saturation of electrical resistivity of solid iron at Earth's

792   core conditions. SpringerPlus, 5, 1–6, https://doi.org/10.1186/s40064-016-1829-x.

793   Pozzo, M., Davies, C., and Alfè, D. (2022) Towards reconciling experimental and

794   computational determinations of Earth's core thermal conductivity. Earth and

795   Planetary Science Letters, 584, 117466,

796   https://doi.org/10.1016/j.epsl.2022.117466.

797   Pozzo, M., Davies, C., Gubbins, D., and Alfè, D. (2012) Thermal and electrical

798   conductivity of iron at Earth's core conditions. Nature, 485, 355–358,

799   https://doi.org/10.1038/nature11031.

800   Pozzo, M., Davies, C., Gubbins, D., and Alfè, D. (2013) Transport properties for liquid

801   silicon-oxygen-iron mixtures at Earth's core conditions. Physical Review, 87, 1–

802   10, https://doi.org/10.1103/PhysRevB.87.014110.

803   Pozzo, M., Davies, C., Gubbins, D., and Alfè, D. (2014) Thermal and electrical

804   conductivity of solid iron and iron-silicon mixtures at Earth's core conditions.

805   Earth and Planetary Science Letters, 393, 159–164,

806   https://doi.org/10.1016/j.epsl.2014.02.047.

807   Ramakrishna, K., Lokamani, M., Baczewski, A., Vorberger, J., and Cangi, A. (2023)

808   Electrical conductivity of iron in Earth's core from microscopic Ohm's law.

809   Physical Review B, 107, 115131, https://doi.org/10.1103/PhysRevB.107.115131.

810   Saha, P., Mazumder, A., and Mukherjee, G.D. (2020) Thermal conductivity of dense hcp

811   iron: Direct measurements using laser heated diamond anvil cell. Geoscience

812   Frontiers, 11, 1755–1761, https://doi.org/10.1016/j.gsf.2019.12.010.

813   Seagle, C.T., Cottrell, E., Fei, Y., Hummer, D.R., and Prakapenka, V.B. (2013) Electrical

814   and thermal transport properties of iron and iron-silicon alloy at high pressure.

815   Geophysical Research Letters, 40, 5377–5381,

816   https://doi.org/10.1002/2013GL057930.

817   Secco, R.A. (2017) Thermal conductivity and Seebeck coefficient of Fe and Fe-Si alloys:

818   Implications for variable Lorenz number. Physics of the Earth and Planetary

819   Interiors, 265, 23–34, https://doi.org/10.1016/j.pepi.2017.01.005.

820   Secco, R.A., and Schloessin, H.H. (1989) The electrical resistivity of solid and liquid Fe

821   at pressures up to 7 GPa. Journal of Geophysical Research, 94, 5887–5894,

822   https://doi.org/10.1029/JB094iB05p05887.

823   Sha, X., and Cohen, R.E. (2011) First-principles studies of electrical resistivity of iron

824   under pressure. Journal of Physics: Condensed Matter, 23, 075401,

825   https://doi.org/10.1088/0953-8984/23/7/075401.

826   Silber, R.E., Secco, R.A., Yong, W., and Littleton, J.A.H. (2018) Electrical resistivity of

827   liquid Fe to 12 GPa: Implications for heat flow in cores of terrestrial bodies.

828   Scientific Reports, 8, 1–9, https://doi.org/10.1038/s41598-018-28921-w.

829   Uher, C. (2004) Thermal Conductivity of Metals. In T.M. Tritt, Ed., Thermal

830   Conductivity, p. 21–91. Springer, U.S.

831   van der Pauw, L.J. (1958) A method of measuring specific resistivity and Hall effect of

832   discs of arbitrary shape. Philips Research Reports, 13, 1–9.

833   Wagle, F., Steinle-Neumann, G., and De Koker, N. (2018) Saturation and negative

834   temperature coefficient of electrical resistivity in liquid iron-sulfur alloys at high

38

835   densities from first-principles calculations. Physical Review B, 97, 94307–94307,

836   https://doi.org/10.1103/PhysRevB.97.094307.

837   Williams, W.S. (1998) The thermal conductivity of metallic ceramics. JOM, 50, 62–66,

838   https://doi.org/10.1007/s11837-998-0131-y.

