Hue University Journal of Science: Natural Science
Vol. 132, No. 1B, 59–64, 2023

pISSN 1859-1388
eISSN 2615-9678

Electrical resistivity of FeSi alloy under high pressure

Nguyen Thi Hong*

Hong Duc University, 565 Quang Trung, Dong Ve Ward, Thanh Hoa, Vietnam

* Correspondence to Nguyen Thi Hong <nguyenthihongvatly@hdu.edu.vn>

(*Received: 12 September 2022; Accepted: 06 December 2022*)

Abstract. The electrical resistivity of FeSi alloy under the influence of pressure is studied based on Matthiessen's rule and the saturation electrical resistivity model. Numerical calculations have been performed for FeSi up to a pressure of 100 GPa and compared with experimental data when possible. These results show that the electrical resistivity of the FeSi alloy diminishes gradually with pressure and saturates at high pressure. Moreover, in this paper, The impurity concentration effects on the electrical resistivity of FeSi alloy have also been investigated. Our numerical calculations, performed at 40 Gpa and 80 Gpa pressures, show that when the Si concentration is less than 20%, the electrical resistivity of the FeSi alloy increase rapidly, and they behave like linear functions of the concentration of Si. Our model gives electrical resistivity values that are in agreement with recent experimental measurements.

Keywords: Electrical resistivity, FeSi, Matthiessen's rule, impurity concentration, high pressure

1 Introduction

To meet the growing need for energy efficiency in power electronics and electric machines as well as the recent demand for even more efficient electric motors and high-voltage transformers, a number of new soft magnetic materials are being investigated. Among them, a Fe-Si alloy with a high Si concentration is already being accepted as a commercially viable soft magnetic material, and is expected to be widely adopted by the industries [1,2].

On a larger scale, Earth's outer and inner cores are mainly composed of iron (~85 wt %) alloyed with niken (~5 wt %) and ~8 to 10 wt % of light elements, respectively, such as Si, O, S, C, and H [3–8]. Convection of the liquid core generates Earth's magnetic field, which is controlled by the thermal conductivity of the core. Therefore, the light elements are important to the database of the thermal state, the structure of the core, as well as the generation and evolution of Earth's magnetic field [3, 4, 9–11], where, Si was determined to account for 5 to 10% of the earth's core [4] and is one of the most promising materials for the main light element of the earth's core. Si is highly abundant cosmochemically, not highly volatile, and forms a continuous solid solution with iron over a wide compositional range. Therefore, the thermal conductivity and electrical conductivity properties of Fe-rich Si alloys have attracted intense interest in recent years [4,12].

Experimental measurements of the electrical resistivity of iron at high pressure (up to the Earth's core pressure) were also made, taking into account the influence of impurities Si, Ni, S, O, and C [3, 4, 13–16]. Gomi *et al.* [15] measured the electrical resistivity of pure Fe and Fe-Si alloy (3.90 at.% Si) to 100 GPa in a diamond-anvil cell (DAC). The authors assumed silicon as the sole alloying element; the Si content in the outer core is

