Electrical resistivity and thermal conductivity of fcc Fe: Implications for the Mercury’s core

*Hitoshi Gomi[1], Takashi Yoshino[1]

1. Okayama University

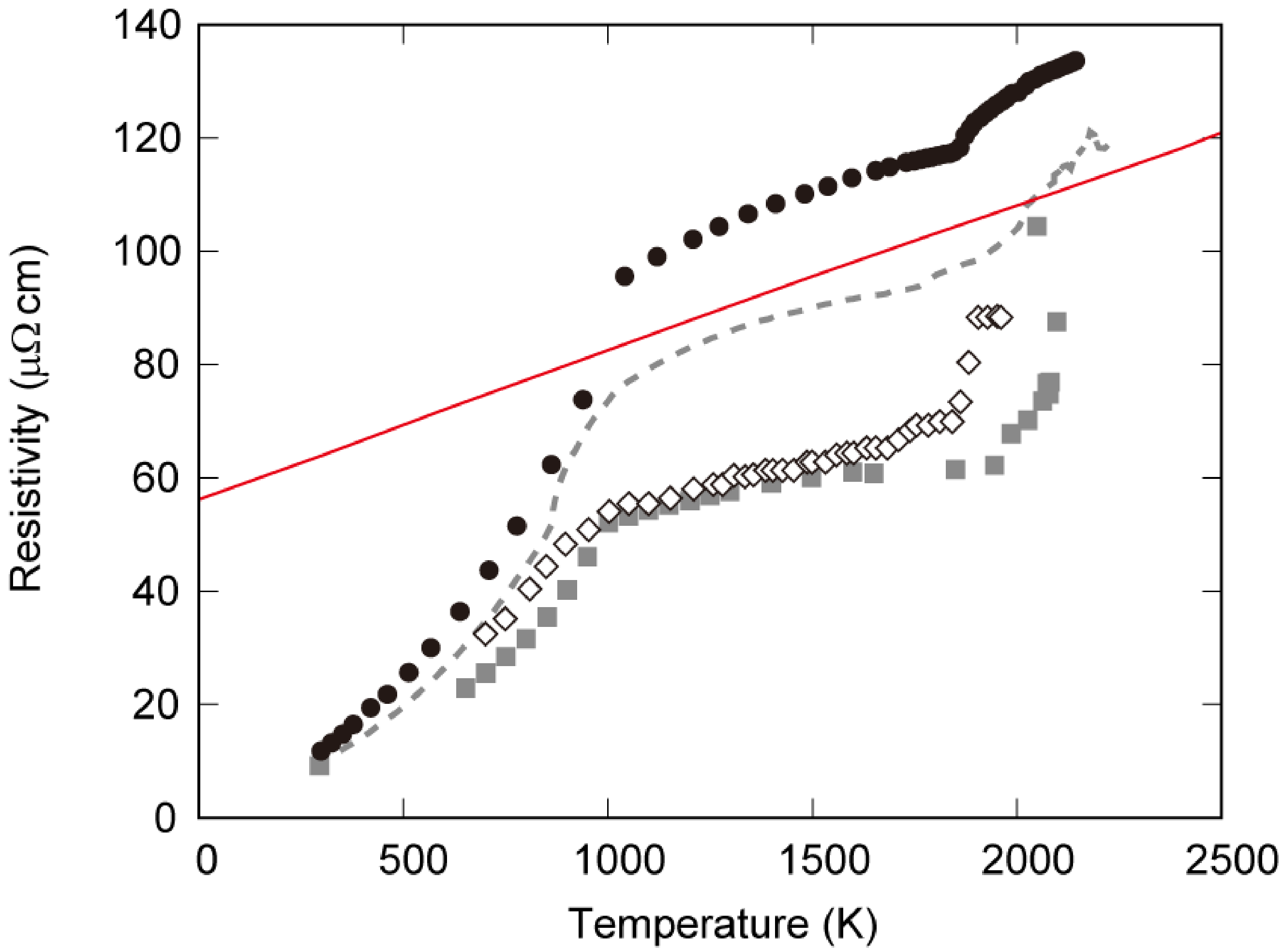
The Mercury’s magnetic field may be sustained by the geodynamo motion in the liquid Fe core. However, its strength is about 1% of that of Earth. This weak magnetic field may implies a partly stratified core. Gomi et al. (2013) pointed out that the geometry of the thermal stratification depends critically on the depth dependency of the thermal conductivity. In this study, we conducted first-principles calculations on the face-centered cubic (fcc) Fe to constrain the electrical resistivity and the thermal conductivity of the Mercury’s core.

We calculated the electrical resistivity and the thermal conductivity of fcc Fe by means of the Korringa-Kohn-Rostoker method combined with the coherent potential approximation (KKR-CPA) (Akai, 1989). The CPA was adopted to treat the disorder effects due to the atomic vibrations and the magnetic fluctuations on the electronic band structure (Glasbrenner et al., 2014; Ebert et al., 2015; Kou and Akai, 2018). Within the alloy analogy model, the thermal atomic displacements were represented by a discrete set of N_v displacement vectors $\Delta R_v(T)$, where $|\Delta R_v(T)|=\sqrt{<u^2>}$ is the root mean square displacement of atoms, which is based on the Debye model without zero point vibration. The lattice parameter and the Debye temperature are obtained from the equation of state of fcc Fe (Tsujino et al., 2013). In addition to the non-magnetic state, the magnetic disorder was simulated by the local magnetic disorder (LMD) approach. The conductivity was calculated by the Kubo-Greenwood formula with the vertex correction.

The calculated electrical resistivities and thermal conductivities with LMD state are consistent with the literature data at 0 GPa (Ho et al., 1972; 1983), whereas the non-magnetic results show smaller resistivity and larger thermal conductivity. This suggests the importance of the magnetic scattering at low pressures. However, our calculation predicts that the magnetic contribution banishes at higher pressures than 20 GPa. Figure 1 compares the present results and previous experiments (gray broken line; Secco and Scholoessin, 1989, gray square; Deng et al., 2013, open diamond; Pommier, 2018, black circle; Silber et al., 2018) on the electrical resistivity at ~5 GPa. Note that, within the fcc stability field, previous measurements have a large variation. Our calculated resistivity values are between Secco and Scholoessin (1989) and Silber et al. (2018).

We further calculated the electrical resistivity and the thermal conductivity of fcc Fe up to 50 GPa and 3000 K. The thermal conductivity increases with increasing pressure and temperature. This means that, if the inner core is absent, the thermal stratification starts from the bottom, and, after the onset of the inner core, a thick thermal stratified layer may develop at the top of the fluid core (Gomi et al., 2013).

Keywords: electrical resistivity, thermal conductivity, Mercury, core, thermal stratification


140
120
100
80
60
40
20
0
Resistivity (μΩ cm)
0
500
1000
1500
2000
2500
Temperature (K)