

1 **Impurity resistivity of the Earth's inner core**

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8

9 **Abstract**

10 Seismic observations suggest that the Earth's inner core has a complex structure (e.g.,
11 the isotropic layer at the top, innermost inner core, and hemispherical dichotomy).
12 These characteristics are believed to reflect the history of dynamics and temperature
13 profile of the inner core. One critical physical property is the inner core's thermal
14 conductivity. The thermal conductivity of metals can be estimated from their electrical
15 resistivity using the Wiedemann-Franz law. Recent high-pressure and temperature
16 experiments revealed that the temperature dependence of electrical resistivity is small
17 for Fe-Si alloys. The small temperature coefficient means that it is essential to
18 determine the impurity resistivity of Fe alloys to constrain the inner core's thermal
19 conductivity. Therefore, this study systematically calculated the impurity resistivities of
20 4- and 6-component alloys at inner core pressure by combining the
21 Korringa-Kohn-Rostoker method with the coherent potential approximation. As a result,
22 we obtained the thermal conductivity of the inner core to be 150-263 W/m/K. The inner
23 core cannot maintain thermal convection with such a high thermal conductivity,
24 resulting in a flat temperature profile. In materials science, it is widely known that
25 polycrystals soften suddenly at high temperatures a few percent below their melting
26 temperature. If such a pre-melting occurs in the inner core, the flat temperature profile
27 due to high thermal conductivity causes variations in the attenuation within the inner
28 core. This may explain the observation that the upper inner core is more strongly
29 attenuated than the innermost inner core.

30 **Plain Language Summary**

31 The center of the Earth is an inner core of solid Fe alloy, which has been grown from
32 the surrounding liquid outer core for about one billion years. Therefore, geoscientists
33 regard it as a time capsule that has recorded the history of the Earth. We determined the
34 thermal conductivity of the inner core, which is important for its history, from computer
35 simulations. We found that the thermal conductivity is high, resulting in a small
36 temperature variation of only less than about 100 K within the present-day inner core
37 with a radius of 1,221 km. Because the surface of the inner core is in contact with the
38 liquid outer core, its temperature equals its melting temperature. The temperature
39 difference between the flat profile and the melting curve becomes larger at the deep
40 inner core because the melting temperature increases with pressure. The deviation from
41 the melting temperature may explain the seismic observation that the upper inner core is
42 softer than the innermost inner core due to the effect of pre-melting, which is
43 well-known in material science.

44 **Key points:**

- 45 ● Impurity resistivity of up to 6-component hcp Fe-based alloys are calculated by the
46 KKR-CPA method.
- 47 ● Linear regression suggests resistivity saturation, leading to the inner core's high
48 thermal conductivity (150-263 W/m/K).
- 49 ● A flat temperature profile of the inner core may be across the boundary due to
50 pre-melting consistent with seismic observation.

51

52 **1. Introduction**

53 At the center of the Earth, there is a solid inner core mainly composed of Fe and Ni
54 alloying with light elements (e.g., Hirose et al., 2021). Even though this inner core is
55 only 0.7% of the Earth's total volume, many characteristic seismic wave observations
56 have been reported (Deguen, 2012; Deuss, 2014). For example, seismic anisotropy and
57 attenuation characterize the uppermost isotropic layer with 60-80 km thick (e.g.,
58 Ouzounis & Creager, 2001; Song & Helmberger, 1995), innermost inner core with the
59 radius of 300-600 km (e.g., Cormier & Li, 2002; Cormier & Stroujkova, 2005; Ishii &
60 Dziewonski, 2002; Li & Cormier, 2002; Pham & Tkalčić, 2023; Stephenson et al.,
61 2021), and hemispherical dichotomy (e.g., Tanaka & Hamaguchi, 1997). All these
62 characteristic observations must be simultaneously explained by dynamics and
63 mineralogy. However, to the best of our knowledge, no single model can explain all
64 observations (Deguen, 2012; Deuss, 2014). Several proposed models can independently
65 explain individual seismic features, but some have exclusive relationships. For example,
66 plume convection in the inner core (Jeanloz & Wenk, 1988; Weber & Machetel, 1992)
67 and translation (Alboussiere et al., 2010; Monnereau et al., 2010) cannot exist
68 simultaneously (Lasbleis & Deguen, 2015; Lythgoe et al., 2015). Thermal conductivity
69 is one of the fundamental properties for understanding the dynamics and temperature
70 profile of the inner core (e.g., Labrosse, 2014; Lythgoe et al., 2015; Yukutake, 1998).

71 The thermal conductivity of metals can be estimated from their electrical resistivity
72 using the Wiedemann-Franz law. Gomi et al. (2013) proposed the model that incorporate
73 the resistivity saturation (Bohnenkamp et al., 2002; Gunnarsson et al., 2003) to
74 constrain the electrical resistivity of Fe-based alloys at the core conditions. Resistivity

75 saturation predicts that the electrical resistivity of Fe alloys will exhibit a weaker
76 temperature dependence than the linear temperature dependence expected from
77 Bloch-Grüneisen law and Matthiessen's rule (Gomi et al., 2013). The temperature
78 dependence of the electrical resistivity of pure Fe is still under debate, both
79 experimental (Ohta et al., 2016; Suehiro et al., 2019; Zhang et al., 2020a) and
80 theoretical (Kleinschmidt et al., 2023; Pozzo & Alfe, 2016; Ramakrishna et al., 2022;
81 2023; Xu et al., 2018) studies. Contrary to the discussion of the temperature dependence
82 of resistivity in pure Fe, different experimental groups have independently reported the
83 breakdown of the Matthiessen's rule and small temperature dependence of the resistivity
84 of Fe-Si alloys (Inoue et al., 2020; Zhang et al., 2022). This implies that it is essential to
85 constrain the impurity resistivity in Fe alloys with high impurity content, such as the
86 inner core.

87 Recently, high-pressure resistivity measurements have been actively reported for binary
88 Fe-based alloys: Ni (Gomi & Hirose, 2015; Lenhart & Secco, 2022; Orole et al., 2022),
89 Si (Berrada et al., 2021; Gomi et al., 2016; Inoue et al., 2020; Zhang et al., 2022), S
90 (Littleton et al., 2021a, b; Manthilake et al., 2019; Pommier, 2018; Pommier et al.,
91 2019), C (Zhang et al., 2018), P (Yin et al., 2020), and H (Ohta et al., 2019). However,
92 the resistivity of multi-component Fe alloys in the Earth's core is difficult to estimate
93 from the binary alloys because of the breakdown of the Mathiesen's rule (Gomi et al.,
94 2016; Gomi & Yoshino, 2018; Inoue et al., 2020; Zhang et al., 2022). Furthermore,
95 experiments on ternary systems are still limited (Berrada et al., 2022; Lenhart et al.,
96 2023; Littleton et al., 2022; Pommier, 2020; Suehiro et al., 2017). In contrast, the
97 coherent potential approximation (CPA) can efficiently compute multi-component

98 alloys. Electrical resistivity of Fe alloys with substitutional impurities has been reported
99 up to ternary systems using the CPA (Gomi et al., 2016; Gomi & Yoshino, 2018; Zidane
100 et al., 2020). These calculations reasonably reproduce the previous experiments using
101 diamond anvil cells (DAC) (Gomi & Hirose, 2015; Gomi et al., 2016; Suehiro et al.,
102 2017; Zhang et al., 2018). Thus, one of the purposes of this study is to calculate the
103 electrical resistivity of Fe-Ni-based alloys with more than two light alloying elements.
104 Another objective of this study is to calculate the electrical resistivity of interstitial
105 impurities, which has yet to be theoretically investigated. Among the light element
106 candidates in the core, H, C, and N may occupy interstitial sites. Gomi et al. (2018)
107 predicted from the band structure of hexagonal close-packed (hcp) and double
108 hexagonal close-packed (dhcp) FeH_x that interstitial H has little effect on electrical
109 resistivity. Also, Ohta et al. (2019) found that the impurity resistivity of H is smaller
110 than the other light element candidates from electrical resistivity measurements of
111 face-centered cubic (fcc) FeH_x at high pressure and temperature using DAC. However,
112 Zidan et al. (2020) calculated the impurity resistivity of hcp Fe alloys with H in the
113 substitutional sites, which exhibit higher than that of other light-element alloys. These
114 results imply that the difference in sites occupied by impurities may significantly affect
115 the electrical resistivity.

116 In this study, we calculate the impurity resistivity of hcp Fe-based alloys from
117 first-principles calculations up to 6-component with impurities in both substitutional
118 and interstitial sites. Then, we performed linear regression on the obtained electrical
119 resistivity data to confirm the saturation behaviour of resistivity. Finally, the thermal

120 conductivity of the inner core is estimated, and the temperature profile of the inner core
121 is discussed.

122 **2. Methods**

123 **2.1 First-principles calculation**

124 Following our previous studies (Gomi et al., 2016; Gomi & Yoshino, 2018), we
125 performed first-principles calculations on hcp Fe-based alloys by using the
126 Korringa-Kohn-Rostoker (KKR) Green function method combined with the coherent
127 potential approximation (CPA), which is implemented in the AkaiKKR
128 (machikaneyama) package (Akai, 1989). The local density approximation (LDA) was
129 used for the exchange-correlation potential (Moruzzi et al., 1978). The crystal potential
130 was approximated by the atomic spherical approximation (ASA). The maximum
131 angular momentum quantum number was set to $l = 3$. Relativistic effects are treated
132 within the scalar relativistic approximation. The electrical resistivity is calculated from
133 the Kubo-Greenwood formula with the vertex correction (Kou & Akai, 2018; Oshita et
134 al., 2009). Two independent resistivity components were computed with respect to the
135 crystallographic orientation, and the polycrystalline average is calculated as $\rho_{\text{poly}} = (2\rho_a$
136 $+ \rho_c)/3$, where ρ_a and ρ_c are the resistivity component perpendicular and parallel to the
137 c -axis, respectively.

138 Previous KKR-CPA studies (Gomi et al., 2016; Gomi & Yoshino, 2018; Zidane et al.,
139 2020) have reported calculations of up to ternary systems containing only substitutional
140 impurities. In this study, we calculated up to 6-component alloys containing
141 substitutional and interstitial impurities. The volume is fixed at $V = 12.91 \text{ \AA}^3$ regardless

142 of composition, which is the volume of hcp Fe at 360 GPa and 300 K (Dewaele et al.,
 143 2006). The axial ratio was fixed to the ideal value for hcp metals ($c/a = 1.633$). First,
 144 calculations were performed for Fe-Ni-based substitutional $\text{Fe}_{0.9-y}\text{Ni}_{0.1}^{\text{s}}\text{L}_y^{\text{s}}\text{Vc}_{1.0}^{\text{i}}$ ternary
 145 alloys to check the effect of adding vacancies (Vc) in the interstitial positions. The
 146 compositions of the ternary alloys are $\text{Fe}_{0.9-y}\text{Ni}_{0.1}^{\text{s}}\text{L}_y^{\text{s}}\text{Vc}_{1.0}^{\text{i}}$, where L^{s} is the light element
 147 ($\text{L}^{\text{s}} = \text{H}, \text{C}, \text{N}, \text{O}, \text{Si}, \text{P}, \text{or S}$) and the superscript s indicate the substitutional element.
 148 The concentration of substitutional light elements was set with 0.05 steps in the range 0
 149 $\leq y \leq 0.3$. Vacancies were introduced at the octahedral interstitial positions. Then,
 150 calculations were performed for FeH_z^{i} and $\text{Fe}_{0.9}\text{Si}_{0.1}^{\text{s}}\text{H}_z^{\text{i}}$ with H in the interstitial
 151 positions. The superscript i means that it is an interstitial element. The H concentration
 152 was set to $0.0 \leq z \leq 1.0$. After these test calculations, we computed the 4- and
 153 6-component alloys. The chemical composition of the 4-component alloys can be
 154 described as $\text{Fe}_{1-x-y}\text{Ni}_x^{\text{s}}\text{L}_y^{\text{s}}\text{L}_z^{\text{i}}$ (Figure 1a), where the substitutional impurities are $\text{L}^{\text{s}} = \text{H},$
 155 $\text{C}, \text{N}, \text{O}, \text{Si}, \text{P}, \text{or S}$, and the interstitial impurities are $\text{L}^{\text{i}} = \text{H}, \text{C}, \text{N}, \text{or O}$. Ni
 156 concentrations were set to $x = 0, 0.05, 0.1, 0.15$. The concentration of the substitutional
 157 light element (L^{s}) is set to $y = 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3$. The interstitial impurity
 158 (L^{i}) concentration was set to $z = 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5$. We
 159 successfully obtained 6105 independent chemical compositions. We further calculated
 160 the 6-component alloys, $\text{Fe}_{1-x-y}\text{Ni}_x^{\text{s}}(\text{Si}, \text{S})_y^{\text{s}}(\text{H}, \text{C})_z^{\text{i}}$, in which two light elements are
 161 alloyed at the substitutional and interstitial sites, respectively (Figure 1b). The Si (y_{Si})
 162 and S (y_{S}) concentrations at the substitution sites were varied in 0.05 steps in the range
 163 where the sum $y = y_{\text{Si}} + y_{\text{S}}$ is $y \leq 0.3$. Similarly, the H (z_{H}) and C (z_{C}) concentrations at

the interstitial sites were varied in 0.1 steps so that the sum $z = z_H + z_C \leq 0.5$. As a result, 1176 independent compositions were obtained for 6-component alloys.

