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Thermal and electrical conductivity of solid iron and iron–silicon mixtures at Earth's core conditions

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ABSTRACT

We report on the thermal and electrical conductivities of solid iron and iron–silicon mixtures ($Fe_{0.92}Si_{0.08}$ and $Fe_{0.93}Si_{0.07}$), representative of the composition of the Earth's solid inner core at the relevant pressure–temperature conditions, obtained from density functional theory calculations with the Kubo–Greenwood formulation. We find thermal conductivities $k = 232$ (237) $W m^{-1} K^{-1}$, and electrical conductivities $\sigma = 1.5$ (1.6) $\times 10^6$ $\Omega^{-1} m^{-1}$ at the top of the inner core (centre of the Earth). These values are respectively about 45–56% and 18–25% higher than the corresponding conductivities in the liquid outer core. The higher conductivities are due to the solid structure and to the lower concentration of light impurities. These values are much higher than those in use for previous inner core studies, k by a factor of four and σ by a factor of three. The high thermal conductivity means that heat leaks out by conduction almost as quickly as the inner core forms, making thermal convection unlikely. The high electrical conductivity increases the magnetic decay time of the inner core by a factor of more than three, lengthening the magnetic diffusion time to 10 kyr and making it more likely that the inner core stabilises the geodynamo and reduces the frequency of reversals.

1. Introduction

This paper follows previous articles (Pozzo et al., 2012, 2013), in which we reported on the electrical and thermal conductivities of liquid iron and iron mixtures at Earth's outer core conditions computed with density functional theory (DFT) and the Kubo–Greenwood (KG) relation. Here we extend those results to the Earth's solid inner core. The conductivities are important in determining the fundamental time scales for diffusion of heat and magnetic field within the inner core.

The study of the inner core is key to understanding the thermal and dynamic processes of the Earth. It formed, and continues to grow, as a result of the Earth's slow cooling, a process central to powering the geodynamo through the release of latent heat and compositional buoyancy resulting from fractionation of light elements into the liquid as it freezes. The inner core is seismically anisotropic (Tromp, 2001) and may contain distinct layers (Ishii and Dziewonski, 2002). Shear flow is required to align crystals and form the anisotropy and solid convection has been invoked as one possible mechanism (Jeanloz and Wenk, 1988). The layering could be a result of thermal convection switching on and shutting off as the temperature gradient rises above, or falls below, the adiabatic gradient (Yukutake, 1998; Buffett, 2009). The thermal conductivity is vital for determining whether the inner core has ever undergone convection.

A conducting inner core has been shown to determine the stability and frequency of polarity reversals in several numerical geodynamo models (Hollerbach and Jones, 1993; Glatzmaier and Roberts, 1995). The geomagnetic field reverses on average a few times in a million years while excursions, events where the polarity reverses briefly but fails to establish the reversed state, are about ten times more frequent (Laj and Channel, 2007). Gubbins (1999) suggested that excursions are a result of the outer core field reversing for too short a time to reverse the field in the inner core. The number of excursions compared to the number of reversals would then depend on the ratio of the magnetic diffusion timescale in the outer and inner cores. More recent dynamo simulations have produced conflicting results, with some showing no effect of conduction in the inner core (Wicht, 2002) and

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others a clear change (Dharmaraj and Stanley, 2012). The different results appear to depend on the different parameters and boundary conditions used in the models (Dharmaraj and Stanley, 2012). In any case, the electrical conductivity is crucial for determining the timescale for magnetic changes in the inner core and the ratio of conductivities between the two cores may be important in determining the degree of stability the inner core imparts on the geodynamo.

The electrical (σ) and thermal (k) conductivities of solid iron have been measured by Gomi et al. (2010) and Konôpková et al. (2011) who found σ of about $10\times10^6\ \Omega^{-1}\,m^{-1}$ at room temperature and up to a pressure of 65 GPa, and k of about $30\ W\,m^{-1}\,K^{-1}$ at 2000 K and up to pressure 70 GPa, respectively. More recently, Deng et al. (2013) measured the electrical resistivity of iron up to 15 GPa and 2200 K. They found a value for the electrical conductivity of $2.2\times10^6\ \Omega^{-1}\,m^{-1}$ at 15 GPa and 1500 K, and a value for the thermal conductivity of about $100\ W\,m^{-1}\,K^{-1}$ at 7 GPa and in the temperature range 600–1300 K. These pressure–temperature conditions are far from those found in the Earth's core. Gomi et al. (2013) measured the electrical resistivity of a solid iron alloy (4 at.% Si) at high-pressure and 300 K finding an electrical conductivity of about $2.5\times10^6\ \Omega^{-1}\,m^{-1}$ at 70 GPa. To extrapolate their results to core temperatures they combined their measurements with the saturation resistivity model, which says that the resistivity of a material stops increasing with temperature once the mean free path of the electrons becomes of the order of the interatomic distance (Gunnarsson et al., 2003). Within this model, their extrapolated values for the electrical and thermal conductivity of $Fe_{78}Si_{22}$ at $T=3750$ (4971) K and $P=135$ (330) GPa, representative of inner core (outer core) boundary conditions, were $0.98\ (1.22)\times10^6\ \Omega^{-1}\,m^{-1}$ and 90 (148) $W\,m^{-1}\,K^{-1}$, respectively. On the theoretical side conductivities of solid iron were calculated by Sha and Cohen (2011) using the low-order variational approximation. They found values of $1.1\text{–}1.8\times10^6\ \Omega^{-1}\,m^{-1}$ and 160–162 $W\,m^{-1}\,K^{-1}$ for σ and k respectively. This approximation is generally valid up to $T=2\Theta_{tr}$, where Θ_{tr} is the temperature corresponding to the average transport frequency, which is estimated to be about 633 K for hcp Fe at 330 GPa. Nevertheless, these results point to relatively high conductivities for the Earth's inner core.

