Electron–electron scattering and thermal conductivity of iron at Earth’s core conditions

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Electron–electron scattering and thermal conductivity of $\epsilon$-iron at Earth’s core conditions

1. Introduction

Earth’s magnetic field plays a crucial role in the survival of the human race. It keeps the ozone layer intact despite the solar wind and therefore protects the Earth from destructive ultraviolet radiation [1]. The magnetic field is generated by self-sustained dynamo action in its iron-rich core [2]. This geodynamo runs on heat from the growing solid inner core and on chemical convection provided by light elements issued from the liquid outer core on solidification [3]. The power supplied to drive the geodynamo is proportional to the rate of inner core growth, which in turn is controlled by heat flow at the core-mantle boundary [4]. This heat flow critically depends on the thermal conductivity of liquid iron under the extreme pressure and temperature conditions in the Earth’s core. For a long time there has been agreement that convection in the liquid outer core provides most of the energy for the geodynamo and has been doing so for at least 3.4 billion years [2, 5].

Recently, such a view has been challenged by first-principles calculations [3, 6], suggesting a much higher capacity for the liquid core to transport heat by conduction and therefore less ability to transport heat by convection [2]. The calculated conductivities have been found to be two to three times higher than the earlier generally accepted estimates, urging for reassessment of the core thermal history and power requirements [3]. Several ideas have been recently put forward to resolve this controversy between low thermal conductivity predicted by $ab\ initio$ calculations and the stability of geodynamo. In particular, magnesium precipitation from the core was suggested to be important to powering Earth’s dynamo [7]. In addition, crystallization of SO$_2$ on top of the core could allow for a secular core cooling rate 3.88 times smaller than is required for unassisted thermal convection alone [8]. Experimental results on the thermal conductivity of $\epsilon$-Fe at high pressure and temperature are so far inconclusive due to a contradictory outcome of different measurements [9, 10].
Convection also plays a crucial role in the current theory of the solid core dynamics, as a radial motion of the inner core matter is invoked to explain the observed seismic anisotropies of the inner core [11–13]. However, \textit{ab initio} calculations [14] similarly predict a too high thermal conductivity for hexagonal close-packed (hcp) \(\epsilon\)-iron generally assumed to form the inner core, thus impeding a significant convection of its solid matter.

The first-principles calculations for liquid and solid iron of [3, 6, 14], unlike previous results, have not relied on any extrapolations, however, they employed the standard density-functional-theory (DFT) framework in which electron–electron repulsion is not properly accounted for as dynamical many-body effects are neglected. Hence, the contribution to resistivity from the electron–electron scattering (EES) of \(d\)-electrons due to correlations was not taken into account in those calculations.

Two earlier works [15, 16] by some of us considered many-body effects in pure Fe and iron-rich FeNi alloys for all three known phases of crystalline iron, hcp \(\epsilon\), body-centered cubic (bcc) and face-centered cubic (fcc), at the conditions of Earth’s inner core employing the density functional theory plus dynamical mean-field theory (DFT+DMFT) method [17, 18]. Electronic correlations were shown to be qualitatively different in those three phases. The \(\epsilon\)-phase was predicted to exhibit a usual Fermi liquid (FL) behavior with a quadratic temperature dependence of the EES rate \(\Gamma\). In contrast, a strongly non-FL behavior of \(\Gamma\) was predicted for the bcc phase of Fe. References [15, 16] focused on evaluating the qualitative temperature dependence of the EES rate; the corresponding thermal and electrical EES resistivities were not calculated. Moreover, a simplified form of the local Coulomb interaction was employed, neglecting so-called spin-flip and pair-hopping processes. This approximation may lead to quantitatively and even qualitatively wrong description of the EES in correlated systems [19, 20].

It is important to clearly elucidate how large the EES contribution to the electrical and thermal resistivity at Earth’s core conditions is. This is the motivation and the main subject of the present work. We perform a detailed and precise DFT+DMFT calculation of the EES rate and transport properties employing a full, rotationally invariant form of the local Coulomb interaction. In result, we establish that \(\epsilon\)-iron at the inner core conditions exhibits a FL EES. This finding is not only of academic interest as the quadratic frequency dependence of the scattering rate characteristic of FLs has a direct bearing on the transport properties. In FLs, the Lorenz number in the Wiedemann–Franz law is suppressed when inelastic scattering dominates over elastic scattering. Thus the EES contribution to the thermal resistivity is enhanced, as demonstrated here by an explicit \textit{ab initio} calculation of the electrical and thermal conductivity in \(\epsilon\)-Fe. The EES contribution to the thermal resistivity is of comparable magnitude to the electron–phonon scattering (EPS) one and should not be neglected. By including both contributions we obtain a substantially reduced value for the total thermal conductivity of pure \(\epsilon\)-Fe at the inner core conditions as compared to previous DFT calculations [14].

