Supplemental Material

Lorenz number and transport properties of Fe: Implications to the thermal conductivity at Earth's core-mantle boundary

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Figures S1 to S4, and Table S1 and S2.

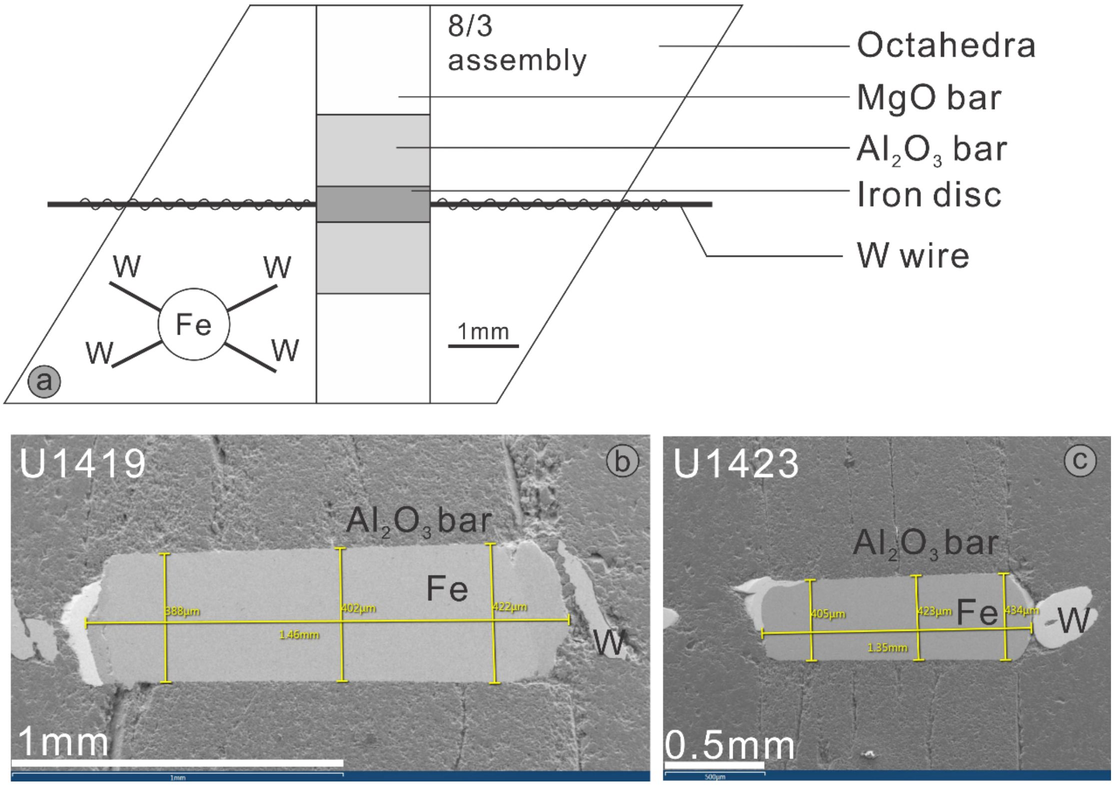

Figure S1. Sample assembly used in resistivity measurement. (a) A sketch map of the configurations of high-pressure assembly (8/3) used in the multi-anvil press. (b, c) The cross-section pictures of the recovered samples using van der Pauw technique.