2.2 Linear regression

We performed linear regression on the resistivities of 6105 compositions obtained from the resistivity calculations of 4-component alloys. If the effect of resistivity saturation is small, the electrical resistivity of multi-component alloys follows Mathiesen's rule.

$$\rho = x\rho_{\text{Ni}^s} + \sum_{\text{L}^s}^{\text{H,C,N,O,Si,P,S}} y_{\text{L}^s} \rho_{\text{L}^s} + \sum_{\text{L}^i}^{\text{H,C,N,O}} z_{\text{L}^i} \rho_{\text{L}^i} \quad (1)$$

Therefore, we considered Matthiesen's rule with a constant term as a linear regression model in this study.

$$\rho = x\rho_{\text{Ni}^s} + \sum_{\text{L}^s}^{\text{H,C,N,O,Si,P,S}} y_{\text{L}^s} \rho_{\text{L}^s} + \sum_{\text{L}^i}^{\text{H,C,N,O}} z_{\text{L}^i} \rho_{\text{L}^i} + \rho_{\text{const}} \quad (2)$$

where the explanatory variables are the concentration of each impurity (x , y_{L^s} , and z_{L^i}), and the regression coefficients are the impurity resistivity (ρ_{Ni^s} , ρ_{L^s} , ρ_{L^i}) and the constant term ρ_{const} .

2.3 Thermal conductivity of the inner core

The temperature dependence of resistivity is small for alloys with large impurity resistivity, such as Fe-Si alloys (Inoue et al., 2020; Zhang et al., 2022). In such cases, the contribution of lattice vibrations to the total resistivity should be small. Thus, Zidane et al. (2020) ignore it. However, in the case of alloys low impurity resistivity (e.g., interstitial H), ignoring the contribution of lattice vibrations may overestimate the thermal conductivity of the inner core. Therefore, following our previous studies (Gomi et al., 2016; Gomi & Yoshino, 2019), we incorporated the effect of lattice vibration on

the impurity resistivity obtained from first-principles calculations. The resistivity of hcp Fe at ambient temperature can be described as follows (Gomi et al., 2013).

$$\rho_{\text{Fe}}(V) = 0.526 \times \left(1.24 - \frac{V}{V_0}\right)^{-3.21} \mu\Omega\text{cm} \quad (3)$$

The ideal resistivity at high temperature can be obtained from the Bloch-Grüneisen law.

$$\rho_{\text{Fe,ideal}}(V, T) = B(V) \left(\frac{T}{\Theta_D(V)}\right)^5 \int_0^{\Theta_D(V)/T} \frac{x^5 dx}{(\exp(x)-1)(1-\exp(-x))} \quad (4)$$

where $B(V)$ is a material constant obtained from Equation (3), $\Theta_D(V)$ is the Debye temperature (Dewaele et al., 2006). However, note that the resistivity of hcp Fe-based alloys saturate at high temperatures (Inoue et al., 2020; Ohta et al., 2016; Suehiro et al., 2019). The saturation resistivity may be calculated by using the following equation with the ambient pressure value $\rho_{\text{sat}}(V_0) = 168 \mu\Omega\text{cm}$ (Bohnenkamp et al., 2002) (Gomi et al., 2013).

$$\rho_{\text{sat}}(V) = \rho_{\text{sat}}(V_0) \left(\frac{V}{V_0}\right)^{\frac{1}{3}} \quad (5)$$

This volume dependence is consistent with recent experiments on hcp Fe-Si alloys (Inoue et al., 2020). Several models have been proposed to describe resistivity saturation at ambient pressure, but no universal one is known (Sundqvist, 2022). In this study, we adopted the model of Cote and Meisel (1978) following our previous studies (Gomi et al., 2016; Gomi & Yoshino, 2018). This model fits well with the resistivity of hcp Fe-Si alloys at high pressures and temperatures (Inoue et al., 2020).

$$\rho_{\text{tot}}(V, T) = \left(1 - \frac{\rho_{\text{tot}}(V, T)}{\rho_{\text{sat}}(V)}\right) \rho_{\text{Fe,ideal}}(V, T) + \rho_{\text{poly}} \exp(-2W(V, T)) \quad (6)$$

$W(V, T)$ can be calculated by the Debye model as follows (Markowitz et al., 1977).

$$W(V, T) = \frac{3\hbar^2 K^2 T^2}{2mk_B \Theta_D^3} \int_0^{\Theta_D(V)/T} \left(\frac{1}{\exp(z)-1} + \frac{1}{2}\right) z dz \quad (7)$$

206 where ρ_{poly} is the polycrystalline average of impurity resistivity obtained from present
 207 first-principles calculations, \hbar is the reduced Plank's constant (the Dirac's constant), m
 208 is the average atomic mass, $K \sim \pi/a$ is electronic wave vector transfer, and a is the
 209 lattice parameter. We estimated the thermal conductivity via the Wiedeman-Franz law.

$$210 \quad k(V, T) = \frac{L_{\text{Somm}} T}{\rho_{\text{tot}}(V, T)} \quad (8)$$

211 Sommerfeld's value L_{Somm} is widely known as an approximation of the Lorenz number.

$$212 \quad L_{\text{Somm}} = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right)^2 \quad (9)$$

213 Although the Lorentz number of Fe alloys at high pressure and temperatures may
 214 deviate from L_{Somm} (Gomi & Hirose, 2015; Kleinschmidt et al., 2023; Pourovskii et al.,
 215 2017), we use L_{Somm} as a representative value.

216 **2.4 Conductive temperature profile of the inner core**

217 Buffett (2009) modeled the temperature profile due to thermal conduction within the
 218 inner core as a function of radial position r and time t from the onset of the inner core.
 219 This study uses this model to calculate the present-day conductive temperature profile.
 220 The density of the inner core is assumed to depend only on the radial position r , using
 221 the polynomial reported by the Preliminary Reference Earth model (PREM)
 222 (Dziewonski & Anderson, 1981). In this subsection, we use $\rho(r)$ as the density of the
 223 inner core. Note that it is not the electrical resistivity. The radius of the inner core,
 224 $r_{\text{ICB}}(t)$, is assumed to be proportional to 1/2 power of time (Buffett, 2009; Labrosse,
 225 2014).

$$226 \quad r_{\text{ICB}}(t) = r_{\text{ICB}p} \left(\frac{t}{t_{\text{IC}}} \right)^{\frac{1}{2}} \quad (10)$$

227 where $r_{\text{ICB}p} = 1221.5$ km is the current radius of the inner core and t_{IC} is the age of the
 228 inner core. The inner-core boundary (ICB) temperature always coincides with the
 229 melting temperature of the inner core material at that radial position $T_M(r)$, which is
 230 modeled based on Lindemann's melting law as follows (Yukutake, 1998).

$$231 \quad T_M(r) = T_{\text{ICB}p} \left(\frac{\rho_{\text{ICB}}}{\rho(r)} \right)^{\frac{2}{3}} \exp \left[2\gamma \left(1 - \frac{\rho_{\text{ICB}p}}{\rho(r)} \right) \right] \quad (11)$$

232 where $T_{\text{ICB}p} = 5500$ K is the present-day ICB temperature (Labrosse, 2014), $\rho_{\text{ICB}p}$
 233 $= \rho(r_{\text{ICB}p})$ is the present-day ICB density, $\gamma = 1.5$ (Vočadlo et al., 2003) is the Grüneisen
 234 parameter. The adiabatic temperature profile can be obtained with the ICB temperature
 235 $T_M(r_{\text{ICB}}(t))$ as a reference.

$$236 \quad T_a(r, t) = T_M(r_{\text{ICB}}(t)) \left(\frac{\rho(r)}{\rho(r_{\text{ICB}}(t))} \right)^\gamma \quad (12)$$

237 The thermal diffusion time $t_d(t)$ is represented as a function of time t via the inner core
 238 radius $r_{\text{ICB}}(t)$.

$$239 \quad t_d(t) = \frac{r_{\text{ICB}}^2(t)}{\kappa} \quad (13)$$

240 where κ is the thermal diffusivity. For simplicity, the physical properties associated with
 241 thermal diffusivity are approximated as independent of radial position r and time t .

$$242 \quad \kappa = \frac{k}{\rho_{\text{average}} C_p} \quad (14)$$

243 where k is the thermal conductivity, $C_p = 750$ J/K/kg is the heat capacity (Gubbins et al.,
 244 2013), and ρ_{average} is the average density of the present-day inner core (Dziewonski &
 245 Anderson, 1981). Finally, the conductive temperature profile is expressed as follow
 246 (Buffett, 2009).

$$247 \quad T_{\text{cond}}(r, t) = T_M(r_{\text{ICB}}(t)) + \frac{T_M(0) - T_M(r_{\text{ICB}}(t))}{1 + \frac{6t_{\text{IC}}}{t_d(t)}} \left[1 - \left(\frac{r}{r_{\text{ICB}}(t)} \right)^2 \right] \quad (15)$$

248 3. Results

249 Figure 2 shows the resistivity results at 0 K for the $\text{Fe}_{0.9-y}\text{Ni}_{0.1}^{\text{s}}\text{L}_y^{\text{s}}$ substitutional alloys
250 obtained from first-principles calculations. The electrical resistivity increased with
251 increasing concentration of substitutional impurities. Si had the most significant effect
252 among the substitutional elements investigated in this study, followed by P and C.
253 Compared with a previous study of hcp $\text{Fe}_{0.9-y}\text{Ni}_{0.1}^{\text{s}}\text{L}_y^{\text{s}}$ (Zidane et al., 2020), the present
254 resistivity is smaller than their values. Zidane et al. (2020) report the axial ratio of hcp
255 Fe-based alloys to be $c/a \sim 1$. However, this value is unrealistically small for metals
256 with hcp structure; their failure to optimize c/a may cause such an overestimation of the
257 resistivity. Zidane et al. (2020) also reported higher impurity resistivity for H compared
258 to other light elements. However, the results of this study show that the impurity
259 resistivity of H at substitutional sites is comparable to that of other light elements.

260 Figure 3(a) shows the resistivity of hcp FeH_z with H occupying the interstitial sites. The
261 compositional dependence of resistivity is concave-down; zero impurity resistivity at z
262 $= 0$ and 1.0 , where no chemical disorder exists, and a maximum resistivity around $y =$
263 0.5 (Figure 3a), consistent with Nordheim's law. However, the resistivity obtained is
264 less than $3 \mu\Omega\text{cm}$, about one order of magnitude smaller than the resistivity of
265 substitutional H (Figure 2). This is because the electrical resistivity of metals is
266 associated with the band broadening due to impurity scattering (Butler, 1985); The local
267 density of states of interstitial H is far below the Fermi level, so the band structure near
268 the Fermi level cannot be affected by H (Gomi et al., 2018). Based on this, Gomi et al.
269 (2018) claimed that the impurity resistivity of FeH_z alloys is almost zero. The present
270 calculations are consistent with this prediction.