839   Xu, J., Zhang, P., Haule, K., Minar, J., Wimmer, S., Ebert, H., and Cohen, R.E. (2018)

840   Thermal conductivity and electrical resistivity of solid iron at Earth's core

841   conditions from first principles. Physical Review Letters, 121, 96601–96601,

842   https://doi.org/10.1103/PhysRevLett.121.096601.

843   Yin, Y., Zhang, Q., Zhang, Y., Zhai, S., and Liu, Y. (2022a) Electrical and thermal

844   conductivity of Earth's core and its thermal evolution-A review. Acta Geochimica,

845   41, 665–688, https://doi.org/10.1007/s11631-021-00523-w.

846   Yin, Y., Wang, L., Zhai, S., and Fei, Y. (2022b) Electrical resistivity of Fe and Fe-3

847   wt%P at 5 GPa with implications for the moon's core conductivity and dynamo.

848   Journal of Geophysical Research: Planets, 127, e2021JE007116,

849   https://doi.org/10.1029/2021je007116.

850   Yokoo, S., Hirose, K., Tagawa, S., Morard, G., and Ohishi, Y. (2022) Stratification in

851   planetary cores by liquid immiscibility in Fe-S-H. Nature Communications, 13,

852   644, https://doi.org/10.1038/s41467-022-28274-z.

853   Yong, W., Secco, R.A., Littleton, J.A.H., and Silber, R.E. (2019) The iron invariance:

854   Implications for thermal convection in Earth's core. Geophysical Research Letters,

855   46, 11065–11070, https://doi.org/10.1029/2019GL084485.

856   Yue, S.-Y., and Hu, M. (2019) Insight of the thermal conductivity of ε-iron at Earth's

857   core conditions from the newly developed direct ab initio methodology. Journal of

858   Applied Physics, 125, 045102, https://doi.org/10.1063/1.5055389.

859   Zhang, C., Lin, J.F., Liu, Y., Feng, S., Jin, C., Hou, M., and Yoshino, T. (2018) Electrical

860   resistivity of Fe-C alloy at high pressure: Effects of carbon as a light element on

861   the thermal conductivity of the Earth's core. Journal of Geophysical Research:

862   Solid Earth, 123, 3564–3577, https://doi.org/10.1029/2017JB015260.

863   Zhang, J., and Guyot, F. (1999) Thermal equation of state of iron and $Fe_{0.91}Si_{0.09}$. Physics

864   and Chemistry of Minerals, 26, 206–211.

865   Zhang, Y., Hou, M., Liu, G., Zhang, C., Prakapenka, V.B., Greenberg, E., Fei, Y., Cohen,

866   R.E., and Lin, J.F. (2020) Reconciliation of experiments and theory on transport

867   properties of iron and the geodynamo. Physical Review Letters, 125, 78501,

868   https://doi.org/10.1103/PhysRevLett.125.078501.

869   Zhang, Y., Luo, K., Hou, M., Driscoll, P., Salke, N.P., Minár, J., Prakapenka, V.B.,

870   Greenberg, E., Hemley, R.J., Cohen, R.E., and others (2022) Thermal

871   conductivity of Fe-Si alloys and thermal stratification in Earth's core. Proceedings

872   of the National Academy of Sciences, 119, e2119001119,

873   https://doi.org/10.1073/pnas.2119001119.

874 **Figure captions**

875 **Figure 1.** The electrical resistivity (**a**) and thermal conductivity (**b**) of iron at room

876 temperature and high pressure conditions. (**a**) shows our measured results at pressures up

877 to 26 GPa (half solid circles, U1419 and U1423) and computed results at pressures up to

878 136 GPa (solid triangles, R1 and R2). The labels exp and calc state the results from

879 experimental measurement and FPMD calculations, respectively. R1 and R2 differ on the

880 input lattice parameters, where the former applied the DFT-based lattice parameters

881 calculated at 0 K and the latter with experimental data measured at 300 K. The arrows in

882 (**a**) and (**b**) note the pressures of the bcc to hcp phase transition and the electronic

883 topological transition (ETT). In (**a**) and (**b**), we see the R1 run exhibits opposite pressure

884 dependency compared to experimental results at 80-136 GPa, indicating the failure of

885 prediction from the calculated lattice parameters at 0 K. In (**b**), all the experimental

886 thermal conductivity values are measured directly in high *P-T* experiments. References:

887 Ez21-(Ezenwa and Yoshino 2021); Go13-(Gomi et al. 2013); Hs20-(Hsieh et al. 2020);

888 Ja02-(Jaccard et al. 2002); Kl23-(Kleinschmidt et al. 2023); Oh18-(Ohta et al. 2018);

889 Se13-(Seagle et al. 2013); Sh11-(Sha and Cohen 2011); Zh18, Zh20-(Zhang et al. 2018,

890 2020).