The paper is organized as follows: we briefly describe our calculational approach in section 2, then the obtained DFT+DMFT results for the EES rate as well as the electrical and thermal conductivity are presented in section 3. A qualitative quasi-classical analysis of the suppression of the Lorenz number in FLs is given in section 4, our conclusions and discussions are presented in section 5.

2. Method

We employed the self-consistent in the charge density DFT+DMFT implementation [21–23] in a full-potential framework [24]. We used the same parameters as in [15] for the lattice (volume 7.05 \(\text{Å}^3\)/atom, the hcp \(\epsilon\)/a ratio 1.6) and construction of the Wannier orbitals (energy window (10.8 eV, 4.0 eV) around the Fermi level). There is a significant spread in the values of local Coulomb interaction for iron reported in the literature. A number of earlier DFT+DMFT works [25–27] chose the parameter \(U\) of about 2 eV. More recent direct calculations within the constrained local-density and random-phase (cRPA) approximations [28, 29] predict the static value of the Slater parameter \(F_0 = U\) in the range between 3 and 4 eV, only about 10% of reduction of the ambient-condition value was obtained in cRPA calculations for the inner-core atomic volume [15]. The 30% increase of the value used in DFT+DMFT calculations with respect to the static cRPA value was suggested in [30] to effectively account for the frequency dependence of the Coulomb vertex. Hence, the value in the range from 4 to 6 eV can be considered as the most reasonable choice for DFT+DMFT calculations employing the static Coulomb vertex. In the present work we, hence, employ the rotationally invariant Coulomb interaction defined by \(F_0 = U = 5.0\) eV and the Hund’s rule coupling \(J = 0.93\) eV previously calculated within cRPA in [15]. The robustness of our main conclusions with respect to the value of interaction parameters was checked by additional test calculations carried out using \(U\) of 4 and 6 eV (see figure S1 of the supplementary material available online at stacks.iop.org/NJP/19/073022/mmmedia). We have employed the around-mean-field (AMF) double counting [31], substituting the AMF double counting with the fully localized-limit one has a negligible impact on the results (see figure S2 of the supplementary material).
The DMFT quantum impurity problem was solved using the hybridization-expansion continuous-time quantum Monte Carlo method [32] as implemented in [33]. The same parameters were used for both hcp and bcc Fe. For each temperature we first performed several tens of DFT+DMFT iterations to reach the self-consistency in the charge density and DMFT self-energy employing $3.8 \times 10^9$ Monte Carlo moves to solve the DMFT impurity problem, each 200 moves followed by a measurement. Subsequently, we performed 20–30 of additional runs (with $15.4 \times 10^9$ Monte Carlo moves and 200 moves/measurement) starting from the same converged value of the DMFT bath Green’s function and resetting the random sequence. The self-energies thus obtained were then averaged to obtain the final high-precision DMFT self-energy, which was analytically continued to the real-energy axis. For the analytical continuation we employed the maximum-entropy (MaxEnt) method in the implementation of [34]. The conductivity was calculated within the Kubo linear-response formalism as described in [23, 35]. Namely, the electrical and thermal conductivity read

\[ \sigma_{\alpha\alpha'} = \frac{\epsilon^2}{k_B T} K_{\alpha\alpha'}^0, \]

\[ \kappa_{\alpha\alpha'} = k_B \left[ K_{\alpha\alpha'}^2 - \frac{(K_{\alpha\alpha'}^1)^2}{K_{\alpha\alpha'}^{\Omega}} \right], \]

where $\alpha$ is the direction (x, y, or z), $k_B$ is the Boltzmann constant. The kinetic coefficients $K_{\alpha\alpha'}^\Omega$ read

\[ K_{\alpha\alpha'}^\Omega = 2\pi \hbar \int d\omega (\beta \omega)^g f(\omega) f(-\omega) \Gamma^{\alpha\alpha'}(\omega, \omega), \]

where $2$ is the spin factor, $f(\omega)$ is the Fermi function, and the transport distribution $\Gamma^{\alpha\alpha'}$ is given by

\[ \Gamma^{\alpha\alpha'}(\omega_1, \omega_2) = \frac{1}{V} \sum_k \text{Tr}(v^\alpha(k) A(k, \omega_1) v^{\alpha'}(k) A(k, \omega_2)), \]

where $V$ is the unit cell volume, $A(k, \omega)$ is the DMFT spectral function and $v^\alpha(k)$ is the velocity, see [23].