271 Figure 3(b) shows the calculated impurity resistivity of the hcp $\text{Fe}_{0.9}\text{Si}_{0.1}\text{H}_z$ alloy. Due to
 272 Si-induced impurity resistivity, the resistivity is not zero even at $z = 0$ and 1.0 , and the
 273 resistivity is higher in $\text{Fe}_{0.9}\text{Si}_{0.1}$ than in $\text{Fe}_{0.9}\text{Si}_{0.1}\text{H}_{1.0}$. The dependence of resistivity on H
 274 concentration shows a concave-down behavior as in the case of FeH_z , but its peak
 275 position is around $z = 0.3$. In the high H concentration region ($z > 0.6$), the resistivity is
 276 lower than that of the H-free $\text{Fe}_{0.9}\text{Si}_{0.1}$. Ohta et al. (2019) conducted electrical resistivity
 277 measurements of fcc FeH_z alloys at high pressure and temperature. They reported that
 278 the resistivity decreases with increasing H concentration in the high H concentration (z
 279 > 0.5) region. The present calculations and previous experiments (Ohta et al., 2019)
 280 show a similar concave-down trend even though the crystal structures, temperatures,
 281 pressures, and chemical compositions differ. As we expect similar behavior for other
 282 interstitial impurities, in subsequent calculations for 4- and 6-component alloys, we
 283 calculated the impurity resistivity only for the compositional range $z \leq 0.5$, where the
 284 resistivity is expected to be larger than in $z = 0$.

285 The resistivity of metals with an hcp structure has two components, parallel (ρ_c) and
 286 perpendicular (ρ_a) to the c -axis of the crystal. At ambient pressure, hcp Sc has a large
 287 anisotropy, with a value of $\rho_a / \rho_c = 2.2$ (Spedding et al., 1971). Balog and Secco (1999)
 288 measured anisotropy in resistivity of hcp Gd up to 1.6 GPa. The anisotropy was $\rho_a / \rho_c =$
 289 2.0 at ambient pressure but decreased linearly with increasing pressure. By
 290 extrapolating this trend, they obtained $\rho_a / \rho_c = 1$ at 20.5 GPa. In contrast, Ohta et al.
 291 (2018) pointed out the presence of high anisotropy in the thermal conductivity
 292 measurements of hcp Fe under high pressure; the value reaches $k_c / k_a = \rho_a / \rho_c = 3$. A
 293 similar high anisotropy $\rho_a / \rho_c = 3.03 \pm 0.37$ has also been reported from recent ab initio

calculations for hcp Fe (Ramkrishna et al., 2022). The present calculation also demonstrates the anisotropic resistivities (Figure 4a). However, they are relatively moderate compared with previous studies (Ohta et al., 2018; Ramkrishna et al., 2022). Figure 4b plots the resistivity ratio as a function of the polycrystalline average of resistivity. Excluding the low resistivity portion, which is close to zero division, the range of anisotropy is $0.63 \leq \rho_a / \rho_c \leq 1.52$, and strong anisotropy of $\rho_a / \rho_c \sim 3$ was not observed. Figure 4c shows the frequency distribution of resistivity anisotropy. In the composition range investigated in this study, $\rho_a / \rho_c \geq 1$ in most cases, but there were also compositions with $\rho_a / \rho_c \leq 1$.

Gomi et al. (2016) computed Fe-Si, Fe-Ni, and Fe-Ni-Si alloys. They identified three features that indicate saturation of resistivity: (1) bending of the composition dependence of resistivity, (2) smearing of the Bloch spectral function in the vicinity of the Fermi level (where the mean free path is close to the interatomic distance), and (3) a breakdown of Matthiessen's rule. Subsequently, Gomi and Yoshino (2018) calculated resistivities for substitutional binary alloys containing Si and other light elements (H, C, N, O, S), as well as Fe-Si-S ternary alloys. Among the three features due to resistivity saturation shown in Gomi et al. (2016), the broadening of the Bloch spectral function was confirmed by Gomi and Yoshino (2018). However, the presence or absence of resistivity bending is not apparent. Also, the breakdown of Matthiessen's rule was confirmed only for the Fe-Si-S ternary alloys. Therefore, it still needs to be verified for the other multi-component alloys. In this study, linear regression was performed on the calculated resistivity of 4-component alloys (Figure 5) to capture the overall trend of electrical resistivity in multi-component alloys. The regression coefficients were

317 obtained (Figure 6). Among the substitutional impurities, Si exhibits the highest
318 impurity resistivity, while the contribution of Ni is small. This result is consistent with
319 our previous studies (Gomi & Hirose, 2015; Gomi et al., 2016; Gomi & Yoshino, 2018).
320 It is also confirmed that the resistivity of substitutional H is as large as that of other light
321 elements and that the resistivity of interstitial H is much smaller than that of
322 substitutional H. In this study, we used Matthiessen's rule with a constant term as a
323 regression model (Equation 2). If Matthiessen's rule holds for the 4-component alloys
324 we calculated, then the constant term should be zero (or very small). However, this
325 study yielded a huge constant term of $33 \mu\Omega\text{cm}$, meaning Matthiessen's rule has broken
326 down. The reason for the breakdown of Matthiessen's rule can be attributed to the
327 saturation of resistivity. From this perspective, the 4-component alloys in Figure 5 can
328 be divided into three categories. The first is the alloys with the resistivity less than about
329 $40 \mu\Omega\text{cm}$, where the actual resistivity deviates from the linear regression line. In this
330 category, the resistivity is far below the saturation resistivity, and Matthiessen's rule
331 may hold. The second is a category with the resistivity of larger than about $40 \mu\Omega\text{cm}$
332 where a bend in the resistivity trend can be seen and agrees with the linear regression
333 prediction. We considered the resistivity saturation is dominant in this category. The
334 third category is where the actual resistivity is more than $\sim 20 \mu\Omega\text{cm}$ higher than the
335 linear regression line. Alloys in this category appears to continue the trend of low
336 resistivity category, which points to the possibility that the compositions in this category
337 become bad metals where resistivity saturation breaks down. If the inner core is a kind
338 of bad metal, then the thermal conductivity of the inner core may be extremely low.
339 Therefore, we looked into the composition of the alloys contained in this category. The

alloys in this category were 32 compositions (~5%) out of 6105 total compositions. Twenty compositions contained H in the substitutional sites; the remaining 12 contained O. However, these are unrealistic for the inner core; H tends to occupy the interstitial sites, and O hardly partitions into the solid inner core (Alfe et al., 2002). A more realistic compositions of the core, 6-component (Fe, Ni, Si, S)(H, C) alloys, are also plotted in Figure 5 together with 4-component alloys. Their resistivities are consistent with those of the 4-component alloys. Non of the 6-component alloys have more than ~20 $\mu\Omega\text{cm}$ large resistivity than the regression line. Therefore, the alloys comprising the inner core are considered to have compositions that follow the standard resistivity saturation.

4. Discussion

The thermal conductivity of the inner core was estimated from the impurity resistivity obtained by first-principles calculations. The thermal conductivities of 6-component $\text{Fe}_{1-x-y}\text{Ni}_x(\text{Si}, \text{S})_y(\text{H}, \text{C})_z^i$ alloys obtained in this study were 120-310 W/m/K at 5500 K. However, some of these 1176 compositions contain too many or too few light elements for the inner core. Therefore, we present the thermal conductivities for five representative compositions. When the only light element in the inner core is interstitial H, the amount of H that satisfies the density of the inner core is about $z = 0.22$ (Gomi & Hirose, 2022). Considering the 5% of Ni present in the core, the thermal conductivity of $\text{Fe}_{0.95}\text{Ni}_{0.05}\text{H}_{0.2}$ is estimated to be $k = 263$ W/m/K. Since interstitial H has negligible impurity resistivity, the thermal conductivity of this composition is the upper limit of the thermal conductivity of the inner core. The amount of C required to satisfy the density defects in the inner core is ~1.5 wt.% (Mookherjee et al., 2011) corresponds to about $z =$

363 0.07. The thermal conductivity of $\text{Fe}_{0.95}\text{Ni}_{0.05}\text{C}_{0.1}$ is $k = 234$ W/m/K, which is lower than
 364 the H-rich alloy. If all light elements in the inner core were substitutional Si, the
 365 concentration would be ~ 7 wt.%Si ($y \sim 0.13$) (Tateno et al., 2015). The thermal
 366 conductivity of $\text{Fe}_{0.8}\text{Ni}_{0.05}\text{Si}_{0.15}$ is computed to be $k = 150$ W/m/K. It is reported that the
 367 effect of Si and S on the density of hcp Fe alloys is similar (Li et al., 2018). We found
 368 that the thermal conductivity of $\text{Fe}_{0.8}\text{Ni}_{0.05}\text{S}_{0.15}$ becomes $k = 154$ W/m/K, slightly higher
 369 than the Si-rich scenario. The thermal conductivity of $\text{Fe}_{0.85}\text{Ni}_{0.05}\text{Si}_{0.05}\text{S}_{0.05}\text{H}_{0.1}$, as an
 370 example with multiple light elements, yielded $k = 166$ W/m/K. Therefore, for realistic
 371 chemical compositions that satisfy the density of the inner core, the range of thermal
 372 conductivities would be 150-263 W/m/K. Zidane et al. (2020) estimated the thermal
 373 conductivity of the inner core to be 110-155 W/m/K. This value is systematically
 374 smaller than this study. The reason may be due to their failure to optimize c/a . Pozzo et
 375 al. (2014) obtained a 232 W/m/K thermal conductivity for $\text{Fe}_{0.93}\text{Si}_{0.07}$. The thermal
 376 conductivity of $\text{Fe}_{0.95}\text{Si}_{0.05}$ obtained from this study, $k = 217$ W/m/K, is slightly lower
 377 than that of Pozzo et al. (2014); Pozzo et al. (2014) reported the Lorentz number as $L =$
 378 $2.7 \times 10^{-8} \text{ W}\Omega/\text{K}^2$. The difference in thermal conductivity may be because the present
 379 study assumes the Sommerfeld value $L_{\text{Somm}} = 2.445 \times 10^{-8} \text{ W}\Omega/\text{K}^2$.

380 Many characteristic seismic observations (seismic velocity, attenuation, and their
 381 anisotropy with depth and hemispherical variations) are known for the Earth's inner
 382 core. However, no single model can explain all of them simultaneously (Deguen, 2012;
 383 Deuss, 2014). Among these observations, the innermost inner core is one of the most
 384 mysterious to understand from mineralogy and inner core dynamics (Deguen, 2012).
 385 The innermost inner core is known as a layer that exists at the center of the inner core

with a radius of 300-600 km, which has a different anisotropy (Ishii & Dziewonski, 2002; Pham & Tkalčić, 2023; Stephenson et al., 2021), and a lower attenuation (Cormier & Li, 2002; Cormier & Stroujkova, 2005; Li & Cormier, 2002) than the upper inner core. Buffet (2009) pointed out that the termination of initial thermal convection could form a layer structure in the inner core. However, using recent high thermal conductivity estimates, including this study, thermal convection is impossible even in the initial inner core (Pozzo et al., 2014). Deguen et al. (2018) pointed out that a double-diffusive translation could be terminated at the early stage of the inner core. The following conditions are required for double-diffusion instability (Deguen et al., 2018).

$$-\frac{\alpha\Delta T}{\beta\Delta\chi} \leq Le \quad (16)$$

where $\alpha \sim 10^{-5} \text{ K}^{-1}$ is the thermal expansion coefficient, $\beta \sim 1$ is the compositional expansion coefficient, $\Delta T \sim -100 \text{ K}$ is the difference in core center temperature from the adiabatic temperature profile, $\Delta\chi$ is the difference in light element concentration between the center and ICB, and $Le = \kappa/D$ is a dimensionless parameter representing the ratio between thermal diffusivity (κ) and diffusion coefficient (D) of light elements, called Lewis number. With a diffusion coefficient of $D \sim 10^{-12} \text{ m}^2/\text{s}$ for light elements (Gubbins et al., 2013), the Le is calculated to be $\sim 2 \times 10^7$ (Deguen et al., 2018). Due to the huge Le , even with a strong thermal stratification ($\Delta T < 0$), a double-diffusive instability exists if there is a slight compositional instability ($\Delta\chi > 0$) (Deguen et al., 2018). For example, even a slight compositional gradient ($\Delta\chi_0 \sim 0.005 \%$) (Labrosse, 2014) created by O that is little partitioned into the inner core would result in the left side of Equation (16) being less than 5 (Deguen et al., 2018). Recent ab initio molecular dynamics studies have indicated that interstitial light elements (H, O, and C) may

