Electrical Resistivity of Substitutional Disordered hcp Fe-Si and Fe-Ni Alloys at High Pressure: Implications for Core Energy Balance. H. Gomi[1], K. Hirose[2], H. Akai[3], Y. Fei[1], [1]Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, DC 20015 (hgomi@carnegiescience.edu), [2]Earth-Life Science Institute, Tokyo Institute of Technology, Meguro, Tokyo 152-8551, Japan, [3]The Institute for Solid State Physics, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8581, Japan.

Introduction: There is a delicate energy balance between the energy requirement for driving a dynamo process in a metallic fluid core and the heat transfer by convection or conduction. A better constrained value of the thermal conductivity of a planetary core is critically important to model the generation of planet magnetic field through self-sustained dynamo and evolution of the core through its history. It also controls the thermal evolution of the planets. The thermal conductivity of the metallic core can be estimated from the electrical resistivity via the Wiedemann-Franz law, $k = LT/\rho$, where k is the thermal conductivity, $L = 2.45 \times 10^{-8}$ WΩ/K^2 is the Lorenz number, T is the temperature and ρ is the electrical resistivity. Gomi et al. [1] demonstrated that the resistivity saturation phenomenon is dominant to determine the resistivity at high temperature and high concentration of impurity elements, pertinent to the core conditions.

The physics of the resistivity saturation is largely investigated by theoretical studies [2]. The basic idea is that the mean free path of conduction electrons should not become shorter than the interatomic distance, which is so-called "Ioffe-Regel condition" [3]. Butler [4] developed the first-principles calculation method of the resistivity of disordered alloys combined with the coherent potential approximation (CPA), which is applied to chemically, thermally and spin disordered metals and alloys [5].

In this study, we focused on chemically disordered iron alloys and demonstrated that the resistivity of planetary cores is largely constrainted by the resistivity saturation.

Methods: We have conducted experiments to measure the electrical resistivity at high pressure in a diamond anvil cell (DAC) up to 90 GPa. A rhenium foil with Al_2O_3 insulating layer was used as gasket material. The sample resistance was obtained by the four-terminal method under a constant DC current of 10 mA with a digital multi-meter (ADCMT 6581). Five separate runs were conducted using iron-silicon alloys with different Si contents. The samples were foils of Fe alloyed with 1wt.%Si (1.97 at.%Si), 2wt.%Si (3.90 at.%Si), 4 wt. %Si (7.65 at.%Si), 6.5 wt.% Si (12.14 at.%Si) and 9 wt.%Si (16.43 at.%Si) (Rare Metallic) with initial thickness of ~10 μm.

We have also performed first-principles calculations by using the AkaiKKR (machikaneyama) package, which employed the Korringa-Kohn-Rostoker (KKR) method with the atomic sphere approximation (ASA) within a framework of the local density approximation (LDA) for exchange-correlation potential. The relativistic effects are taken into account within the scalar relativistic approximation. The wave functions are calculated up to $l = 3$, where l is the angular momentum quantum number. The coherent potential approximation (CPA) is adopted to treat the substitutional disorder effect on the electronic band structure [6]. The electrical resistivity is calculated from the Kubo-Greenwood formula [4].

Results: Figure 1 shows the measured electrical resistivity of iron-silicon alloys as a function of pressure at 300 K with different Si contents. A sharp resistivity enhancement was observed across the bcc-hcp phase boundary, which is consistent with previous studies [1, 7]. The resistivities of iron-silicon alloys are very close to that of Gomi et al. [1] and Seagle et al. [7] at around 20 GPa, but slightly lower than Gomi et al. [1] at higher pressure. The resistivity increases linearly with increasing silicon impurity concentration as predicted by the Matthiessen's rule.

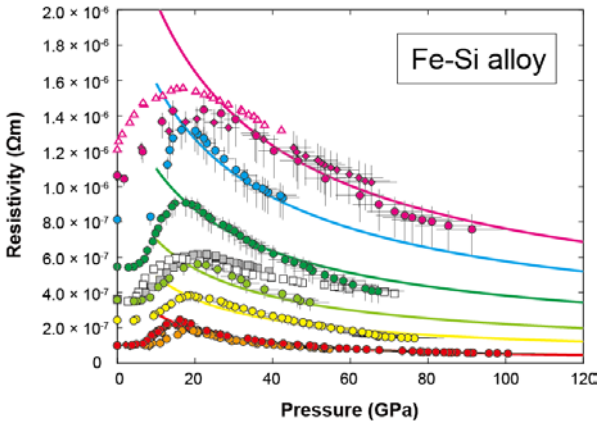

Fig.1 Electrical resistivity of iron-silicon alloys as a function of pressure. Yellow (1 wt.% Si), light green (2 wt.% Si), deep green (4 wt. % Si), blue (6.5 wt.% Si) and purple (9 wt.% Si) circles and diamonds are present measurement. Previous measurements conducted by Gomi et al. [1] (Red and orange circle for pure Fe and gray and white square for 2 wt.% Si alloy) and Seagle et al. [7] (purple triangle for 9 wt.% Si alloy) were also plotted for comparison.