To estimate the stochastic error of the real frequency self-energy and the resulting conductivities we employed a statistical bootstrap approach. Namely, we randomly picked imaginary-frequency self-energy from the calculated set used to compute the averaged high-precision self-energy for subsequent analytical continuation as described above. Thus we created about twenty trial sets of the same length (about 20 self-energies). By averaging self-energy within each set and then performing Maximum Entropy analytical continuation on the result we obtained an estimate of the variance of the real-axis self-energy and EES rate. We subsequently carried out transport calculations for each such averaged self-energy to obtain the standard deviation of the conductivities.

3. Results

First we analyze the temperature dependence of the inverse quasiparticle life-time

\[ \Gamma_m = -Z_{m0} \text{Im}[\Sigma_m(\omega = 0)], \]

where $\Sigma_m(\omega = 0)$ is the value of DMFT self-energy for the orbital $m$ at zero frequency and $Z_{m0}$ is the corresponding quasi-particle residue, $Z_{m0} = \left(1 - \frac{\Delta E_m(\omega = 0)}{\Delta E} \right)^{-1}$. The resulting dependence of $\Gamma$ versus $T$ is plotted in figure 1. One may notice a clearly parabolic FL shape of $\Gamma(T)$ for all three inequivalent orbitals of the 3d shell of Fe in the hcp lattice. Correspondingly, $\Gamma$ scales linearly as a function of $T^2$, see inset in figure 1. To obtain $\Gamma$ plotted in figure 1 we have analytically continued the imaginary-frequency DMFT self-energy $\Sigma(i\omega_n)$, where $\omega_n$ is the fermionic Matsubara frequency $\omega_n = \pi (2n + 1) k_B T$ and $k_B$ is the Boltzmann constant, to the real-frequency axis. The standard deviation for $\Gamma$ at $T = 5800$ K estimated as described in section 2 is about 3%.

Our results for the scattering rate $\Gamma$ shown in figure 1 are obtained from the analytically continued DMFT self-energy. It is well known that the analytical continuation methods needed to obtain the real-frequency data from imaginary-frequency self-energy are quite sensitive to the details of the procedure (e.g. the number of Matsubara frequencies included into the Pade approximant [36], the way high frequency noisy tails are treated and the way the stochastic error is estimated in the initial imaginary-time data in the case of the MaxEnt etc). However, a qualitative but definite conclusion about the Fermi or non-FL nature of a system can be inferred directly from the imaginary-frequency self-energy without resorting to any analytical continuation. This is done by employing the so-called ‘first-Matsubara-frequency’ rule. As demonstrated, e.g., in [37], in a FL the imaginary part of electronic self-energy, $\Sigma$, at the first Matsubara point within a local approximation like DMFT must be proportional to the temperature, $T$, i.e. $\text{Im}[\Sigma(i\pi k_B T)] = \lambda T$, where $\lambda$ is a real constant. In figure 2(a) we plot $\text{Im}[\Sigma(i\pi k_B T)]$ as a function of temperature for all inequivalent orbitals in hcp and bcc Fe. One may clearly see that in the $\epsilon$ phase $\text{Im}[\Sigma(i\pi k_B T)]$ is almost perfectly proportional to $T$, in contrast to bcc Fe, where it exhibits significant deviations from the ‘first-Matsubara-frequency’ rule [15]. This deviation is especially pronounced for
Figure 1. Orbitally resolved values of the inverse quasi-particle lifetime $\Gamma$ in $\epsilon$-Fe as a function of temperature $T$. The curves are fits $AT^2$ to the calculated data. The values of $\Gamma$ were extracted from real-axis self-energies obtained by the maximum-entropy method [34]. Inset: $\Gamma$ versus $T^2$. The curves are linear-regression fits to the data.

