Transport properties of iron at the Earth’s core conditions: the effect of spin disorder

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Abstract

The electronic and thermal transport properties of the Earth’s core are crucial for many geophysical models such as the geodynamo model of the Earth’s magnetic field and of its reversals. Here we show, by considering bcc-iron and iron-rich iron-silicon alloy as a representative of the Earth’s core composition and applying the first-principles modeling that the spin disorder at the Earth’s core conditions not considered previously provides an essential contribution, of order $20 \, \mu \Omega \, \text{cm}$, to the electrical resistivity. This value is comparable in magnitude with the electron-phonon and with the recently estimated electron-electron scattering contributions. The origin of the spin-disorder resistivity (SDR) consists in the existence of fluctuating local moments that are stabilized at high temperatures by the magnetic entropy even at pressures at which the ground state of iron is non-magnetic. We find that electron-phonon and SDR contributions are not additive at high temperatures. We thus observe a large violation of the Matthiessen rule, not common in conventional metallic alloys at ambient conditions.

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I. INTRODUCTION

The temperature dependence of the resistivity is one of the most important properties of metals. At ambient conditions, the resistivity of metals and their alloys consists of three contributions: (i) the residual resistivity $\rho_{\text{imp}}$ which is due to the scattering of conduction electrons on impurities and other structural defects with a very weak temperature dependence; (ii) the phonon contribution $\rho_{\text{ph}}$, and (iii) the contribution $\rho_{\text{mag}}$ which is due to the scattering on magnetic fluctuations in ferromagnetic metals and in alloys with local moments. In an ideal ferromagnet $\rho_{\text{imp}} = 0$ while $\rho_{\text{ph}}$ varies linearly with temperature $T$ above the Debye temperature and usually even below it down to fairly low temperatures. The contribution due to magnetic fluctuations reaches its maximum at the Curie temperature, $T_c$, and then remains constant. Its value corresponding to scattering of charge carriers on static disordered moments is called the spin-disorder resistivity (SDR), $\rho_{\text{SDR}}$. The SDR is an important feature of ferromagnetic metals and the bcc-iron at ambient conditions is a textbook example with $\rho_{\text{mag}}$ at $T_c$ of about $80 \mu\Omega \text{cm}$, four times larger than its phonon part. It should be noted that the temperature dependence of $\rho_{\text{mag}}$ below $T_c$ obeys reasonably well the $T^2$ law.

At the Earth’s core conditions, i.e., at pressures about 350 GPa and temperatures 5000 K – 6000 K, one naturally expects dominating scattering on phonons, $\rho_{\text{ph}}$, on which many authors studying resistivity have concentrated. We refer readers to a recent extensive review. We mention in particular studies of Pozzo and Alfè which employ ab initio molecular dynamics simulations. Their estimate of $\rho_{\text{ph}}$ about $50 \mu\Omega \text{cm}$ seems to agree reasonably well with the result of a very recent measurement employing the laser-heated diamond-anvil cell. The estimated value of $\rho_{\text{ph}}$ is few times smaller than the traditional estimates based on the extrapolation of the shock compression data. Possible effects of electron correlations under Earth’s core conditions were investigated recently. There are indications of a Fermi-liquid behavior of hcp and fcc phases and a non-Fermi-liquid behavior of the bcc phase. The resistivity, $\rho_{\text{ec}}$, caused by electron correlations was calculated for hcp phase and the value $\rho_{\text{ec}} = 16 \mu\Omega \text{cm}$ was reported. It should be noted that a reliable experimental estimate of the resistivity at the Earth’s core conditions is a highly demanding task.