The Earth's solid core is slightly less dense than pure iron under the same pressure–temperature conditions, and therefore must contain some small fraction of light impurities (Poirier, 1994). These light impurities partition at the inner core boundary (ICB) in a way that is governed by their chemical potentials in the solid and the liquid phases. First principles calculations of the chemical potentials of silicon, sulphur and oxygen established that oxygen partitions almost completely into the liquid, and therefore the composition of the solid must be based on a silicon/sulphur mixture (Alfè et al., 2007). This partitioning is also responsible for a decrease of the temperature of the mixture compared to the melting temperature of pure iron.

Here we compute the conductivities of pure solid iron at pressures close to that at the ICB, $p=329$ GPa, and to the centre of the Earth, $p=364$ GPa, at the DFT melting temperature of pure iron $T_m=6350$ K (Alfè et al., 2002; Alfè, 2009; Anzellini et al., 2013). We have also computed the conductivities of $Fe_{0.92}Si_{0.08}$ and $Fe_{0.93}Si_{0.07}$ mixtures. These two mixtures are in equilibrium with liquid mixtures $Fe_{0.82}Si_{0.10}O_{0.08}$ and $Fe_{0.79}Si_{0.08}O_{0.13}$, and correspond to ICB solid–liquid coexisting temperatures of 5700 and 5500 K, respectively (Alfè et al., 2007; Pozzo et al., 2012, 2013).

This paper is organised as follows. In Section 2 we describe the techniques used in the calculations. The results for the thermal and electrical conductivities for pure solid iron and two iron–silicon mixtures are presented in Section 3. The implications of the results are discussed in Section 4. Conclusions follow in Section 5.

2. Techniques

The DFT technical details used in this work are identical to those used in (Alfè et al., 2012; Pozzo et al., 2012, 2013). First principles simulations were performed using the VASP code (Kresse and Furthmuller, 1996), with the projector augmented wave (PAW) method (Blöchl, 1994; Kresse and Joubert, 1999) and the Perdew–Wang (PW91) functional (Wang and Perdew, 1991; Perdew et al., 1992). For the molecular dynamics calculations, the PAW potential for oxygen, silicon and iron have the $2s^2 2p^4$, $3s^2 3p^2$ and $3p^6 4s^1 3d^7$ valence electronic configurations respectively, and the core radii were 0.79, 0.8 and 1.16 Å. Earlier tests (Pozzo et al., 2012, 2013) showed that the conductivities of pure iron and those of the mixtures are unaffected by using an iron PAW potential with the $4s^1 3d^7$ valence configuration instead, and so to compute the conductivities this is what we used. Single particle orbitals were expanded in plane-waves with a cutoff of 380 eV. Electronic levels were occupied according to Fermi–Dirac statistics, with an electronic temperature corresponding to the temperature of the system. An efficient extrapolation of the charge density was used to speed up the *ab initio* molecular dynamics simulations (Alfè, 1999), which were performed on 288-atom cells and sampling the Brillouin zone (BZ) with the Γ point only. The temperature was controlled with an Andersen thermostat (Andersen, 1980) and the time step was set to 1 fs. We ran simulations for typically 8–13 ps, from which we discarded the first ps to allow for equilibration. We then extracted more than 20 configurations (more precisely, 40 for pure solid iron and 24 for the solid iron–silicon mixtures) separated in time by 0.25 ps, which guarantees that they are statistically uncorrelated, and calculated the conductivities on these ionic configurations using the KG formula, as implemented in VASP by Desjarlais et al. (2002). We used two **k**-points in the BZ, which guarantees convergence of the conductivities to better than 1.5%. For specific details of the calculations we refer to Pozzo et al. (2013).

3. Results

3.1. Iron

We begin our discussion by presenting the electrical and thermal conductivities of pure iron. We computed them at the three different temperatures, 6350, 5700 and 5500 K, and two pressures close to ICB pressure and the pressure at the center of the Earth. Results are displayed in Fig. 1 and also reported in Table 1. The conductivities of pure iron at Earth's outer core conditions have been reported before (Pozzo et al., 2012, 2013), but for convenience we re-plot them here on the same figure. The temperature profiles are displayed in the bottom panel of Fig. 1: they are constant in the inner core and adiabatic in the outer core. The values for the electrical and thermal conductivities in pure solid iron are in the range $1.76\text{–}1.97\times10^6\ \Omega^{-1}\,m^{-1}$ and 286–330 $W\,m^{-1}\,K^{-1}$, respectively, with the low/high values corresponding to ICB/Earth's centre pressure–temperature conditions. The electrical conductivities increase by ~13–20% going from the liquid to the solid, with the largest increase corresponding to the lowest temperature. This is expected as the electronic mean free path increases with increasing order. A solid is more ordered than a liquid, and order increases with decreasing temperature.

In metals the thermal conductivity is related to the electrical conductivity via the empirical Wiedemann–Franz (WF) law (Wiedemann and Franz, 1853): $k=T\sigma L$, where L is a constant of proportionality known as the Lorenz parameter, equal to $2.44\times10^{-8}\ W\,\Omega\,K^{-2}$ in the ideal case of a free electron metal. The linear increase of k with temperature is due to the linear increase of the electronic specific heat with temperature: hotter electrons