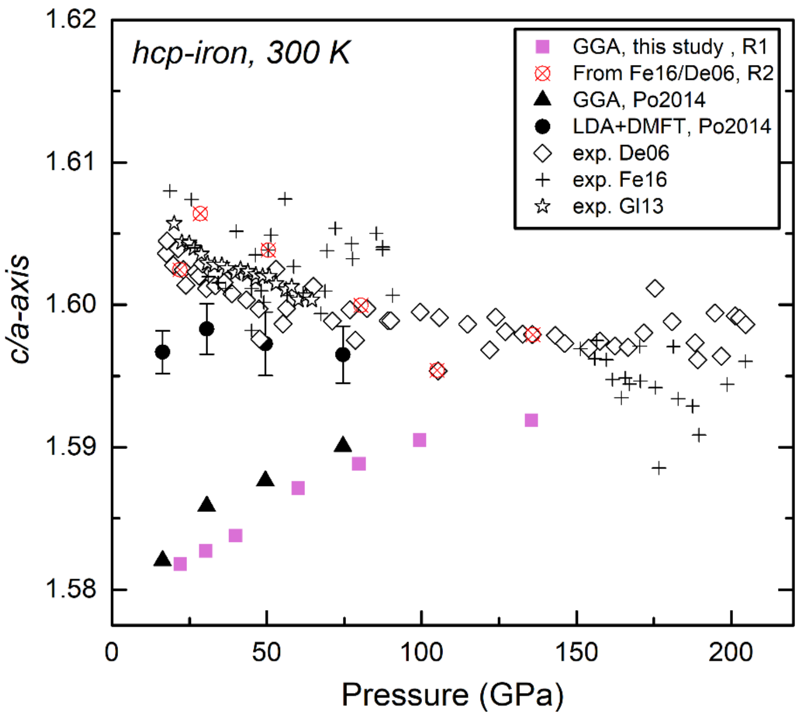

Figure S2. The lattice parameter ratios (*c/a*) obtained in computational and experimental studies at high pressure and ambient temperature conditions. References: De06-(Dewaele et al. 2006), Fe16-(Fei et al. 2016), Gl13-(Glazyrin et al. 2013), Po2014-(Pourovskii et al. 2014). Our optimized lattice parameters have similar *c/a* ratios and positive pressure dependence as results from Pourovskii et al. (2014). However, the *c/a* ratio have a negative pressure dependence as determined by experiments. With the local-density approximation (LDA) plus dynamical mean-field theory (DMFT) method, the computation predicts similar *c/a* ratios for hcp iron as experiments.

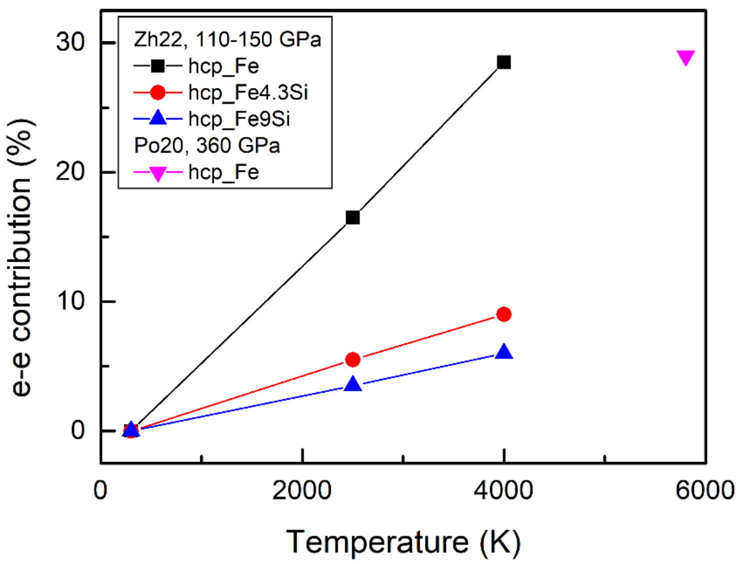

Figure S3. The computed contribution of electron-electron scattering (EES) to the electrical resistivity of hcp iron and Fe-Si alloys under high pressure-temperature conditions. The computational method is first-principles molecule dynamics along with dynamical mean-field theory. All the data are from literature (Po20-Pourovskii et al. 2020; Zh22-Zhang et al. 2022). The impact of EES on the transport property is treated as a correction on the Lorentz number in this study.

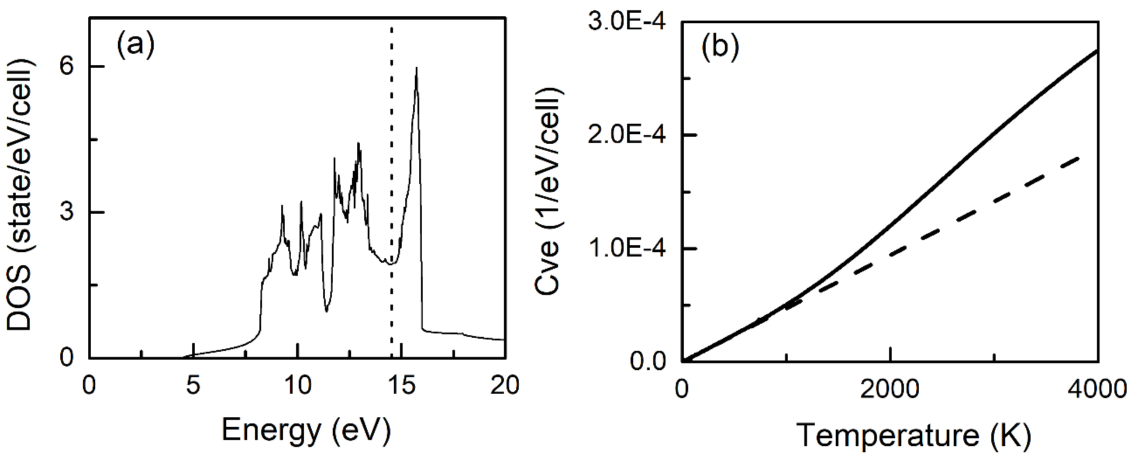

Figure S4. The density of states (DOS) (a) and the electronic specific heat (Cve) (b) for hcp iron at 134 GPa. The DOS is calculated within the unit cell and a Gamma-centered k-mesh of 36×36×18. The dotted line in (a) is the Fermi energy. The solid and dashed lines in (b) are numerical and Sommerfeld values of electronic specific heat, respectively, calculated from the DOS in (a). The numerical values of Cve increase more rapidly than the Sommerfeld value at high temperatures.