Figure 2. Fermi-liquid scaling of the DMFT self-energy in $\epsilon$-Fe. (a) The imaginary part of the DMFT self-energy at the first Matsubara point $\omega_1 = i\pi k_B T$ versus temperature for hcp and bcc Fe. Note that $|\text{Im}[\Sigma(i\pi k_B T)]|$ being proportional to $T$ is a signature of a Fermi-liquid [37]. The lines are the linear regression fits to the calculated points for corresponding 3d orbitals of Fe. (b) The rescaled imaginary part of the DMFT self-energy at the real axis, $\text{Im}[\Sigma(\omega)]/(\pi k_B T)^2$, versus $\omega/(\pi k_B T)$. The real-frequency self-energies are obtained by the MaxEnt analytic continuation method [34]. One sees that all self-energies collapse into a single curve described by a parabolic fit (the dotted line) defined by the quasiparticle weight $Z = 0.7$ and the characteristic Fermi-liquid temperature scale $T_0 = 13$ eV.
the $e_{g}$ states of the bcc phase. Indeed, the density of $e_{g}$ states in $\alpha$-Fe feature a large peak in the vicinity of the Fermi level due to a van Hove singularity [38]. This pronounced peak leads to suppression of low-energy hopping [39] resulting in a strongly correlated non-FL behavior of the bcc phase, similarly to the cases of Sr$_2$RuO$_4$ [39] and FeSe [40]. Therefore, our analysis on the basis of the ‘first-Matsubara-frequency’ rule confirms the FL state of $\epsilon$-Fe at Earth’s core conditions. We note that this conclusion is further corroborated by a weak temperature dependence of the calculated quasiparticle weight $Z$, as well as by the ratio $\frac{T}{G}$. Varying the value of $U$ between 4 and 6 eV has no impact on the FL nature of $\alpha$-Fe, see figure S1 of the supplementary material.

Moreover, our real-frequency self-energies for different temperatures collapse into a curve consistent with the dependence $C \cdot (\omega^2 + (\pi k_B T)^2)$ expected for a FL, see figure 2(b). From this plot we extracted the upper bound $T_{FL}$ for the FL regime of the transport following [41]. Namely, the constant of proportionality $C$ can be written as $1/(Z\pi k_B T_0)$ with the characteristic scale $T_0 \sim 10T_{FL}$, where $T_{FL}$ is the temperature where resistivity ceases to follow a strict $T^2$ temperature dependence [41]. The rather high value of $k_B T_0 = 13$ eV that corresponds to a $T_{FL} = 14\ 000$ K supports our finding that hcp-Fe at the Earth-core conditions is a FL in spite of the quite high temperature (of about 6000 K) expected for Earth’s core. Hence, the FL behavior is still robust at those conditions, in spite of the large absolute value of core’s temperature.

Figure 3(a) displays our calculated contribution of the EES to the electrical resistivity. One clearly observes that it increases quadratically with increasing temperature up to at least 6000 K, corresponding to Earth’s core conditions. The obtained value of about $1.6 \times 10^{-5}$ $\Omega$ cm at 5800 K is rather insignificant compared to the EPS contribution of about $5.3 \times 10^{-5}$ $\Omega$ cm predicted by DFT calculations [14] indicating that the EES cannot strongly influence the electrical resistivity in hcp-Fe at Earth’s core conditions.
In figure 3(b) we display the corresponding thermal conductivity due to EES. One may notice that this conductivity is not very high: its average magnitude of 540 Wm⁻¹K⁻¹ at 5800 K is comparable to the figure ~300 Wm⁻¹K⁻¹ obtained in [1-6] for the electron–phonon thermal conductivity. By including both scattering effects the total conductivity is reduced to about 190 Wm⁻¹K⁻¹, hence, the corresponding resistivity is enhanced by about 60%. The standard deviation of the thermal and electrical conductivity evaluated by the statistical bootstrap method is below 1%. It is somewhat lower than that for the scattering rate, T, apparently, because the random stochastic error in the real-frequency self-energy diminishes when effectively averaged over a range of frequencies contributing into conductivity.

4. Lorenz number in the Boltzmann formalism

In fact, this large EES contribution is directly related to the FL behavior of ε-Fe. One may demonstrate this by simple analytical calculations [42, 43] in the Boltzmann formalism [44] within the relaxation time approximation, where the conductivity σ and the thermal conductivity κ read:

\[\sigma = e^2 \int d\epsilon \Phi(\epsilon)(-f'(\epsilon))\tau(\epsilon),\]

\[\kappa = \frac{1}{T} \int d\epsilon e^2 \Phi(\epsilon)(-f'(\epsilon))\tau(\epsilon) - \frac{\left(\int d\epsilon e \Phi(\epsilon)(-f'(\epsilon))\tau(\epsilon)\right)^2}{T \int d\epsilon \Phi(\epsilon)(-f'(\epsilon))\tau(\epsilon)},\]