409 become a superionic state (He et al., 2022). In this case, the diffusion coefficient of
 410 these light elements reaches the order of $D \sim 10^{-8} \text{ m}^2/\text{s}$ (He et al., 2022; Wang et al.,
 411 2021; Yang et al., 2022), resulting in a Lewis number down to the order of 10^3 . However,
 412 this value is still sufficiently high for double-diffusive instability. Therefore, the
 413 double-diffusive instability is determined only by the sign of $\Delta\chi$. Zhang et al. (2020b)
 414 performed atomistic simulations with machine learning potentials to constrain the
 415 solid-liquid partitioning of S. Their results show that, in contrast to Gubbins et al.
 416 (2013), there is little pressure dependence on the S partition coefficient. If the S
 417 concentration in the outer core increases with inner core growth, the S partitioning into
 418 the inner core yields compositional stratification ($\Delta\chi_S \leq 0$). The partition coefficient of a
 419 light element in a multi-component system may depends on the concentration of the
 420 coexisting light element. For example, Hasegawa et al. (2021) conducted high-pressure
 421 experiments on a Fe-Si-C system in a DAC. They found that the partition of Si to the
 422 solid phase increases with increasing C concentration in the liquid phase. If the core
 423 composition can be approximated by a Fe-Si-C ternary system, the outer core C
 424 concentration increases with the inner core growth. In this case, the Si concentration in
 425 the inner core also increases toward the top of the core, so Si causes compositional
 426 stratification within the inner core ($\Delta\chi_{Si} \leq 0$). It is worth mentioning that, as Deguen et
 427 al. (2018) point out, temporal changes in the composition of the liquid reacting with the
 428 inner core behave complicated due to the following two reasons; precipitation of MgO
 429 and SiO₂ (Badro et al., 2016; Hirose et al., 2017; O’Rourke & Stevenson, 2016)
 430 decreases the concentration of light elements in the liquid. Forming a dense layer at the
 431 bottom of the outer core makes the composition of the liquid reacting with the inner

432 core depleted in light elements compared with the average composition of the outer core.
433 Thus, early termination of double-diffusive translation is possible for the origin of the
434 innermost inner core. However, in this case, translation cannot explain the
435 hemispherical dichotomy, and other models are needed (e.g. Aubert et al., 2008;
436 Gubbins et al., 2011). Kuwayama et al. (2008) pointed out the possibility of an fcc-hcp
437 phase transition in Fe-Ni alloys within the inner core. In this scenario, the innermost
438 inner core is composed of hcp Fe-Ni alloy, and the upper inner core is fcc. Recently, the
439 possibility of delayed crystallization of the inner core due to super-cooling has been
440 proposed (Huguet et al., 2018). If this is the case, a substantial amount of melt is
441 trapped in the innermost inner core, whereas compaction of a solid matrix extract melts
442 in the upper inner core (Lasbleis et al., 2020). These are the possible origins of the
443 boundary with different physical properties inside the inner core.

444 In this study, we propose a new mechanism that make a boundary with different
445 physical properites in the inner core due to the pre-melting. Recently, Yamauchi and
446 Takei (2020) reported that the grain boundary pre-melting could explain the sharp
447 lithosphere-asthenosphere boundary observed in the oceanic mantle. The similar
448 bounday is possible in the inner core. Due to grain boundary pre-melting, polycrystals
449 rapidly soften slightly below the melting temperature (e.g., Cantwell et al., 2014). Its
450 characteristic temperature T_{PM} is several percent below the melting temperature
451 (Martorell et al., 2013; Nadal & Poac, 2003; Yamauchi & Takei, 2016). In the
452 polycrystalline Sn experiments by Nadal and Poac (2003), a sharp decrease in shear
453 modulus occurred within 1% of the melting temperature ($T_{PM} > 0.99 T_M$). Yamauchi and
454 Takei (2016) showed from experiments on polycrystalline Borneol ($C_{10}H_{18}O$), a mantle

455 analog composed of organic materials, that softening occurs at $T_{\text{PM}} > 0.92 T_{\text{M}}$. Martorell
 456 et al. (2013) calculated the elastic constants of single-crystal hcp Fe without grain
 457 boundaries by using the first principles calculations up to melting temperature at inner
 458 core pressure. They found a decrease in the shear modulus at $T_{\text{PM}} > 0.96 T_{\text{M}}$. Martorell
 459 et al. (2013) argued that pre-melting occurs throughout the inner core assuming the
 460 adiabatic temperature profile. However, suppose the thermal conductivity of the inner
 461 core is high and the resultant temperature gradient is flat. In that case, the difference
 462 between the melting temperature and core conductive temperature profile increases as
 463 one goes deeper into the inner core, and pre-melting may not occur at the center. Figure
 464 7 shows the temperature profile of the inner core as a function of the thermal
 465 conductivity with the age of the inner core to be $t_{\text{IC}} = 1.0$ Gyr. The higher the thermal
 466 conductivity, the smaller the temperature gradient within the inner core. For the present
 467 inner core to be thermally convective, the temperature determined by thermal
 468 conduction must be higher than that determined by the adiabatic temperature gradient
 469 (Yukutake, 1998). Therefore, the present-day inner core cannot maintain thermal
 470 convection if the thermal conductivity is higher than 40 W/m/K. This critical value is
 471 much lower than the present estimates ($k = 150\text{-}263$ W/m/K), making the present-day
 472 inner core likely to be thermally stable. With such high thermal conductivity, the
 473 temperature profile of the inner core would be flat. The temperature difference between
 474 the present-day ICB and the center was estimated to be less than 110 K. Let us compare
 475 the conductive temperature profiles with the pre-melting temperature. In Figure 7,
 476 profiles for 99, 98, 97, and 96% of T_{M} are plotted in addition to the melting curve. If $k =$
 477 160 W/m/K, $t_{\text{IC}} = 1.0$ Gyr, and $T_{\text{PM}} = 0.97 T_{\text{M}}$, pre-melting does not occur at radius $r \leq$

478 600 km in the inner core (Figure 7), which may explain the observation that seismic
 479 attenuation is stronger in the upper inner core and weaker at the innermost inner core
 480 (Cormier & Li, 2002; Cormier & Stroujkova, 2005; Li & Cormier, 2002). We plotted
 481 the temperature at the center of the core as a function of core thermal conductivity and
 482 the inner core age (Figure 8). $T = 5711$ K, calculated from adiabat (Equation 12), is a
 483 criterion for thermal instability. Therefore, we plotted the region with $T < 5711$ K as
 484 blue and $T > 5711$ K as red. In the range of present thermal conductivities, the inner
 485 core should be thermally stable, meaning no thermally-driven plume convection or
 486 thermally-driven translation. In this situation, the temperature profile of the inner core
 487 becomes flat, determined by conduction. Although the T_{PM} of the inner core is currently
 488 essentially unconstrained, if the $T_{\text{PM}} \sim 0.97 T_{\text{M}}$, then a boundary due to pre-melting can
 489 exist in the inner core. This pre-melting boundary could explain the difference in
 490 seismic attenuation between the upper inner core and the innermost inner core (Cormier
 491 & Li, 2002; Cormier & Stroujkova, 2005; Li & Cormier, 2002). It should be worth
 492 mentioning that this pre-melting model can easily be combined with other models to
 493 explain other seismic observations (e.g., double-diffusive translation for hemispherical
 494 dichotomy) because it depends only on the present-day temperature profile.

495 **5. Summary and conclusion**

496 We computed the impurity resistivity of hcp Fe-based 4- and 6-component alloys by
 497 means of KKR-CPA method combined with the Kubo-Greenwood formula. The results
 498 exhibit anisotropy $0.63 \leq \rho_a / \rho_c \leq 1.52$, where ρ_c and ρ_a are resistivities parallel and
 499 perpendicular to the c -axis, respectively. Interstitial H contributed little to resistivity,
 500 consistent with prior experiments (Ohta et al., 2019). Impurities at substitutional sites

501 showed systematically greater resistivity than impurities at interstitial sites. We
502 performed linear regression on the resistivity of the 4-component alloys. The results
503 show the breakdown of Matthiessen's rule due to resistivity saturation. This trend was
504 also observed for hcp (Fe, Ni, Si, S)(H, C) 6-component alloys, which have a more
505 realistic chemical composition of the inner core. The Wiedemann-Franz law was applied
506 to estimate the thermal conductivity of the inner core to be $k = 150\text{-}263$ W/m/K. This
507 value is systematically higher than the previous calculation (Zidane et al., 2020). With
508 the present thermal conductivity values, we calculated the temperature profile due to
509 thermal conduction in the present-day inner core using the model developed by Buffett
510 (2009). The conductive temperature profile is flat, indicating that the inner core cannot
511 maintain thermal convection. Polycrystalline solids are known to soften rapidly at
512 temperatures above a few percent below the melting temperature due to grain boundary
513 pre-melting (e.g., Nadal & Poac, 2003; Yamauchi & Takei, 2016). When the
514 temperature profile is flat, pre-melting occurs only in the upper inner core. This could
515 explain the observations that the attenuation is stronger in the upper inner core and
516 weaker in the innermost inner core (Cormier & Li, 2002; Cormier & Stroujkova, 2005;
517 Li & Cormier, 2002).

518

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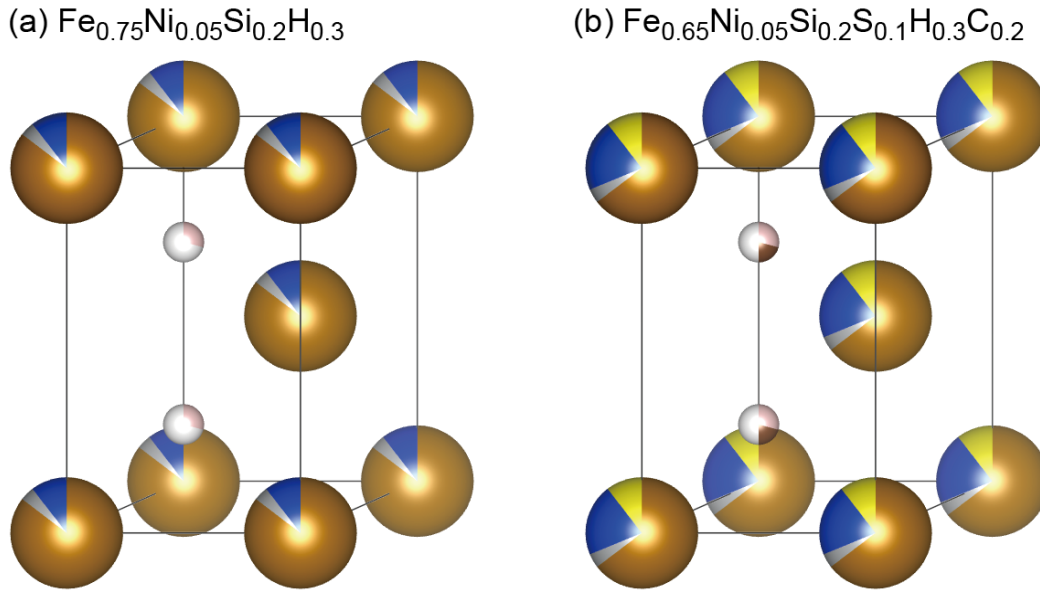
841 **Acknowledgements**

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843 22K03754, and 21H04968.