DOI: 10.26459/hueunijns.v132i1B.6937

estimated to be 22.5 at.% to account for the 10% core density deficit [17]. The total electrical resistivity of $Fe_{78}Si_{22}$ is 1.02 (+ 0.04/-0.11) × 10^{-6} Ωm for Core mantle boundary (CMB) conditions (135 GPa, 3750 K) and 8.20 (+0.54/-1.31) x 10^{-7} Ωm for inner core boundary (ICB) conditions (330 GPa, 4971 K). Y. Zhang *et al.* [3] directly measured the electrical resistivity of the alloys hcp-Fe-4.3 wt% Si (or $Fe_{0.92}$ $Si_{0.08}$) and Fe-9 wt% Si (or $Fe_{0.84}Si_{0.16}$) to ~136 GPa and 3000 K. The thermal conductivity of hcp Fe_9Si is found to be ~100 to 110 $W.m^{-1}.K^{-1}$ for liquid Fe_9Si at ~140 GPa and 4000 K. Recent studies also reported that the thermal conductivity is around 100 $W.m^{-1}.K^{-1}$ at conditions near CMB [18,19]. Meanwhile, another study reported a moderate thermal conductivity of 50 to 70 $W.m^{-1}.K^{-1}$ for Fe-5 wt% Ni-8 wt% Si alloy at conditions near CMB (~ 140 GPa and 4000 K) [20-21]. For the Fe-8 wt% Si alloy, the conductivity results are ~20 $W.m^{-1}.K^{-1}$ at ~132 GPa and 3000 K. However, the thermal conductivity of solid Fe-6,5 wt% Si at ~99 GPa and 2000 K is ~66 $W.m^{-1}.K^{-1}$ [20]. Thus, the studies on the thermal conductivity (electrical resistivity) of FeSi alloys at high pressure, especially at the Earth core pressure condition, are still controversial. There is no consensus among these past/previous results.

In this work, we study the effect of impurity concentration and pressure on the electrical resistivity of FeSi alloy. For such a goal, the influence of Si impurity concentration on the resistivity of the alloy is calculated based on Matthiessen's rule. To calculate the resistivity of alloys with a large doping concentration at high pressure, we use the suggestions of Côte and Meisel in which the electrical resistivity of the alloy system is not only depends on the impurity resistivity and temperature effects described by the Bloch-Grüneisen formula, but also on the effect of resistivity saturation in the estimates of core resistivity [15].

2 Materials and Methods

Conduction in metals is hindered by the scattering of charge carriers due to the quantum vibrations of the lattice (phonons) and by their collisions with each other. Metals are generally considered good conductors; they allow current to flow through easily because, in their structure, there are many freely moving electrons. Metals will be alloys after adding some other metals and/or non-metals to get better properties. Non-metals are poor conductors. When we add non-metals to metals, the change in crystal structure will decrease their ability to conduct electricity. This causes an increase in resistivity. Consequently, alloy(s) has/have greater resistivity than metal(s).

Firstly, the dependence of the resistivity of the FeSi alloy on the concentration of Si will be studied based on Matthiessen's rule [14], which was introduced in 1864 [14]. Matthiessen *et al.* discovered that most of the change in resistivity by temperature in a two-component alloy is equivalent to the resistivities of two conductive components that are completely independent and parallel to each other. When the concentration of a component decreases, the role of that component will become less important. From this result, they concluded that the addition of impurities concentrations will only add a constant amount to the total resistivity of pure metal, while the ingredient, depending on the temperature of resistivity, will not be affected.

$$\rho_{tot} = \rho_{pure} + \rho_i\left(C_i\right), \quad (1)$$

where $\rho_i\left(C_i\right)$ is the electrical resistivity of the impurity at 0 ^{0}C, ρ_{pure} is the electrical resistivity caused by phonon-phonon scatterring in pure iron. Here, Matthiessen's rule will be applied and improved by the idea that $\rho_i\left(C_i\right)$ is directly proportional to C_i [22].

The resistivity caused by phonon scatterring in a metal is calculated by the expression of Bloch-Grüneisen's law

$$\rho_{\text{pure}}(V,T)=\rho(0)+B(V)\left(\frac{T}{\theta_D(V)}\right)^5\int_0^{\theta_D(V)}\frac{x^5dx}{\left(e^x-1\right)\left(1-e^{-x}\right)}, \tag{2}$$

with the note that we neglected residual resistivity caused by imperfections $\rho(0)$. The value of $B(V)$ can be derived from the expression showing the dependence of resistivity of iron on pressure at room temperature [15]

$$\rho_{\text{pure}}(V,300\,\text{K})=5,26\times\left(1,24-\frac{V}{V_0}\right)^{-3.21}\times10^{-9}\ (\Omega\text{m}). \tag{3}$$