where \(\epsilon\) is the energy measured with respect to the chemical potential, \(\Phi(\epsilon)\) is the transport function, \(f\) is the Fermi function and \(\tau\) is the relaxation time. Often the energy dependence of \(\tau\) is neglected (what is considered to be a good approximation for EPS in Fe above its Debye temperature of about 1000 K [45]). If one additionally neglects the energy dependence of the transport function and evaluates the elementary integrals, one gets the Wiedemann–Franz law \(\kappa/(\sigma T) = \frac{\pi^2}{3} (\frac{\mu}{k})^2 = L_0\), where the standard Lorenz number \(L_0\) is \(2.44 \times 10^{-8}\) WΩK⁻². In the case of a FL, however, the energy dependence of the scattering rate is very strong

\[1/\tau(\epsilon) = 1/\tau(\epsilon = 0) \cdot (1 + \epsilon^2/(\pi k_B T)^2).\]

This leads to a modification of the Wiedemann–Franz law in the case of EES

\[\kappa/(\sigma T) = L_0 / 1.54 = L_{FL}.\]

Accordingly, the conductivity and thermal conductivity from equations (5) and (6) will be smaller by 0.82 and 0.53, respectively, if compared with that obtained by neglecting the energy dependence of the scattering rate, i.e. by putting \(1/\tau(\epsilon) = 1/\tau (\epsilon = 0)\) into equations (5) and (6). The stronger effect of the frequency-dependence of \(\tau(\omega)\) on the thermal conductivity as compared to \(\sigma\) is due to the additional power \(\epsilon^2\) in the numerator of the transport integrals for \(\kappa\).

One may estimate the impact of this effect on the overall thermal conductivity of ε-Fe by summing up the contributions from electron–electron and EPS. To obtain the later we evaluated the ratio \(\kappa/\tau\) using the BoltzTraP [46] code. By adopting for the conductivity with EPS, \(\kappa_{e-\text{ph}}\), the value of about 300 Wm⁻¹K⁻¹ obtained by DFT calculations of [14] for the temperature range from 5700 to 6200 K, we estimated the electron–phonon quasiparticle lifetime \(\tau_{e-\text{ph}}\) = \(1.11 \times 10^{-15}\) s. Assuming a frequency-independent EPS one obtains for the total lifetime at 5800 K:

\[\frac{1}{\tau_{\text{tot}}} = \frac{1}{\tau_{e-\text{ph}}} \left[ 1 + \frac{\tau_{e-\text{ph}}}{\tau (\epsilon = 0) (1 + \epsilon^2/(\pi T k_B)^2) \right].\]

Using the EES lifetime extracted from the average value of self-energy at zero frequency, 0.09 eV one obtains \(3.66 \times 10^{-15}\) s for \(\tau (\epsilon = 0) = \hbar/(2\Sigma(0))\) and 0.303 for the ratio \(\tau_{e-\text{ph}}/\tau (\epsilon = 0)\). Inserting \(\tau_{\text{tot}}\) into (6) and carrying out the integration assuming, for simplicity, a constant value for the transport function one obtains the reduction of \(\kappa\) by a factor of 0.61 as compared to pure EPS, \(\tau_{e-\text{ph}}/\tau (\epsilon = 0) = 0\). Hence, the thermal conductivity is reduced from 300 to 183 Wm⁻¹K⁻¹. This value is very close to the one obtained by adding the electron–electron thermal scattering calculated directly within DMFT (figure 3(b)) for \(T = 5800\) K to the electron–phonon contribution, \(\kappa_{\text{tot}} = 1/(\kappa_{e-e} + \kappa_{e-\text{ph}}) = 190\) Wm⁻¹K⁻¹.

The Lorenz number depends on the magnitude of the EES compared to that of the other scattering processes. As an illustration of this, we consider an elastic, temperature independent scattering whose magnitude we set to \(1/\tau_{e-\text{ph}}\) at 5800 K and plot the Lorenz number as a function of the ratio of electron–electron and total scatterings in figure 4. At high temperatures the EES that in a FL increases quadratically with temperature dominates and the Lorenz number approaches the pure FL result of 2.14 (\(k_B/e)^2\). At low
temperatures the EES is insignificant and the standard Lorenz number of $L_0$ is recovered instead.

Using the conventional value $L_0$ of the Lorenz number together with our calculated $\sigma$ would lead one to a substantially larger thermal conductivity (see figure 3(b)), and hence an incorrect conclusion that the electron–electron contribution to the thermal scattering is insignificant.