844 **Data Availability Statement**

845 Datasets for this study are available online <https://doi.org/10.5281/zenodo.7929259>.

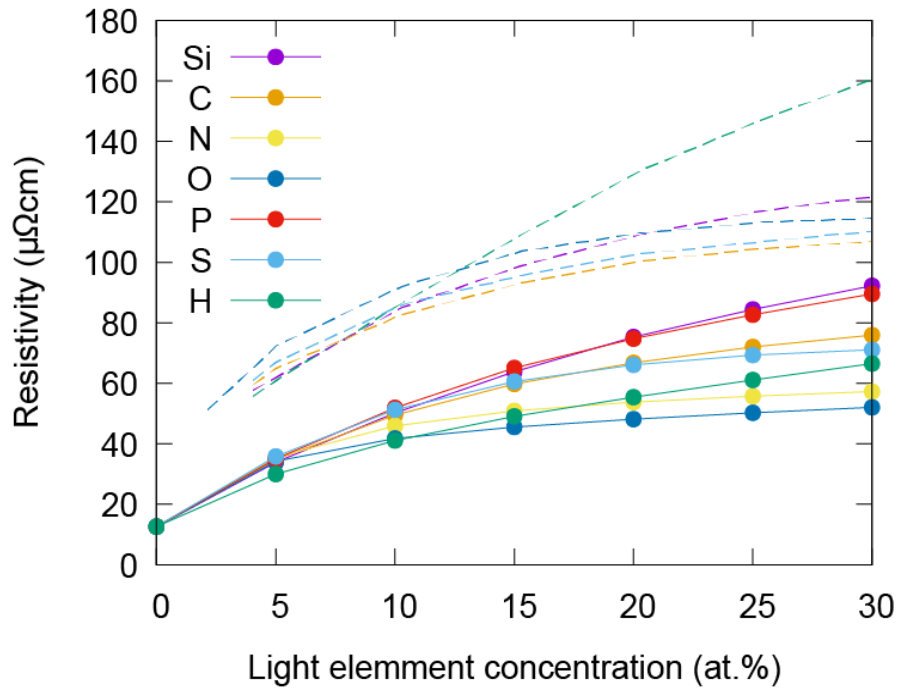
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847

848 **Figure 1.** The crystal structure of hcp Fe-based alloy is illustrated using the VESTA
 849 program (Momma & Izumi, 2011). (a) $\text{Fe}_{0.75}\text{Ni}_{0.05}\text{Si}_{0.2}\text{H}_{0.3}$ alloy, which is an example of
 850 a 4-component alloy. Ni (silver) and Si (blue) enter the substitutional site of hcp Fe
 851 (brown), whereas H (pink) occupies the octahedral interstitial site. (b)
 852 $\text{Fe}_{0.65}\text{Ni}_{0.05}\text{Si}_{0.2}\text{S}_{0.1}\text{H}_{0.3}\text{C}_{0.2}$ alloy, which is an example of a 6-component alloy. Note that
 853 Ni, Si, and S (yellow) enter the substitutional site simultaneously, and H and C (dark
 854 brown) are simultaneously located at the interstitial site.

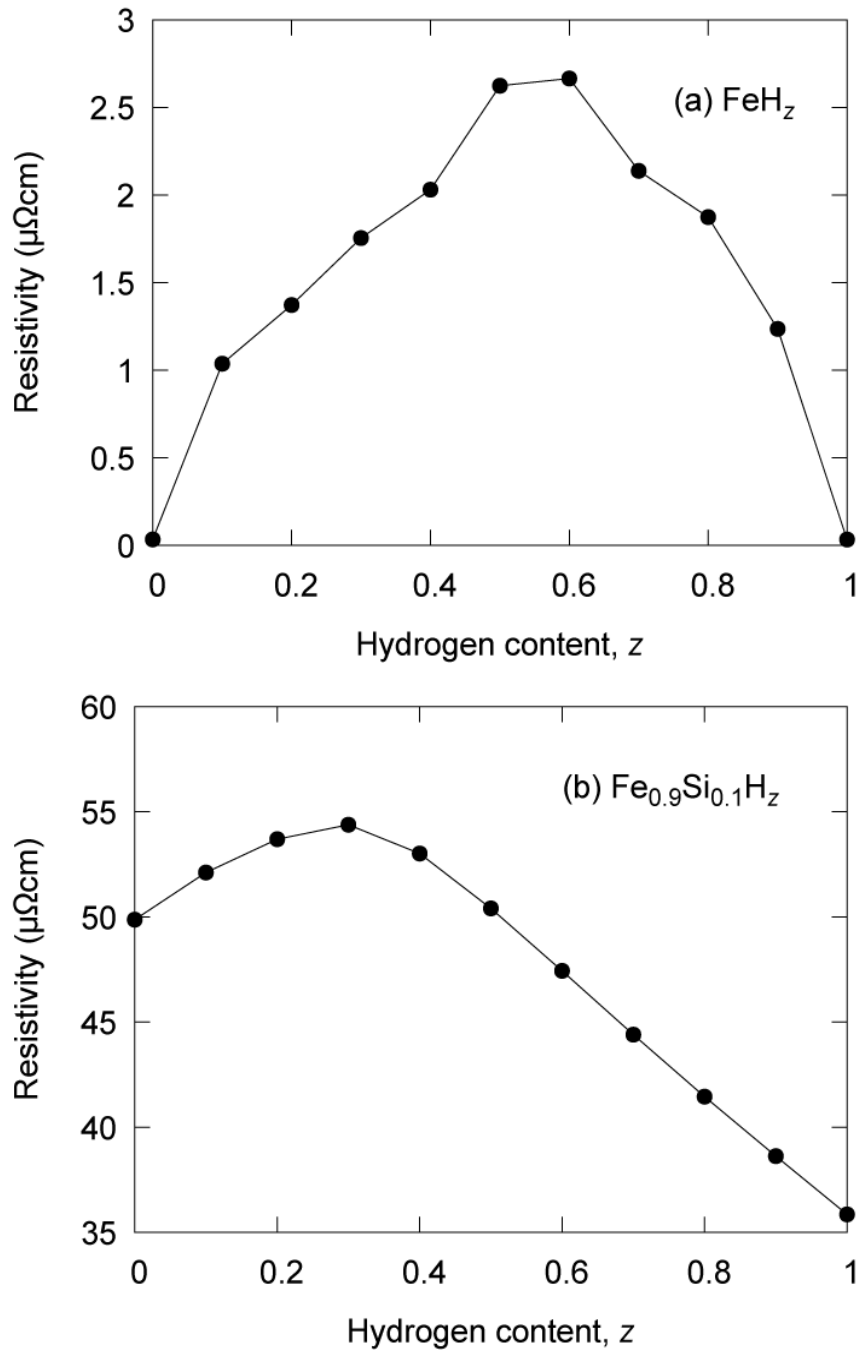
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857 **Figure 2.** The resistivity of hcp $\text{Fe}_{0.9-x}\text{Ni}_{0.1}\text{L}_x^i$ substitutional ternary alloys.
 858 Substitutional light element is Si (purple), C (orange), N (yellow), O (blue), P (red), S
 859 (cyan), or H (green). Solid lines with circles are present calculations. Broken lines are
 860 previous calculations (Zidane et al., 2020). Note that Zidane et al. (2020) overestimated
 861 the resistivity.

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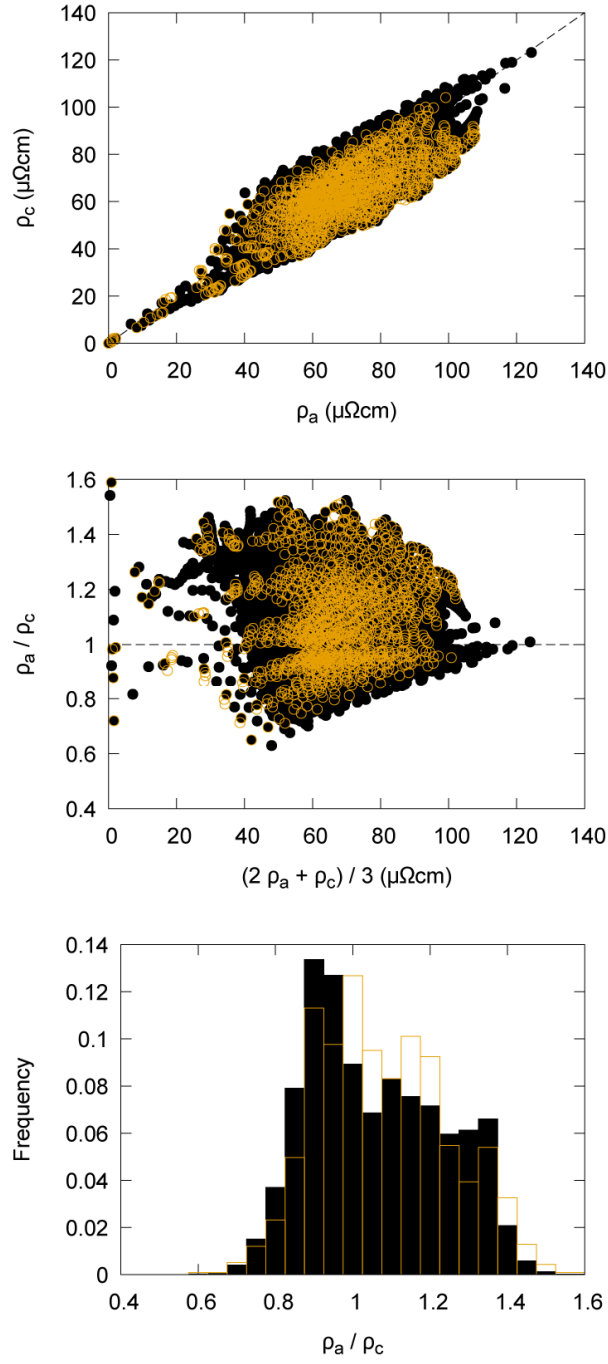


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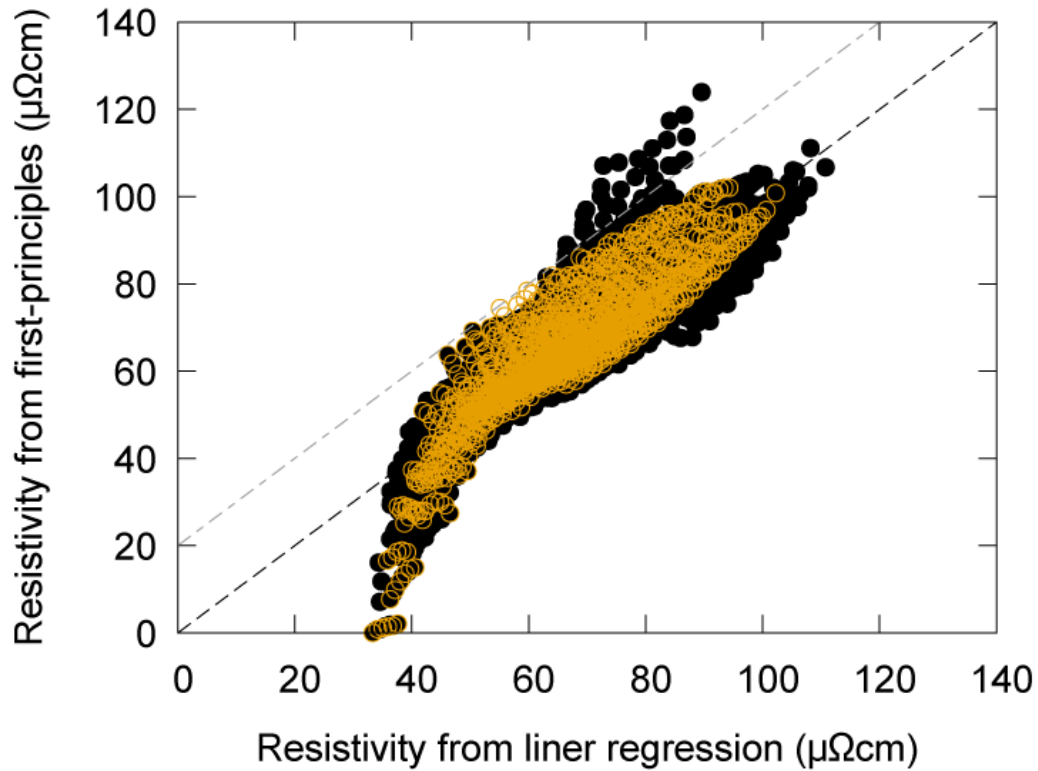
864 **Figure 3.** The resistivity of hcp (a) FeH_z (b) $\text{Fe}_{0.95}\text{Ni}_{0.05}\text{H}_z$, and (c) $\text{Fe}_{0.9}\text{Si}_{0.1}\text{H}_z$ alloys as

865 functions of H content, z .

