Electrical resistivity of substitutionally disordered hcp Fe-Si and Fe-Ni alloys: Chemically-induced resistivity saturation in the Earth's core

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The thermal conductivity of the Earth's core can be estimated from its electrical resistivity via the Wiedemann-Franz law. However, previously reported resistivity values are rather scattered, mainly due to the lack of knowledge with regard to resistivity saturation (violations of the Bloch-Grüneisen law and the Matthiessen's rule). Here we conducted high-pressure experiments and first-principles calculations in order to clarify the relationship between the resistivity saturation and the impurity resistivity of substitutional silicon in hexagonal-close-packed (hcp) iron. We measured the electrical resistivity of Fe-Si alloys (iron with 1, 2, 4, 6.5, and 9 wt.% silicon) using four-terminal method in a diamond-anvil cell up to 90 GPa at 300 K. We also computed the electronic band structure of substitutionally disordered hcp Fe-Si and Fe-Ni alloy systems by means of Korringa-Kohn-Rostoker method with coherent potential approximation (KKR-CPA). The electrical resistivity was then calculated from the Kubo-Greenwood formula. These experimental and theoretical results show excellent agreement with each other, and the first principles results show the saturation behavior at high silicon concentration. We further calculated the resistivity of Fe-Ni-Si ternary alloys and found the violation of the Matthiessen's rule as a consequence of the resistivity saturation. Such resistivity saturation has important implications for core dynamics. The saturation constrains an upper limit of the resistivity, and the saturation resistivity value has almost no temperature dependence. As a consequence, the core thermal conductivity has a lower bound and exhibits a linear temperature dependence. We predict the electrical resistivity of the Earth's core to be about 1.0 $\times 10^{-6}$ Ω m, which corresponds to the thermal conductivity of 100 and 135 W/m/K at 4000 K and 5500 K, respectively. Such high thermal conductivity suggests high isentropic heat flow, leading to young inner core age (< 1 Gyr old) and high initial core temperature. It also strongly suppresses thermal convection in the core, which results in no convective motion in the inner core and possibly thermally stratified layer in the outer core.

Keywords: core, electrical resistivity, resistivity saturation, diamond-anvil cell, KKR-CPA, thermal conductivity