In contrast to existing theoretical studies of electrical resistivity due to phonons and electron correlations, the role of spin polarization and magnetic fluctuations in transport
properties of iron at the Earth’s core conditions remains unexplored. First-principles total energy calculations\textsuperscript{13} clearly show that the long-range magnetic order does not exist. On the other hand, authors of Ref.\textsuperscript{13} demonstrated the existence of fluctuating Fe-local moment larger than 1 \(\mu_B\) for bcc Fe as well as for fcc Fe and hcp Fe using the classical model of local spin fluctuations (LSF). One can understand this result as a stabilizing effect of the magnetic entropy. A similar effect exists also at ambient conditions, e.g., for fcc Ni in paramagnetic region\textsuperscript{14}. In particular, the issue here was an estimate of the size of fluctuating local Ni-moment just above \(T_c\), i.e., in the paramagnetic state. A conventional description of the paramagnetic state using the disordered local moment (DLM) approach\textsuperscript{15} gives a zero local moment. The combination of the DLM with the fixed spin-moment (FSM) approach\textsuperscript{14} yields the total energy that increases with the value of the fixed local moment \(m_{Ni}\) on Ni atoms, but the presence of magnetic entropy leads to a minimum of the free energy for the value of \(m_{Ni}\) about 0.4 \(\mu_B\) in a very good agreement both with the LSF calculations\textsuperscript{16} and the neutron diffuse scatterings experiments.

The purpose of the present paper is a first-principles study of the electrical resistivity of iron-based systems due to the spin disorder relevant under the Earth’s core conditions. We focus not only on the SDR itself, but also address the combined effect of several possible scattering mechanisms, namely, phonons, spin disorder, and impurities.

II. THEORY

The electronic structure was determined from first principles by using the tight-binding linear muffin-tin orbital (TB-LMTO) method and the local spin-density approximation. The effect of disorder was included in the framework of the coherent potential approximation (CPA). The CPA is used to include the effect of substitutional impurities (Si in the present work) and also to describe the paramagnetic state in terms of disordered local moments (DLM state)\textsuperscript{15}. The effect of phonon disorder is treated within the multicomponent CPA. Statistical mechanics of disordered moments is based on the magnetic entropy proposed by Heine and Joynt\textsuperscript{17} and Grimvall\textsuperscript{18}. We refer the reader to the Supplemental material\textsuperscript{19} for details.
A. Electron transport

The DLM-FSM method yields the selfconsistent potentials needed to calculate the SDR using the Kubo-Greenwood approach. It should be noted that the DLM approach is closely related to the conventional alloy theory employing the CPA. Calculated SDR of fcc Ni at ambient conditions agrees well with the experiment (SDR is about $15 \mu\Omega\text{cm}$). We use the same computational approach also for estimate of the SDR at the Earth’s core conditions.

We need to determine $\rho_{ph}$ for comparison with the SDR and to investigate if individual contributions to the total resistivity are additive – in other words if the Matthiessen rule is valid. We employ a simple yet quantitative model to include the effect of phonons. Their effect is accounted for by frozen random displacements of atomic positions.

A good agreement of calculated and measured $T$-dependent resistivity was obtained for $\rho_{ph}$ at ambient conditions if the root-mean-square (r.m.s.) displacements $\sqrt{\langle u^2 \rangle}$ for a given temperature are estimated from the Debye theory. We refer the reader to the Supplemental material for details. It is important to note that results are also in a good agreement with a more sophisticated ab initio molecular dynamics approach for bcc Fe at ambient conditions. However, a straightforward extension of the Debye theory to the Earth’s core condition is not justified as demonstrated recently. This theory yields large displacements, for example, for bcc Fe $\sqrt{\langle u^2 \rangle} = 0.80$ bohr at 5500 K. The relation between the temperature and displacements under the Earth’s core conditions can be estimated using other approaches: (i) Lindemann’s melting condition $\sqrt{\langle u^2 \rangle} = \rho r_m$, where $\rho$ is a constant and $r_m$ is an interatomic distance for bcc Fe it gives $\sqrt{\langle u^2 \rangle} = 0.30$ bohr. (ii) Molecular dynamics simulations, the value $\sqrt{\langle u^2 \rangle} = 0.59$ bohr was reported for hcp Fe. The values estimated by these methods are rather scattered so we show calculated resistivities simply as a function of r.m.s. displacements.