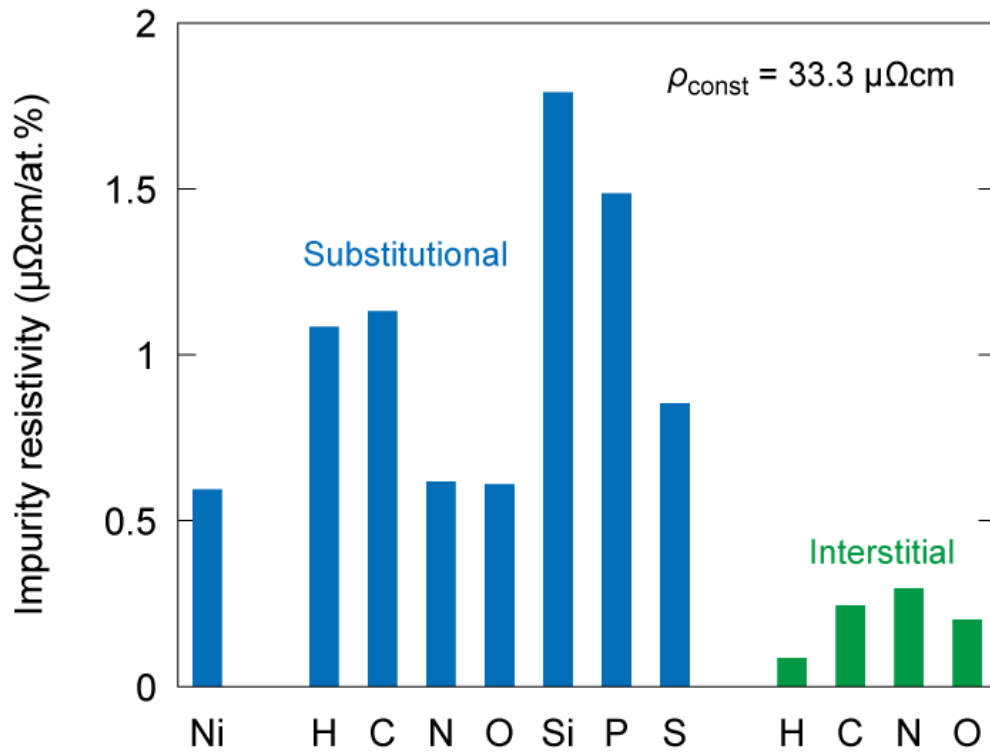
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867
868 **Figure 4.** Anisotropic impurity resistivity of hcp Fe-based alloys with 4- (black) and
869 6-component (orange) alloys. (a) impurity resistivity parallel (ρ_c) and perpendicular (ρ_a)
870 to the c -axis. (b) Resistivity ratio. (c) Histogram of the resistivity ratio (ρ_a / ρ_c).
871



872
 873 **Figure 5.** Result of the linear regression for 4-component alloys (black filled circle).
 874 6-component alloys (orange open circle) are consistent with 4-component alloys. Black
 875 broken line indicates the regression line, and gray dotted-broken line represents the
 876 resistivity 20 $\mu\Omega\text{cm}$ higher than the regression line.
 877

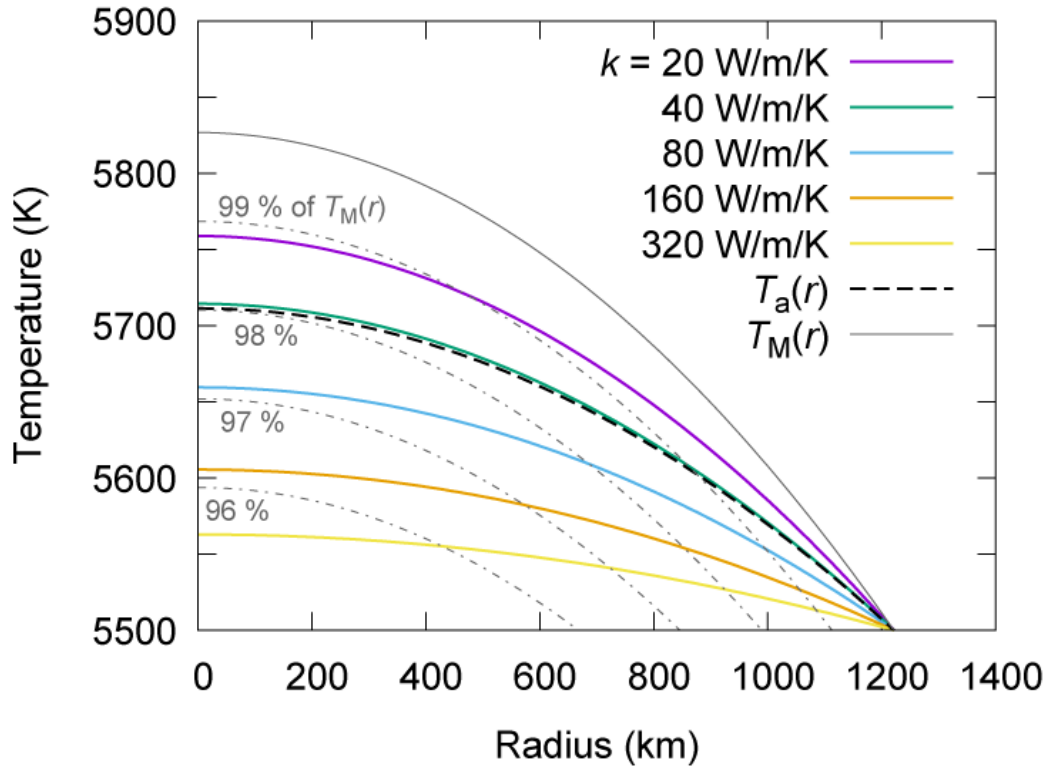


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879 **Figure 6.** Regression coefficients for the impurity resistivity 4-component alloys.

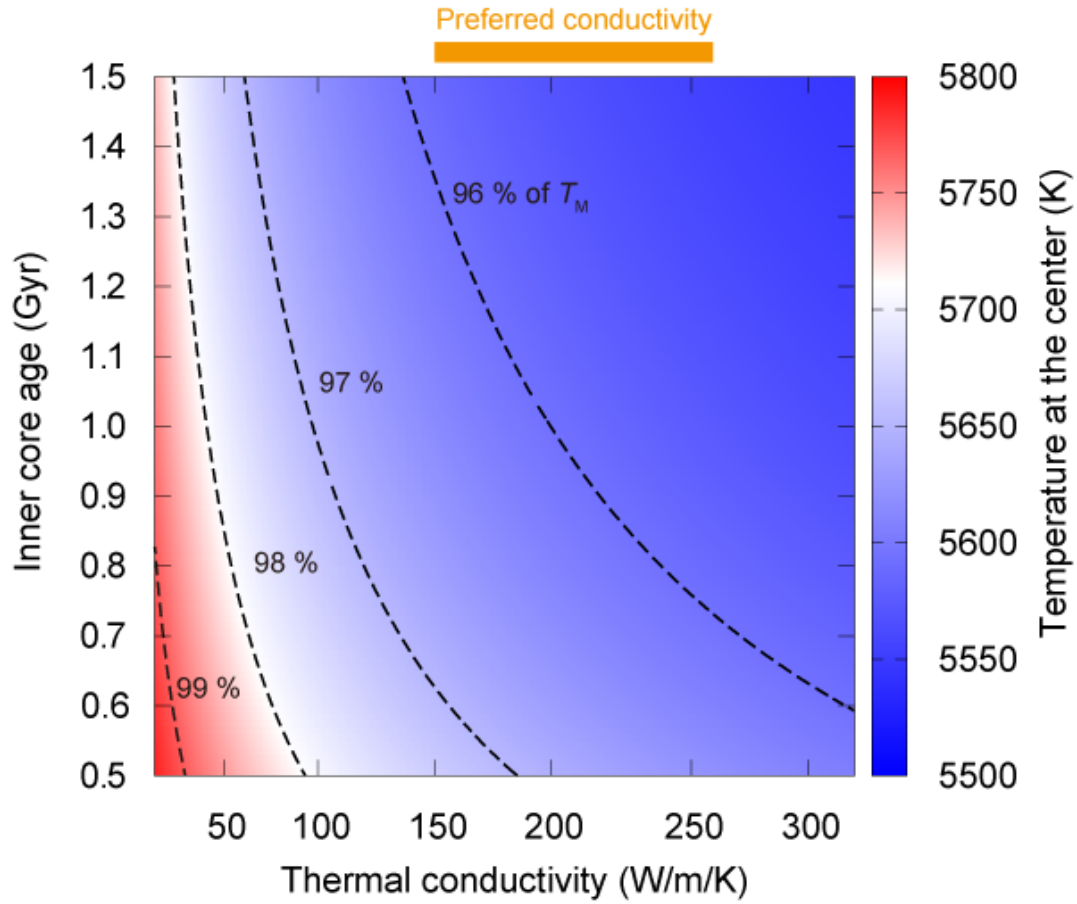
880 Substitutional impurities are indicated as blue and interstitial impurities are green.

881



882
883 **Figure 7.** The present-day temperature profile within the inner core with the inner-core
884 age of 1 Gyr. Thick solid lines indicate the conductive temperature profile with thermal
885 conductivity of 20 (purple), 40 (green), 80 (cyan), 160 (orange), and 320 W/m/K
886 (yellow). The broken line represents the adiabatic temperature profile. For thermal
887 convection to occur, the temperature must be higher than the adiabat. The solid gray line
888 represents the melting temperature. Gray dotted broken lines are 99, 98, 97, and 96 % of
889 the melting temperature.

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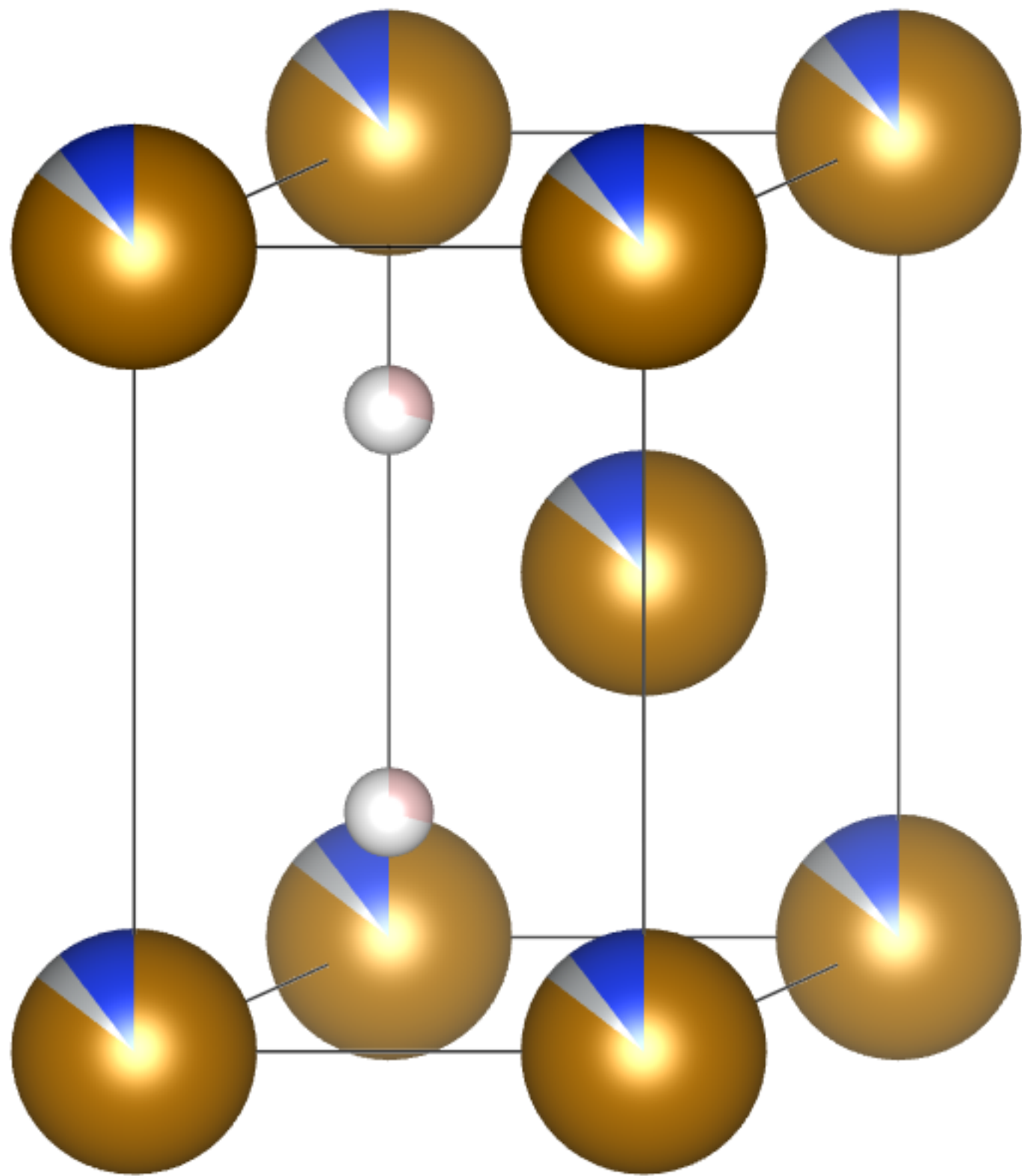


891

892 **Figure 8.** The present-day temperature at the center of the inner core as a function of
 893 thermal conductivity and inner-core age. The red region indicates thermal instability,
 894 whereas the blue area tends to become thermal stratification. Broken lines are
 895 iso-temperature curves corresponding to 99, 98, 97, and 96 % of the melting
 896 temperature. The preferred thermal conductivity range (150-263 W/m/K) is indicated as
 897 the orange band.