The electrical resistivities of iron-silicon and iron nickel alloys are calculated by using the Kubo-Greenwood formula [4] at several volumes, equivalent to experimentally determined room-temperature volumes of pure hcp iron at 0, 40, 80 and 120 GPa, respectively [8]. Figure 2 shows the electrical resistivities of iron-silicon and iron-nickel alloys. The electrical resistivity increases with increasing impurity content up to about 50 at%, then the resistivity decreases to zero. To simplify, we considered the average as the resistivity of bulk polycrystalline alloys: $(2\rho_x + \rho_z)/3$ where ρ_x and ρ_z are the resistivity calculated perpendicular and parallel to the *c*-axis, respectively.

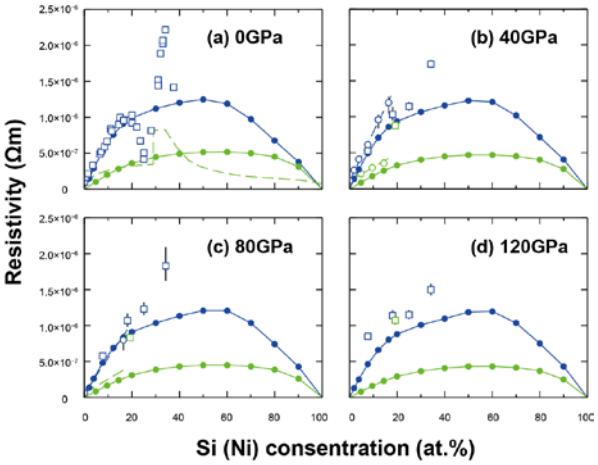

Fig.2 Present (circile) and previous (square) electrical resistivity of iron-silicon (blue) and iron-nickel (green) alloys as a function of silicon and nickel concentration. The open symbols indicate experimental results and the filled symbols represent values from first-principles calculations.

Discussion: Figure 2(a) summarized the electrical resistivities of iron-silicon and iron-nickel alloys at ambient pressure. Blue open square symbols indicate the measured resistivity of single-phase iron-silicon alloys at ambient temperature [9 and references therein]. The resistivity increases with increasing silicon concentration within the bcc stability field, and then the resistivity decreases because of formation of Fe_3Si component with DO_3 structure. A local minimum is observed at the stoichiometric composition. They also found unexpected high resistivity at $\chi_{Si} \approx 35$ at.%, which may be related to the DO_3 structure. Literature values of iron nickel solid solutions at 300 K are plotted as green broken line [10]. Impurity resistivity of nickel in iron is smaller than that of silicon. The resistivity is increases with increasing nickel impurity concentration within the bcc stability field. The discontinuity in resistivity at $\chi_{Ni} \approx 30$ at.% is attribute to the phase transition from bcc to fcc. Then, the resistivity decreases with increasing the nickel content. First-principles results on hcp iron-nickel solid solutions are plotted as solid green circles for comparison. Figures 2 (b, c, d) show comparison of our experimental results with first-principles calculations and previous shock compression experiments [11]. Our experimental and first-principles results of iron-silicon alloys show excellent agreement with each other. Furthermore, previous shock wave data [11] are in general agreement with our results, except for the value at 34.2 at.% Si, although these data are taken along Hugoniot. This is consistent with the prediction from the saturation theory that temperature dependence should become small at high resistivity [1]. In addition, the first-principles result of iron-silicon alloys clealy shows a kink at $\chi_{Si} \approx 15$ at.%, which is considered to be the result of the resistivity saturation. Because both thermally and chemically disordered alloys follow the resistivity saturation, electrical resistivity should become about 1×10^{-6} Ωm at strongly disordered condition.

Terrestrial planetary cores consists of iron-nickel alloys with different amounts of impurity such as Si depending on the accretion consitions and size of the planets. This study provides systematic data and theoretical predictions that reveal the effect of Ni and Si concentractions on the electrical resistivity over a wide pressure range. The derived thermal conductivity values via the Wiedemann-Franz law can be directly used to model conductive energy losses from the core to power the dynamo. Understanding the effect of Si on the thermal conductivity is particularly important for Mercury because Si could be a major light element in the core [12,13]. Sigificant increase in resistivity with Si impurity would substantially low the capacity for the core to transport heat by conduction.

References: [1] Gomi et al. (2013) PEPI. [2] Gunnarsson et al. (2003) Rev. Mod. Phys. [3] Gurvitch (1981) PRB. [4] Butler (1985) PRB. [5] Glasbrenner et al. (2014) PRB. [6] Akai (1989) J. Phys.: Cond. Mat. [7] Seagle et al. (2013) GRL [8] Dewaele et al. (2006) PRL [9] Varga et al (2002) J. Phys.: Cond. Mat. [10] Ho et al. (1983) J. Phys. Chem. Ref. [11] Matassov (1977) PhD thesis. [12] Fei et al. (2011) 42nd *LPSC Abstract #194.* [13] Malavergne V. *et al.* (2010) *Icarus, 206,* 199-209.