The stable phase in the Earth’s solid core is still under discussion. The bcc-phase or the bcc-phase stabilized by sulphur or silicon impurities, treated in the present study, are probable candidates, although hcp Fe is also possible, whereas fcc Fe seems less probable. The presence of impurities is needed to explain the density of the Earth’s core which is smaller than if it consisted from pure iron. The main aim of the present study is to understand the effect of spin fluctuations on transport so that a specific choice of the particular phase is less important.
B. Computational details

All calculations were done using the scalar-relativistic TB-LMTO method while the effects of spin disorder and of atomic disorder were treated within the CPA. The transport properties are determined using the Kubo-Greenwood approach implemented in the framework of the TB-LMTO-CPA method. The \( spd_f \)-basis set was employed. We assumed the volume reduction 0.6:1 with respect to the ambient case (Wigner-Seitz radius is 2.250 bohr, or bcc lattice constant 2.418 Å). The change of the LMTO structure-constant matrix due to the atomic displacements can be recast into a change of the potential functions of atoms located formally at the sites of the undistorted crystalline lattice. This model is treated in the multicomponent CPA. The reader can find computational details in the Supplemental material.

III. RESULTS AND DISCUSSION

A. Local moments

The local Fe-moments as a function of temperature \( T \) calculated using the DLM-FSM and the Heine-Joynt magnetic entropy are shown in Fig. 1 together with the values taken from Ref. [13]. We see a good agreement between the results of the LSF and DLM-FSM methods although the DLM-FSM moments are slightly smaller than the LSF ones. We refer the reader to a recent paper, Ref. [32], for a general discussion of both approaches. Results indicate the existence of robust local Fe-moments stabilized by the magnetic entropy which monotonically increase with temperature and which show a saturation at high temperatures. The values of order 1.1–1.3 \( \mu_B \) for temperatures 5000–6000 K, typical for the Earth’s core, are found.

B. Spin-disorder resistivity

The SDR’s based on the DLM-FSM approach are shown in Fig. 2 as a function of the temperature for the same volume as in Fig. 1. We see a monotonic increase of SDR with temperature while without the stabilizing effect of the magnetic entropy the SDR is zero. The SDR values of order 20 \( \mu\Omega \text{ cm} \) are obtained for temperatures in the Earth’s core. Such
a value of the SDR contribution is about 2.5 times smaller than the phonon contribution, but larger than that coming from the electron correlations\textsuperscript{12}. It is interesting to note that for small values of the r.m.s. deviations the calculated behavior is similar to that at ambient conditions. In agreement with calculations using first-principles molecular dynamics\textsuperscript{5} we observe saturation at high temperatures corresponding to the Earth’s core conditions. It is interesting to compare the present result to that for bcc Fe at ambient conditions. First, the dominating contribution at $T_c=1050$ K is the SDR, about four-times larger than that due to phonons. Second, the Matthiessen rule in bcc Fe is obeyed quite well at ambient conditions, although even here the theory predicts some violation\textsuperscript{33}.

C. Combined effect of spin disorder and phonons

Such result raises a natural question about the value of the total resistivity calculated assuming the validity of the Matthiessen rule, i.e., the additivity of $\rho_{\text{ph}}$ and $\rho_{\text{SDR}}$ or calculated when the effects of both phonons and spin disorder are included together on the same footing. The temperature dependence of resistivity of systems with local moments is very challenging problem even at ambient conditions\textsuperscript{20,31,33}. The situation is somewhat simpler if we can limit ourselves to the paramagnetic region, i.e., to the case of the largest possible spin disorder at a given temperature, or better, for a specific local moment. We have chosen the moment size corresponding roughly to 5500 K, and calculated total resistivities corresponding to various r.m.s. displacements using the multicomponent CPA approach\textsuperscript{20,31}. We refer the reader to Supplemental material\textsuperscript{19} for details. The results are shown in Fig. 3a together with the case with phonons only. For comparison, the total resistivity assuming the validity of the Matthiessen rule, $\rho_M = \rho_{\text{ph}} + \rho_{\text{SDR}}$, is also shown. We employ $\rho_{\text{SDR}}$ calculated at $T = 5500$ K\textsuperscript{23}. The estimated value for $\sqrt{\langle u^2 \rangle}$ is about 0.59 bohr, to which corresponds $\rho_{\text{ph}}$ about 75 $\mu\Omega$ cm. This is about 50% larger value than that calculated for hcp Fe in Ref. 5 or estimated experimentally although for a smaller pressure (see Fig. 3 in Ref. 8). We ascribe this discrepancy to a simplified phonon model used here (see Supplemental material\textsuperscript{19} for details) and the missing knowledge of actual r.m.s. displacement. The most remarkable result is, however, a strong violation of the Matthiessen rule seen in Fig. 3a: while the SDR is about 20 $\mu\Omega$ cm, the net increase of the $\rho_{\text{tot}}$ is only 2 $\mu\Omega$ cm. Even if we choose $\rho_{\text{ph}}$ around 50 $\mu\Omega$ cm, same as that calculated in Ref. 8 which corresponds to the present r.m.s.
displacement of 0.35 bohr, the net increase is still only $9 \mu\Omega\text{cm}$.

