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The thermal state in the Earth's liquid outer core, insight from theoretical predictions for the electrical and thermal conductivity of iron and iron-silicon alloys

YUAN YIN[1], LIN WANG[2], SHUANGMENG ZHAI[1] AND YUN LIU[1]

[1]Institute of Geochemistry, Chinese Academy of Sciences
[2]Bayerisches Geoinstitut, University Bayreuth
Presenting Author: yinyuan@mail.gyig.ac.cn

The electrical resistivity (ρ) and thermal conductivity (κ) of iron and its alloys are crucial in determining the thermal state of the Earth's core and the geodynamo. However, discrepancies remain between experimental and computational studies. To address this issue, we systematically investigated the transport properties of hcp Fe and Fe-9wt%Si alloy under high pressure-temperature conditions. According to the Kubo-Greenwood formula and density function theory, we calculated the electrical resistivity and electronic thermal conductivity of pure iron under high P-T conditions, which results agree well with previous experimental studies. Under high pressure conditions. the electronic thermal conductivity of hcp iron initially decreases rapidly with increasing temperature and slightly increases with rising temperature at above 2000 K. We carefully investigated the Lorentz number of hcp iron and found that the thermal disorder effect has a greater impact on the electronic thermal conductivity than the electron-electron scattering effect at high temperature conditions, causing the increase in thermal conductivity. At the Earth's core-mantle boundary (CMB), the thermal conductivity of solid hcp iron is calculated to be about 120 W/m/K.

Moreover, utilizing the deep potential method, we performed the deep potential molecular dynamic simulations to compute the lattice thermal conductivity of hcp Fe-9wt%Si alloys under high P-T conditions through the Green-Kubo formula. At room temperature and high pressure conditions, the values of electronic and phononic parts of thermal conductivity are of the same magnitude. The total thermal conductivities at room temperature conditions align with previous experimental results. At the Earth's CMB conditions, liquid hcp Fe-9wt%Si alloys have a thermal conductivity of about 100 W/m/K, which is slightly smaller than that of pure liquid iron at the same conditions.