891

892 **Figure 2.** The electrical resistivity (**a**) and thermal conductivity (**b**) of hcp iron at high *P-*

893 *T* conditions. In (**a**), the experimental data from Zhang et al. (2020) only display the error

894 bar at the highest temperature. Solid and dashed lines are Bloch-Grüneisen fitting lines

895 from Zhang et al. (2020). In (**b**), the numbers near the symbol note the pressures, and the

896 pressure error is in parentheses. The grey short-dashed line and region (noted as WFL)

897   show the predicted thermal conductivity range of solid hcp iron at 105 and 136 GPa via

898   the Wiedemann-Fanz law in this study, in which the resistivity data is the Bloch-

899   Grüneisen fitting data from Zhang et al. (2020), and the Lorentz number is from this

900   study. The data of grey short-dashed lines are calculated with L values of 2.20×10^{-8}

901      $W\Omega K^{-2}$ and the grey regions are calculated with L values from 2.0 to 2.4×10^{-8} $W\Omega K^{-2}$.

902   The red solid triangles state the calculated electronic thermal conductivity from this study,

903   whereas the open inverted triangles are data with an EES correction. References: Ko16-

904   (Konôpková et al. 2016); Ko19-(Korell et al. 2019); Oh23-(Ohta et al. 2023); Sa20-

905   (Saha et al. 2020); Xu18-(Xu et al. 2018); Zh20-(Zhang et al. 2020).

906

907   **Figure 3.** The Lorenz numbers of Fe at room-temperature (**a**) and high temperature (**b**)

908   conditions. (**a**) The grey horizontal dash-dot, dash-dot-dot, and dash lines represent

909   Lorenz numbers of the theoretical value ($L_0 = 2.44 \times 10^{-8}$ $W\Omega K^{-2}$), iron with disordered

910   lattice structure (2.28×10^{-8} $W\Omega K^{-2}$), and iron with ordered lattice structure (1.57×10^{-8}

911      $W\Omega K^{-2}$), respectively (Pourovskii et al. 2020). The experimental Lorentz number is

912   computed from experimental resistivity (Seagle et al. 2013; Zhang et al. 2020) and

913   experimental thermal conductivity (Hsieh et al. 2020; Konôpková et al. 2016; Saha et al.

914   2020) data. (**b**) Symbols of plus, cross and open square denote the Lorentz numbers after

915   electron-electron scattering (EES) correction. The black short dash and short dot curves

916   are part of the Lorentz number of hcp iron from the theoretical calculation studies by

917   Gomi and Yoshino (2018) and Pourovskii et al. (2017), respectively. The results from

918   Pourovskii et al. (2017) include the EES effect while those from Gomi and Yoshino

919   (2018) do not. Some error bars of results from this study are smaller than the symbol size.

920   The dash-dot line denotes the L_0 value. The inset in (**b**) shows an enlarged view of all

921   theoretically calculated Lorentz numbers with EES correction, and the y-axis is the ratio

922   of calculated and theoretical *L*. References: de12-(de Koker et al. 2012), Go18-(Gomi

923   and Yoshino 2018), Hs20-(Hsieh et al. 2020), Ko16-(Konôpková et al. 2016), Po17-

924   (Pourovskii et al. 2017), Sa20-(Saha et al. 2020); Se13-(Seagle et al. 2013); Xu18-(Xu et

925   al. 2018); Zh20-(Zhang et al. 2020).

926

927   **Figure 4.** The thickness of the potential thermally stratified layer beneath CMB varies

928   with the total heat flow across the CMB (Q_{cmb}). The grey dashed line is the calculated

929   inner core age from Li et al. (2022). Open circles represent the thickness when the

930   thermal conductivity at CMB is ~100 W/m/K from the study by Zhang et al. (2022). The

931   vertical light-yellow area represents the most likely Q_{cmb} values at present-day CMB.