D. Combined effect of spin disorder and other scattering mechanisms

Now we discuss the combined effect of substitutional impurities, phonons, and spin fluctuations. There are indications that nickel, silicon, oxygen, sulfur and other impurities exist in the Earth’s core\textsuperscript{27,34,35}. Nickel is perhaps the most prominent one and the study of its effects was so far limited to the non-magnetic case, see, e.g., Ref.\textsuperscript{36}. It is possible to include two or more magnetic elements (Fe and Ni), but it would require significantly more demanding computations. As we make no attempt to study the effect of impurities systematically we selected a non-magnetic Si to illustrate the role of chemical disorder. We take a disordered bcc Fe-rich alloy with silicon impurities, specifically Fe$_{0.92}$Si$_{0.08}$ as an example. Alloys at Earth’s core conditions were not studied within the LSF approach. We therefore extend the present DLM-FSM theory to substitutional alloys assuming zero moments on Si impurities.

The combined effect of phonons and Si impurities was studied using the first-principles molecular dynamics\textsuperscript{34}. The calculated resistivities were $51 \mu\Omega\text{cm}$ for hcp Fe and $63 \mu\Omega\text{cm}$ for solid solution Fe$_{0.92}$Si$_{0.08}$ at Earth’s core conditions. We have evaluated resistivity due to the combined effect of impurities, spin fluctuations, and phonons. We assumed a random distribution of Si atoms on the bcc lattice (no clustering or local environment effects) and described the effect of phonons in terms of effective r.m.s. displacements similarly as in the case of pure iron. The displacements of Fe and Si atoms in the alloy differ, but we made no attempt to take this fact into account, we just assumed an effective r.m.s. displacement common for both atomic species and determined resistivity as a function of it for the SDR calculated at $T = 5500$ K. The fluctuating moment in disordered alloy calculated using the DLM-FSM method is $1.114 \mu_B$. It is slightly smaller than that calculated for pure bcc Fe at the same temperature, namely, $1.143 \mu_B$ which in turn is smaller than that obtained by the LSF approach (see Fig. 1).

Results of our calculations are summarized in Fig. 3b in which the total resistivity including impurities, effect of phonons, and spin disorder is shown together with a resistivity of the non-magnetic alloy Fe$_{0.92}$Si$_{0.08}$ due to impurities and phonons only. In the latter case the value $\sqrt{\langle u^2 \rangle} = 0$ corresponds to impurity disorder alone (about $28 \mu\Omega\text{cm}$). The general conclusion is the same as for pure iron case: the relative weight of the spin disorder
in the total resistivity decreases with temperature, or $\sqrt{\langle u^2 \rangle}$ and it approaches that with impurities and phonons only. The calculated resistivities for pure iron and its alloy due to phonons only are 54 and 65 $\mu\Omega \text{cm}$ (for $\sqrt{\langle u^2 \rangle} = 0.35$ bohr), respectively, which agrees well with the values 51 and 63 $\mu\Omega \text{cm}$ obtained by the molecular dynamics simulations$^{34}$. A strong violation of the Matthiessen rule at Earth’s core conditions was verified also by using a finite-relaxation time model. We refer the reader to the Supplemental material$^{19}$ for details.