5. Conclusions and discussion

In conclusion, our DFT+DMFT calculations predict that EES in $\varepsilon$-iron is FL-like at Earth’s core conditions. The quadratic frequency dependence of this scattering leads to a reduction of the Lorenz number, hence, the thermal conductivity is suppressed with respect to predictions of the conventional Wiedemann–Franz law. As a result, the EES contribution to the thermal resistivity is comparable to the electron–phonon one. By taking them both into account, we obtained a significant reduction of the thermal conductivity of the $\varepsilon$ phase at the inner core’s condition, therefore contributing to stabilizing the convection. Our findings, hence, lend support to explanations of the inner core anisotropy in terms of convection processes.

In the present study we employ the single-site DMFT approach, hence effects due to non-local correlations are not included. Those effects were inferred to be important for transport in $\varepsilon$-Fe under moderate pressure at about 10 GPa, for which the single-site DFT+DMFT calculations substantially underestimate the magnitude of EES [47]. This significant non-local contribution is related to the proximity of $\varepsilon$-Fe to a magnetic instability believed to be located below the $\alpha \to \varepsilon$ transition point at about 12 GPa, as a magnetically ordered $\varepsilon$ phase has so far never been reliably observed experimentally [48]. The proximity of any magnetic instabilities can hardly be expected at the pressure and temperature of the inner core, hence the non-local correlations should be far less important at those conditions. However, this should certainly be investigated carefully in future work, when the transport calculations within the novel methods for accurate simultaneous treatment of both local and non-local many-body effects [49–53] become computationally feasible for the 5-band case of iron. An alternative approach can be a combination GW and DMFT [54], which is also computationally heavy, or even applying GW alone. A recent comparative study of the GW, DFT+DMFT and GW+DMFT found that in weakly correlated FL systems dynamical correlation effects within GW+DMFT are mostly local, and non-local effects are generally static [55]. The local correlations captured by DMFT are thus crucial for correctly describing the EES and, correspondingly, its contribution to transport. Of course, additional studies of the transport in iron with GW would be very interesting as well. We can argue with certainty that for $\varepsilon$-Fe under ambient and low-pressure conditions the experimental EES is larger than the one found in the DMFT method. Accordingly our results should be considered as a lower bound to the electronic contribution to thermal resistivity, the actual value may be even larger. Hence, our conclusion that the electron correlations reduce significantly the thermal conductivity of iron at the inner core conditions may only be strengthen by additional scattering due to non-local effects, e.g., the long-wavelength spin-fluctuations [56].
The obtained reduction of the thermal conductivity is insufficient to explain the stability of convection by itself. The additional suppression of Lorenz number due to EES is also still insufficient to reconcile recent measurements of electrical [10] and thermal [9] conductivity in iron at extreme conditions. With both electron–electron and EPS included we obtain a reduced value of total Lorenz number of about $2.04 \times 10^{-8} \text{Wm}^{-1}\text{K}^{-2}$ compared to the standard value of $2.44 \times 10^{-8} \text{Wm}^{-1}\text{K}^{-2}$ and the thermal conductivity is reduced to about 190 $\text{Wm}^{-1}\text{K}^{-1}$ for $\epsilon$–Fe at the inner core conditions, compared to the value of about 300 $\text{Wm}^{-1}\text{K}^{-1}$ due to EPS only [14]. This reduced value is still though significantly higher than 50 $\text{Wm}^{-1}\text{K}^{-1}$ inferred from measurements by Konopkova et al. [9]. On the other hand, the extremely low values of $\kappa_{\text{tot}} \sim 50 \text{Wm}^{-1}\text{K}^{-1}$ may not be required to reconcile theoretical calculations of the thermal conductivity with geophysical observations [7, 8]. Moreover, it is likely that the thermal disorder, and the admixture of significant quantities of nickel or light elements [7], that we did not take into account may further increase the EES and hence decrease the thermal conductivity. Indeed, DFT+DMFT calculations of hcp Fe–Ni alloy at the inner core conditions point out at an enhanced scattering rate $\Gamma$ for iron sites having Ni nearest neighbors [16]. The impact of alloying, crystalline order and thermal vibrations on the electron–electron contribution to the electrical and thermal conductivity should thus be investigated in future work, when such calculations will become feasible.

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References

[34] Beach K S D 2004 arXiv:cond-mat/0403055
[38] Maglic R 1973 Phys. Rev. Lett. 31 546