932   Numbers next to the symbols and lines represent different thermal conductivity (70, 90,

933   and 100 W/m/K) at CMB. Though the thermal conductivity of liquid iron is ~95-114

934   W/m/K at the CMB, the alloying of iron and light elements (silicon and oxygen) may

935   reduce the thermal conductivity to 70-90 W/m/K (Pozzo et al. 2022; Li et al. 2022), and

936   thus the most possible thermal conductivity at CMB is around 70-90 W/m/K. The black

937   dashed area represents the thickness of thermally stratified layer beneath the CMB when

938   the thermal conductivity at CMB varies from 70 to 90 W/m/K.

43

Table 1. Pressure, electrical resistivity (ρ), electronic thermal conductivity (κ_{el}), and Lorentz number (L) for hcp iron in this study.

Pressures[※] (GPa)	Temperature (K)	ρ ($\mu\Omega\cdot$cm)	κ_{el} (W/m/K)	L (10^{-8} WΩK^{-2})	Pressures (GPa)	Temperature (K)	ρ ($\mu\Omega\cdot$cm)	κ_{el} (W/m/K)	L (10^{-8} WΩK^{-2})
Room temperature (300 K)									
R1*					R2				
22	-	10.65(102)	77.84(570)	2.61(13)	22	-	9.69(110)	92.82(1179)	2.73(15)
30	-	8.64(64)	99.24(950)	2.69(11)	29	-	8.13(133)	107.58(1857)	2.65(10)
40	-	8.09(58)	105.92(639)	2.67(12)	50	-	6.88(53)	115.77(743)	2.56(14)
60	-	6.14(49)	133.79(634)	2.59(15)	80	-	6.54(71)	110.64(1109)	2.35(21)
80	-	5.81(52)	127.09(1051)	2.37(11)	105	-	5.91(66)	116.58(662)	2.26(25)
100	-	6.52(72)	115.19(785)	2.43(21)	136	-	5.72(65)	128.56(844)	2.36(38)
136	-	7.66(55)	85.57(478)	2.12(10)					
High pressure-temperature									
98.5	1562	37.86(279)	105.32(737)	2.53(2)	132	2725	55.79(287)	130.20(525)	2.66(4)
98.6	3521	80.01(333)	137.33(578)	3.13(3)	134	4114	79.58(359)	157.76(840)	3.06(3)

[※]Pressure-temperature conditions and lattice parameters are referred to Dewaele et al. (2006); Anzellini et al. (2013); and Fei et al. (2016) for iron.