Figure 1.

(a) $\text{Fe}_{0.75}\text{Ni}_{0.05}\text{Si}_{0.2}\text{H}_{0.3}$



(b) $\text{Fe}_{0.65}\text{Ni}_{0.05}\text{Si}_{0.2}\text{S}_{0.1}\text{H}_{0.3}\text{C}_{0.2}$

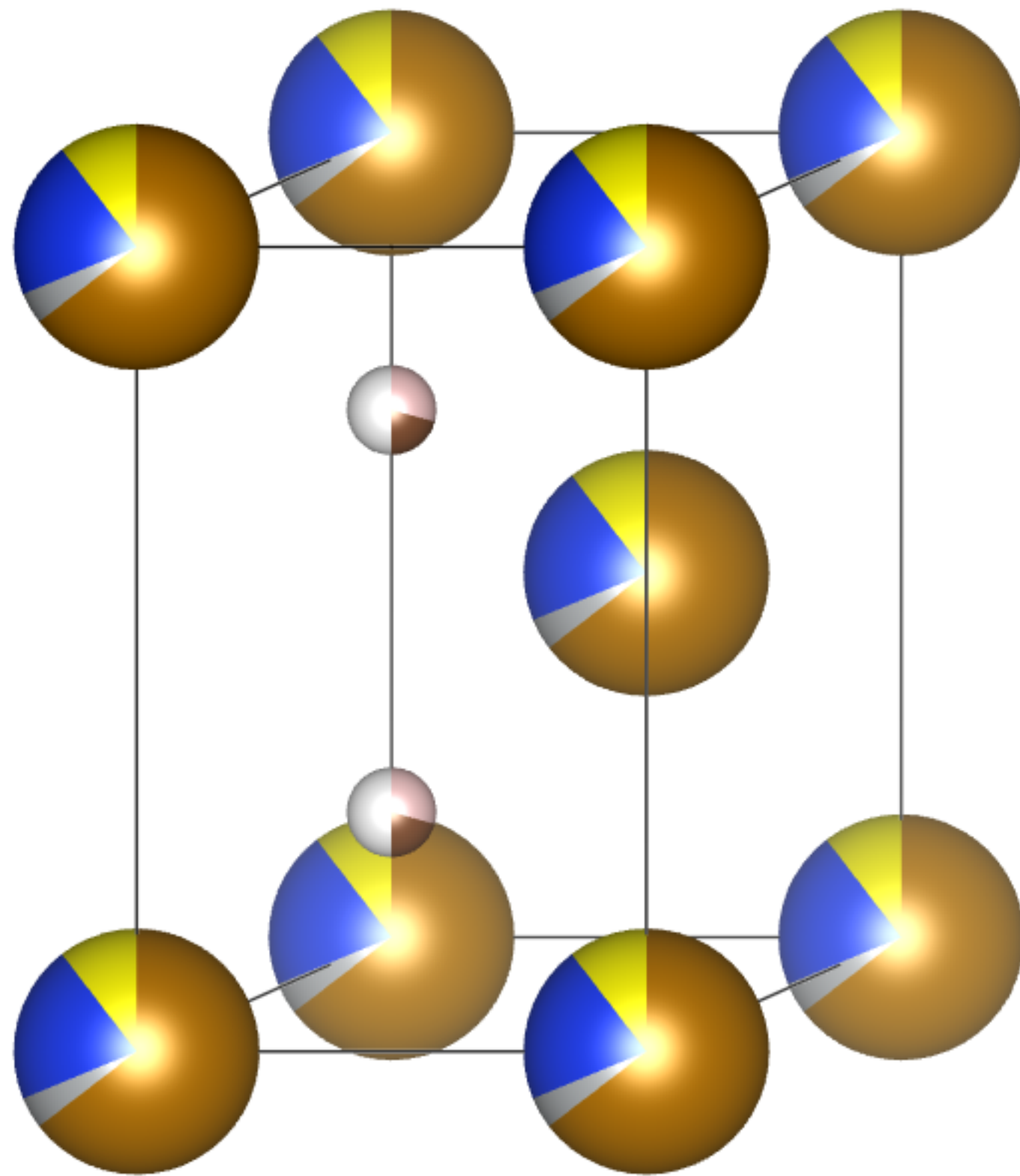


Figure 2.

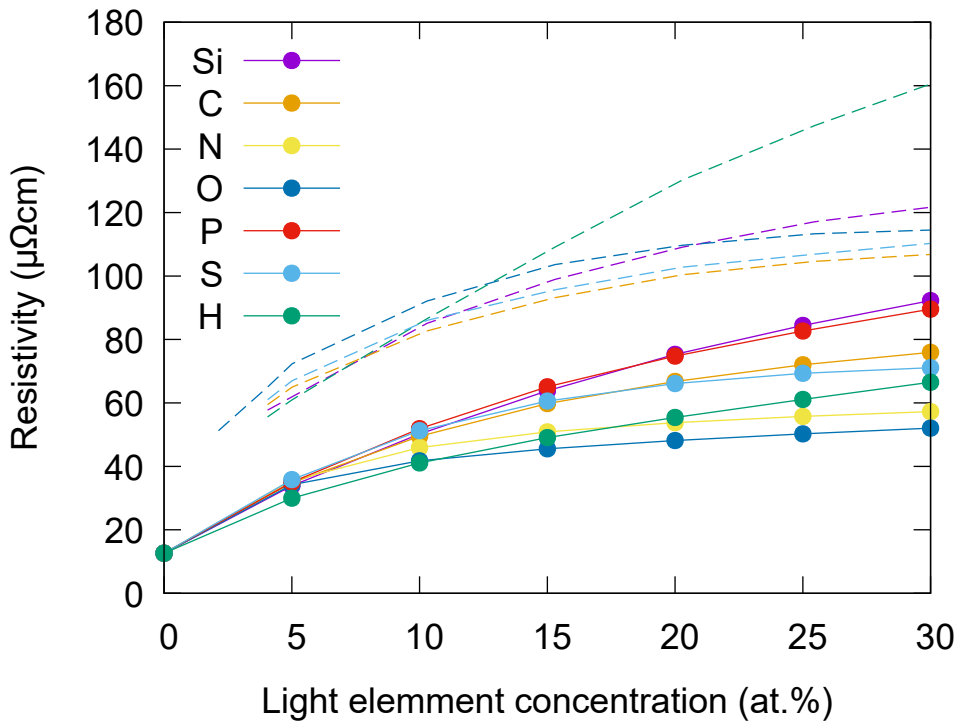


Figure 3.

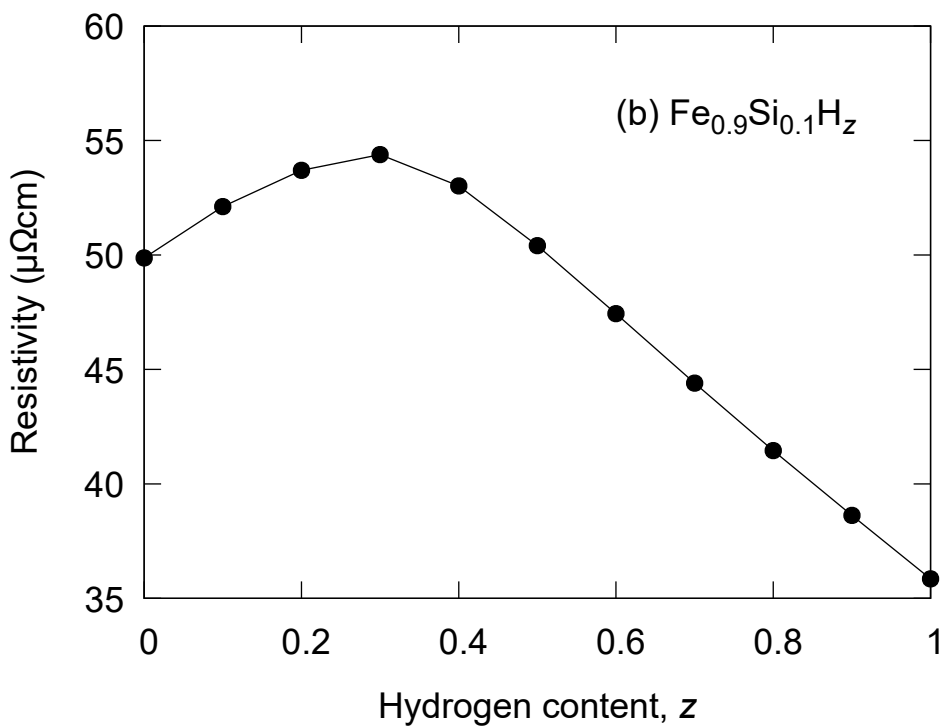
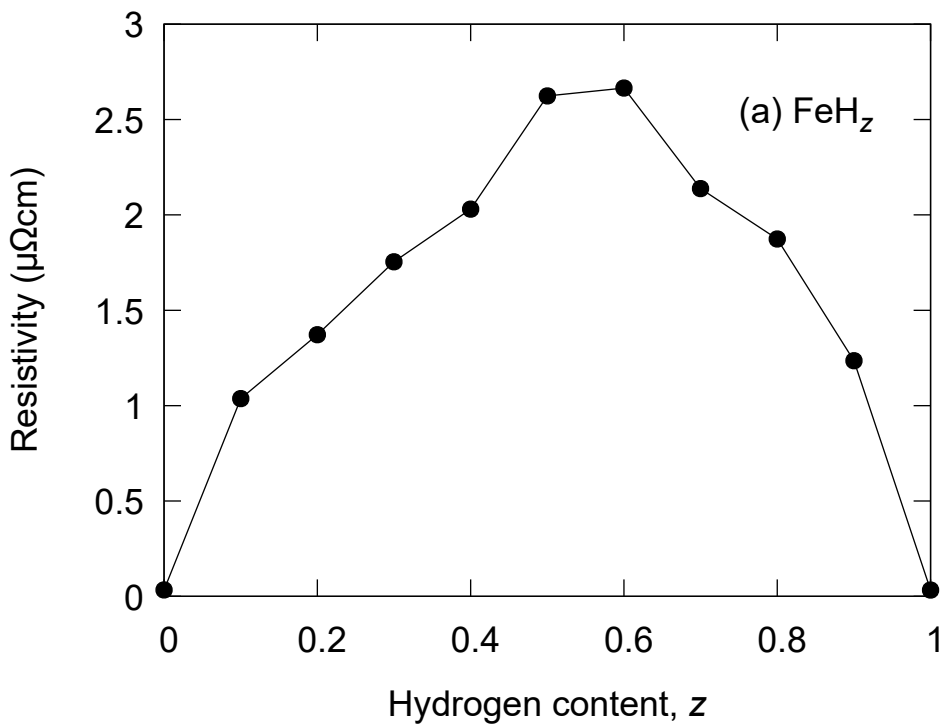


Figure 4.

