Electron-phonon contribution to electrical resistivity of hcp Fe

*Haruhiko DEKURA¹, Taku Tsuchiya¹

1.Geodynamics Research Center, Ehime University

Determination of electron transport property of the Earth's core is a key to understanding its thermal property. Electrical resistivity (ρ) of a solid metal comprises electron-phonon and electron-electron scattering mechanisms. Two recent first-principles studies however show a significant difference in the electron-phonon contribution (ρ_{el-ph}) of hcp Fe (M. Pozzo, C. Davies, D. Gubbins, and D. Alfe, Nature, 485, 355, 2012; P. Zhang, R. E. Cohen, and K. Haule, Nature, 517, 605, 2015). While Pozzo *et al.* reported ρ_{el-ph} smaller than the conventional estimates (e.g. F. D. Stacey and O. L. Anderson, Phys. Earth Planet Int, 124, 153, 2001), Zhang *et al.* showed approximately two times larger ρ_{el-ph} than Pozzo *et al*'s and closer to the conventional values. To aim for verifying these previous studies, we develop a technique to compute electron-phonon interaction and ρ_{el-ph} of metals based on the density-functional perturbation theory. In this talk, in addition to our technical advantage, preliminary results on the electrical resistivity of hcp Fe under high-*P*, *T* condition are presented.

Keywords: Earth's core, Electron transport property, First-principles calculation