*The lattice parameters used in R1 simulation are calculated at 0 K while R2 simulation are from experiments. All lattice parameters are listed in Table S1.
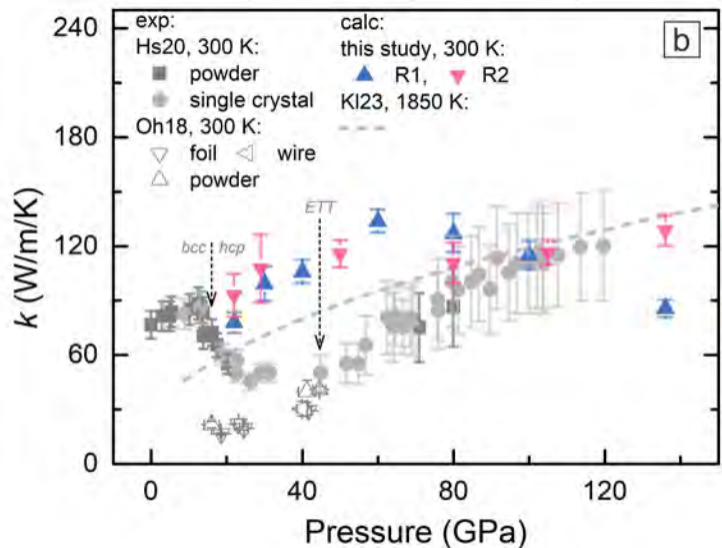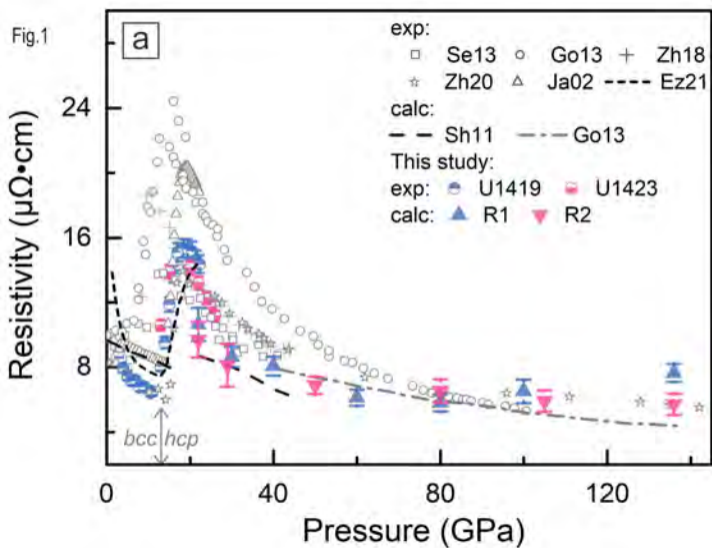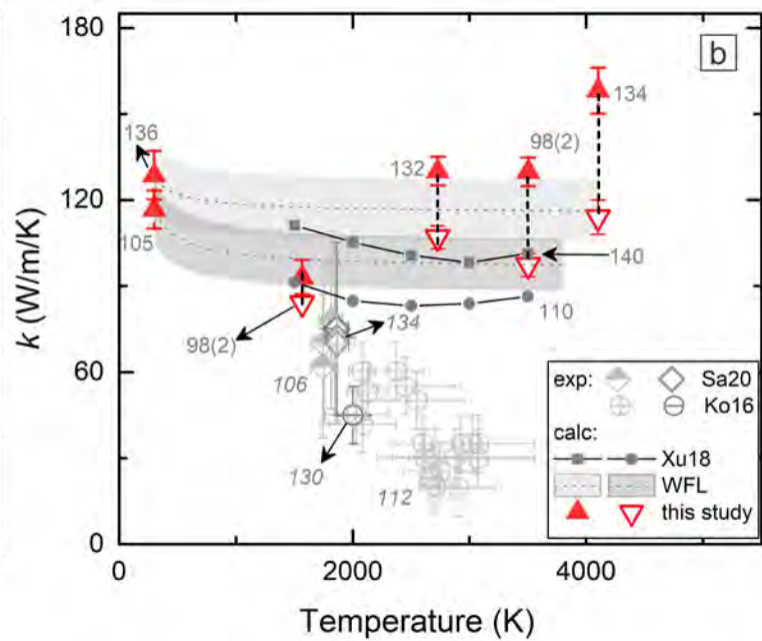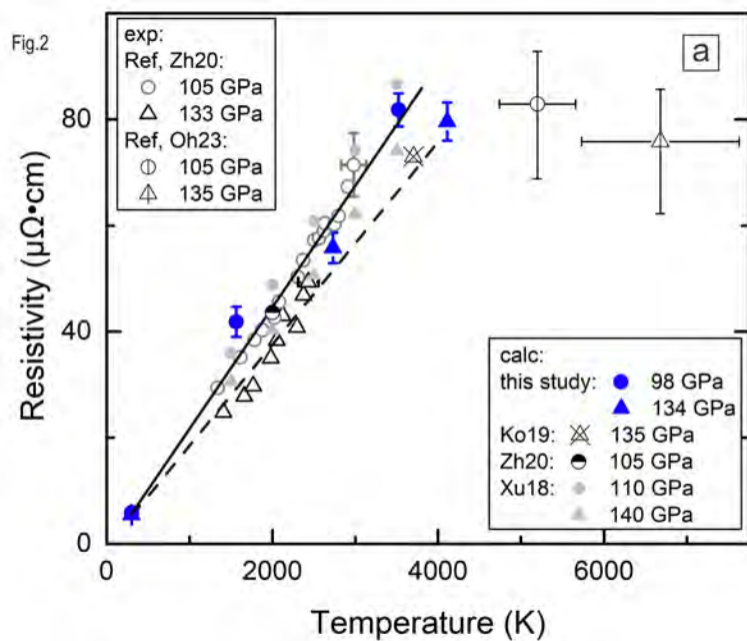
Fig.1

Fig.2

Fig.3

Fig.4