Impurity resistivity of fcc and hcp Fe-based alloys: Geodynamo energy balance in super-Earths

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

1. Okayama University

It is widely known that the Earth’s Fe dominant core contains a certain amount of light elements such as H, C, N, O, Si and S (e.g. Hirose et al., 2013). The electronic band structure of Fe provides fundamental thermodynamic quantities (e.g. Boness et al. 1986). Gomi et al. (2016) calculated the band structure of substitutionally disordered hcp Fe-Si and Fe-Ni alloys, which suggest the broadening of the band structure due to Si is related to the impurity resistivity. However, only a few studies have investetaged the effect of alloying. In this study, we report the results of first-principles calculations on the band structure and the impurity resistivity of substitutionally disordered hcp and fcc Fe based alloys.

The first-principles calculation was conducted by using the AkaiKKR (machikaneyama) package, which employed the Korringa-Kohn-Rostoker (KKR) method with the atomic sphere approximation (ASA). The local density approximation (LDA) was adopted for the exchange-correlation potential (Moruzzi et al., 1978). The coherent potential approximation (CPA) was used to treat substitutional disorder effect (e.g. Akai, 1989). We mainly focused on Si, Ni, C, N, O and S impurity elements. The impurity resistivity is calculated from the Kubo-Greenwood formula with the vertex correction (Butler, 1985; Oshita et al., 2009; Gomi et al., 2016).

In dilute alloys with 1 at.% impurity concentration, calculated impurity resistivities of C, N, O, S are comparable to that of Si. On the other hand, in concentrated alloys up to 30 at%, Si impurity resistivity is the highest followed by C impurity resistivity. Ni impurity resistivity is the smallest. N, O and S impurity resistivities lie between Si and Ni. Impurity resistivities of hcp-based alloys show systematically higher values than fcc alloys. We also calculated the electronic specific heat from the density of states (DOS). For hcp and fcc Fe, the results show the deviation from the Sommerfeld value at high temperature, which is consistent with previous calculation (Boness et al., 1989). However, the degree of deviation becomes smaller with increasing impurity concentration.

The violation of the Sommerfeld expansion is one of possible sources of the violation of the Wiedemann-Franz law (Gomi and Hirose, 2015; Secco et al., 2017), but the present results predict that the effect may not significant. Therefore, we conclude that the combination of the Wiedemann-Franz law and the resistivity saturation (Gomi et al., 2013; Ohta et al., 2016) can reasonably predict the thermal conductivity of the Earth’s and planetary cores.

Based on the present thermal conductivity model, we calculated the conductive heat flux at the top of terrestrial cores, whose density is modeled by Tachinami et al., (2011). We found that it increases with increasing planetary mass, which implies that massive terrestrial planets, with more than ~2 times Earth mass, cannot maintain thermal convection.

Keywords: band structure, density of states, impurity resistivity, Linde’s rule, KKR-CPA