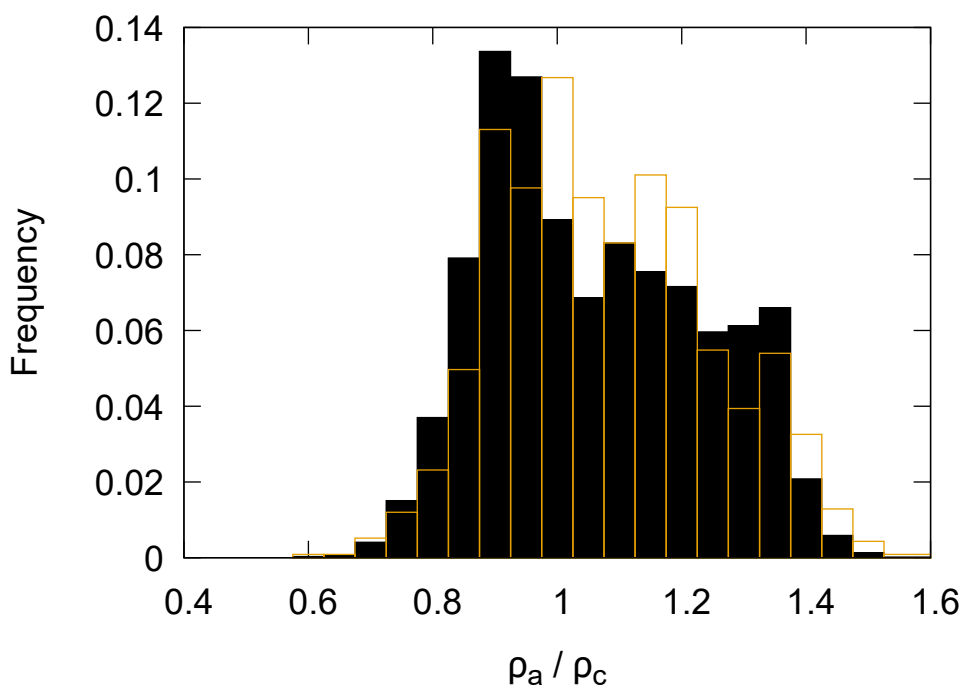
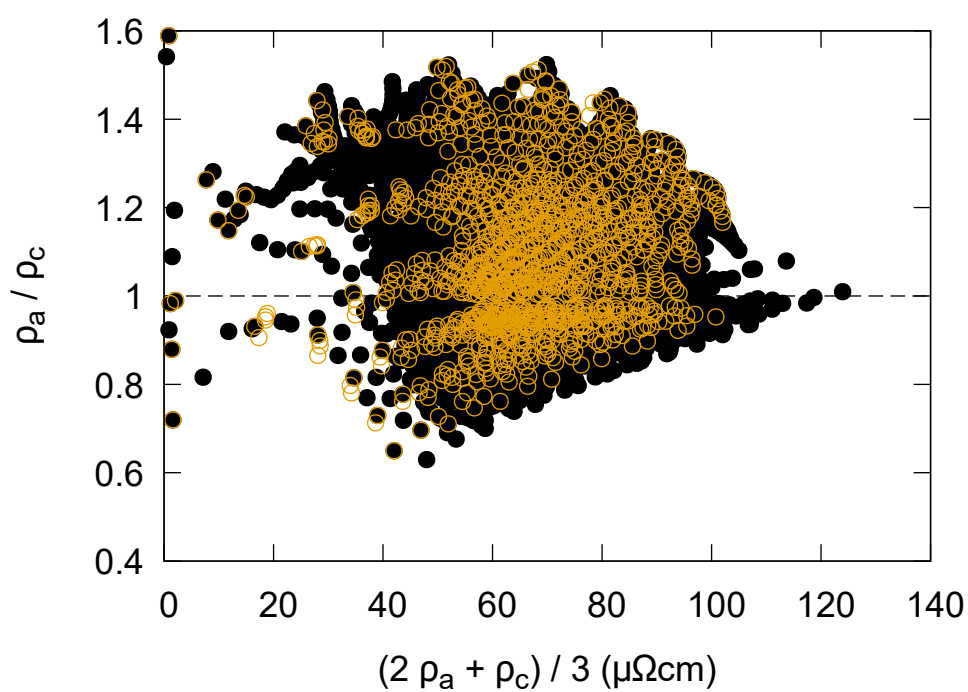
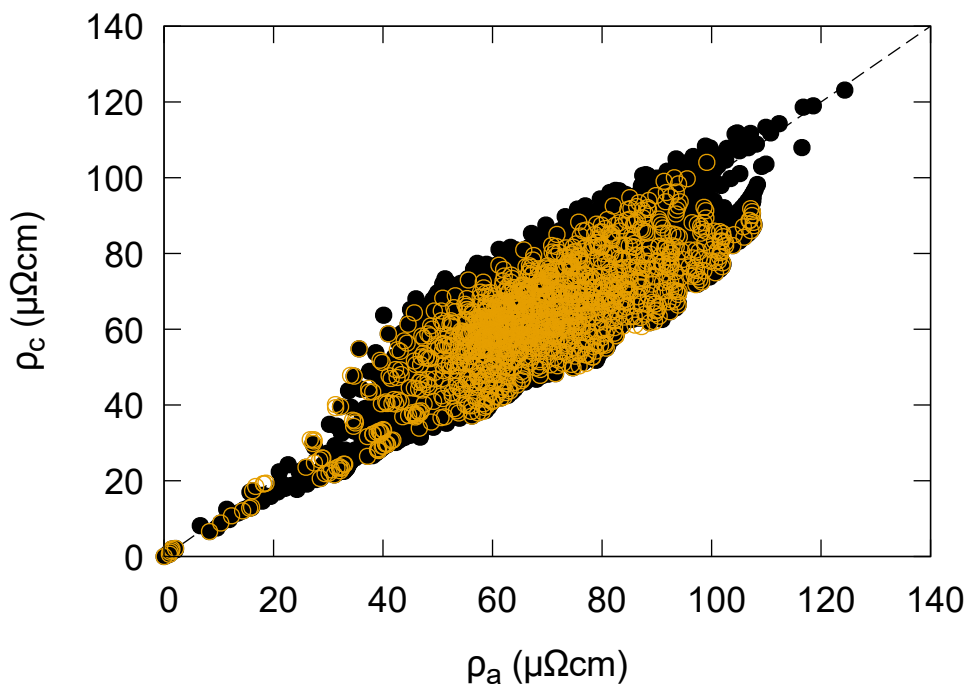


Figure 5.

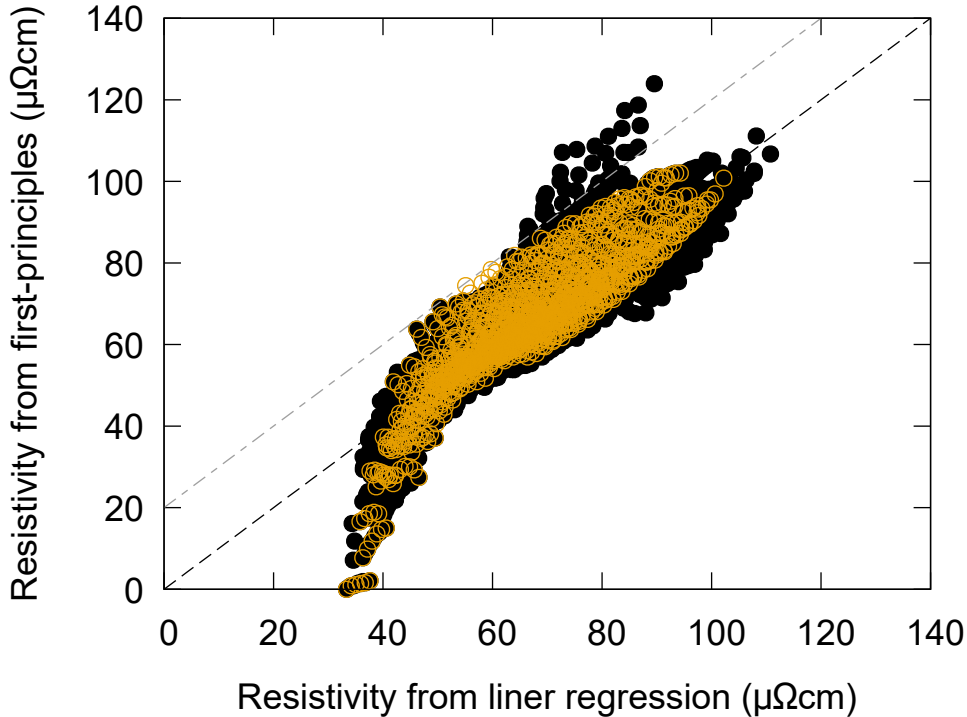


Figure 6.

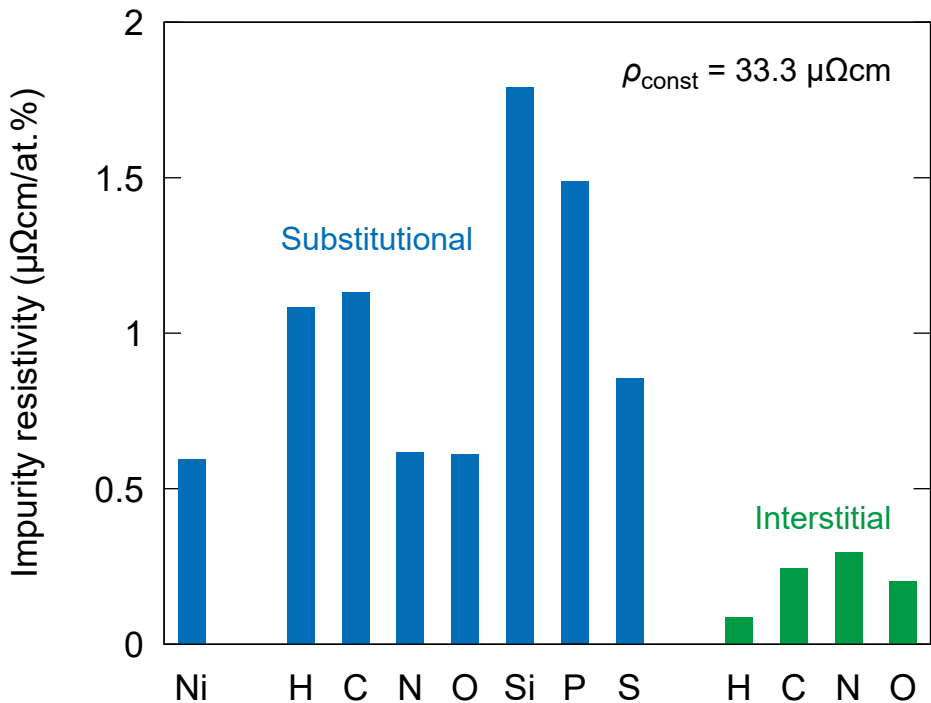


Figure 7.

Temperature (K)

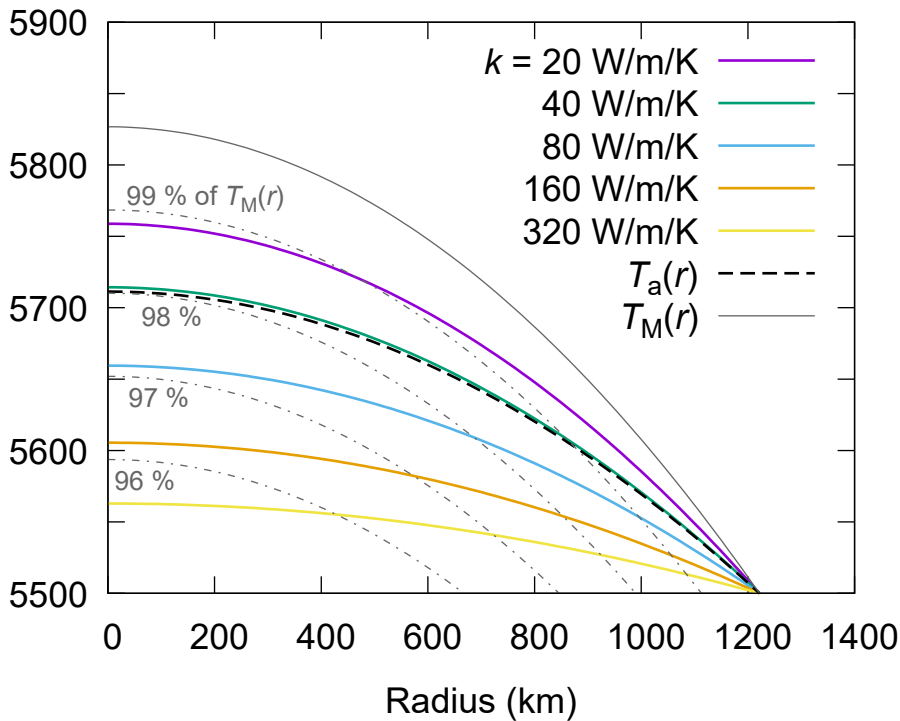


Figure 8.