Table S1. The pressure-temperature conditions and lattice parameters used in our computations.

References	Pressure (GPa)	Temperature (K)	a(Å)	c(Å)	volume (Å^3)	c/a
hcp_iron (Fei et al. 2016)	21.93	300	2.4405	3.9108	20.1714	1.6024
	28.60	300	2.4178	3.8839	19.6617	1.6064
	50.54	300	2.3761	3.8108	18.6320	1.6038
	80.37	300	2.3265	3.7224	17.4491	1.6000
hcp_iron (Dewaele et al. 2006)	105.00	300	2.2927	3.6578	16.6508	1.5954
	136.00	300	2.2564	3.6055	15.8974	1.5979
hthp_hcp_iron (Anzellini et al. 2013)	98.5	3521	2.294	3.704		1.6146
	132	2725	2.277	3.681		1.6166
	134	4114	2.334	3.776		1.6178
hthp_hcp_iron (Fei et al. 2016)	98.59	1562	2.3113	3.7096		1.6049

Table S2. Critical parameters used to estimate the stratification depth (Li et al. 2022; Zhang et al. 2022)

Parameters	Symbol	Value	Units
Thermal expansivity	α	1×10^{-5}	K^{-1}
Compositional expansivity	β	1.1	
Core radius	Rc	3480	km
Inner core radius	Ri	1221	km
Shell thickness	D	2259	km
Length scale	Dx	1180	km
Composition length scale	χ_i	8×10^{-9}	
Wavelength of light element plumes	λ	100	m
Density difference across the ICB	$\Delta\rho$	600	kg/m^3
Gravity at ICB	g_i	4.4	m/s^2
solid viscosity	η	1×10^{21}	Pa·s
Length scale	D_N	6340	km
Length scale	D_{Fe}	7000	km
Grüneisen parameter	γ_c	1.3	
Average core temperature	Tc	5014	K
Mass of the core	Mc	1.93×10^{24}	kg
Thermal conductivity at CMB	k	70-90	W/m/K
specific heat	C_p	840	$Jkg^{-1}K^{-1}$

SI References

Anzellini, S., Dewaele, A., Mezouar, M., Loubeyre, P., and Morard, G. (2013) Melting of iron at Earth's inner core boundary based on fast X-ray diffraction. Science, 340, 464–466, https://doi.org/10.1126/science.1233514.

Dewaele, A., Loubeyre, P., Occelli, F., Mezouar, M., Dorogokupets, P.I., and Torrent, M. (2006) Quasihydrostatic equation of state of Iron above 2 Mbar. Physical Review Letters, 97, 29–32, https://doi.org/10.1103/PhysRevLett.97.215504.

Fei, Y., Murphy, C., Shibazaki, Y., Shahar, A., and Huang, H. (2016) Thermal equation of state of hcp-iron: Constraint on the density deficit of Earth's solid inner core. Geophysical Research Letters, 43, 6837–6843, https://doi.org/10.1002/2016GL069456.

Glazyrin, K., Pourovskii, L.V., Dubrovinsky, L., Narygina, O., McCammon, C., Hewener, B., Schünemann, V., Wolny, J., Muffler, K., Chumakov, A.I., and others (2013) Importance of correlation effects in hcp iron revealed by a pressure-induced electronic topological transition. Physical Review Letters, 110, 117206–117206, https://doi.org/10.1103/PhysRevLett.110.117206.

Li, W.J., Li, Z., He, X.T., Ma, Z., Fu, Z.G., Lu, Y., Wang, C., and Zhang, P. (2022) Ab initio calculations on thermal conductivity of Fe-Ni-O fluid: Constraints on the thermal evolution of Earth's core. Earth and Planetary Science Letters, 589, 117581, https://doi.org/10.1016/j.epsl.2022.117581.

Pourovskii, L.V., Mravlje, J., Ferrero, M., Parcollet, O., and Abrikosov, I.A. (2014) Impact of electronic correlations on the equation of state and transport in ε -Fe. Physical Review B, 90, 1–5, https://doi.org/10.1103/PhysRevB.90.155120.

Pourovskii, L.V., Mravlje, J., Pozzo, M., and Alfè, D. (2020) Electronic correlations and transport in iron at Earth's core conditions. Nature Communications, 11, 5–12, https://doi.org/10.1038/s41467-020-18003-9.

Zhang, Y., Luo, K., Hou, M., Driscoll, P., Salke, N.P., Minár, J., Prakapenka, V.B., Greenberg, E., Hemley, R.J., Cohen, R.E., and others (2022) Thermal conductivity of Fe-Si alloys and thermal stratification in Earth's core. Proceedings of the National Academy of Sciences, 119, e2119001119, https://doi.org/10.1073/pnas.2119001119.