With increasing temperature or with addition of further scattering mechanisms we observe a saturation of resistivity. The contributions of individual scattering mechanisms to the total resistivity are not additive and the Matthiessen rule is violated. This phenomenon is well-known and it is closely related to the Ioffe-Regel rule which states that the mean free path of charge carriers cannot exceed the interatomic distance$^{37}$.

Thermal and transport processes inside the Earth’s core are central to the notion of the geodynamo which is powered by the release of latent heat. These processes are not independent, but mutually related (Wiedemann-Franz law). Our results show that due to the spin disorder the electrical resistivity can have higher value than expected on the basis of previous calculations while the thermal conductivity will be smaller. Although the properties of the liquid core cannot be directly derived from the properties of the inner core, similar changes of outer core parameters can be anticipated. One can thus expect that the effects of the spin disorder will finally act in favor of a stronger advection in the outer core.

**IV. CONCLUSIONS**

In summary, we have estimated from first principles a contribution to the resistivity of bcc Fe and of Fe-rich bcc FeSi alloy which is due to the presence of fluctuating spin moments stabilized at the Earth’s core conditions by the magnetic entropy which was not considered in previous studies. The existence of fluctuating moments larger than 1 $\mu_B$, predicted earlier by the LSF approach, was confirmed by the present approach using the DLM-FSM method and the Heine-Joynt entropy also for FeSi alloys. We used the multicomponent CPA method including vertex corrections to treat on equal footing three scattering mechanisms, namely, the scattering on spin disorder, on the atomic substitutional disorder, and on atoms displaced from their equilibrium positions.
The estimated value of the SDR is about $20 \, \mu \Omega \, \text{cm}$ for bcc Fe. Very rough estimates of other contributions, namely, $\rho_{\text{ph}}$ from phonons and $\rho_{\text{ec}}$ from electron correlations are $\rho_{\text{ph}} \approx 50 \, \mu \Omega \, \text{cm}$ and $\rho_{\text{ec}} \approx 16 \, \mu \Omega \, \text{cm}$. The contribution from alloy disorder $\rho_{\text{dis}}$ depends on the type and concentration of impurities, for bcc Fe$_{0.92}$Si$_{0.08}$ alloy we found $\rho_{\text{dis}} \approx 28 \, \mu \Omega \, \text{cm}$. All these contributions should be considered simultaneously as they are not additive and a pronounced saturation is present. This fact demonstrates a strong violation of the Matthiessen rule at the Earth’s core conditions. Consequently the microscopic origins of the transport properties of iron at the Earth’s core conditions are markedly different from those at ambient conditions, where the violation of the Matthiessen rule is much weaker and, in addition, the SDR part dominates in the paramagnetic state.

The implications for geophysical phenomena are twofold: (i) the appearance of magnetic moments changes the electronic structure, which can lead to modifications of all physical properties, and, (ii) in particular, it brings a new contribution to electrical resistivity and thus it can influence thermal conductivity. These quantities are important parameters in the theory of the geodynamo and play a significant role in the thermal history of the Earth.

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FIG. 1. Fluctuating values of the local Fe-moment $|m_{Fe}|$ in bcc iron as a function of the temperature for the Earth’s core atomic volume (Wigner-Seitz radius is 2.25 bohr): (i) the LSF model\textsuperscript{13} (empty circles); and (ii) the present DLM-FSM model (full circles).
FIG. 2. Calculated SDR in bcc Fe as a function of the temperature for the same atomic volume as in Fig. 1 with fluctuating local moments obtained from the DLM-FSM model.
FIG. 3. The resistivity due to phonons as a function of the r.m.s. displacement $\sqrt{\langle u^2 \rangle}$ calculated for a model based on the multicomponent CPA\textsuperscript{20,31} for the Earth’s core conditions: (a) Ideal bcc Fe with phonons only (filled circles), with phonons and the SDR contribution for $T = 5500$ K calculated including both effects together on equal footing (filled triangles), and assuming the validity of the Matthiessen rule (empty circles); and (b) Disordered bcc Fe\textsubscript{0.92}Si\textsubscript{0.08} alloy with phonons only (filled circles), with phonons and the SDR contribution for $T = 5500$ K including both effects together with alloy disorder on equal footing (filled triangles).
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