One of the remarkable points is that the experimental results of Gomi and his colleagues on FeSi and FeNi alloys [23-24] show that Matthiessen's rule is only suitable for dilute alloys. Therefore, in this research, to find out the dependence of the resistivities of alloys on pressure, we will apply the theory that allows us to calculate the resistivities of alloys based on the model of saturation resistivity that was considered by Côte and Meisel [13], and modeled by Gomi *et al.* [23-24]

$$\rho_{tot}(V,T)=\left(1-\frac{\rho_{tot}(V,T)}{\rho_{sat}(V)}\right)\rho_{pure}(V,T)+ \\ +\rho_i(V)\exp\left(-2W(V,T)\right), \tag{4}$$

where $\rho_{tot}(V,T)$ is the total resistivity of alloys, $\rho_{sat}(V)$ is the saturation resistivity, and $\exp\left(-2W(V,T)\right)$ is the Debye-Waller factor that can be determined from Debye or experiments.

For the resistivity of impurities, we use the value of the resistivity $\rho_i(V)$ of Si that is fitted to the respective experimental values [23]

$$\rho_{Si}(V)=4,34\times\left(2,56-\frac{V}{V_0}\right)^{-7,79}\times10^{-6}\ (\Omega\text{m/at.\%}). \tag{5}$$

For the saturation the electrical resistivity $\rho_{sat}(V)$, Gomi *et al.* showed that it is directly proportional to $V^{1/3}$. This means that the saturation of the electrical resistivity $\rho_{sat}(V)$ can be calculated as [15, 25]

$$\rho_{sat}(V)=\rho_{sat}(V_0)\left(\frac{V}{V_0}\right)^{1/3}=\rho_{sat}(V_0).\eta^{1/3}. \tag{6}$$

To determine the influence of pressure on resistivity, we will apply the Vinet equation that shows the relationship between pressure – volume - temperature [26]

$$P=3B_0\left(\frac{V}{V_0}\right)^{-2/3}\left[1-\left(\frac{V}{V_0}\right)^{1/3}\right]\times \\ \times\exp\left\{\frac{3}{2}\left(B_0^{'}-1\right)\left[1-\left(\frac{V}{V_0}\right)^{1/3}\right]\right\}, \tag{7}$$

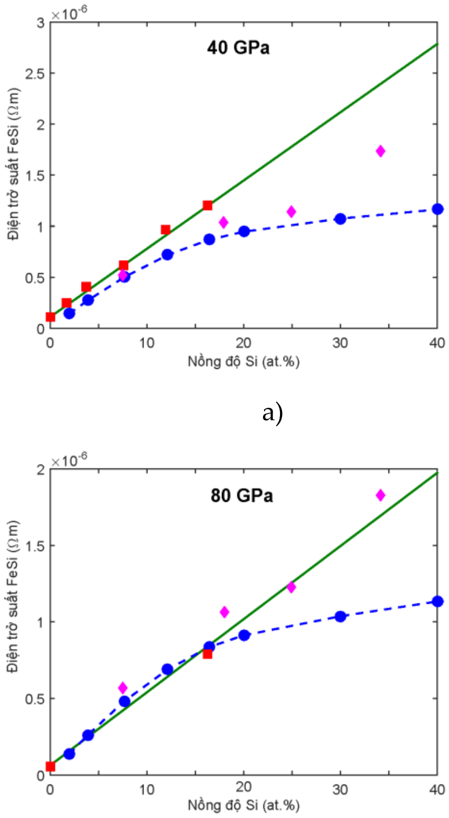
where B_0, $B_0^{'}$ is, respectively, the isothermal bulk compression module and the first order of its derivative.

3 Results and discussions

In the following, the expressions established in the previous section will be applied to numerically calculate FeSi alloys up to 100 GPa. For this purpose, the Debye temperature $\theta_D(V)$ is assumed to be constant in the studied pressure range. The Debye-Waller coefficient is obtained experimentally in Gomi's work [23]: $\theta_D(V)=710$ K, $\exp\left(-2W(V,T)\right)\approx0.95$. The isothermal bulk modulus and its first-pressure derivative are also approximated for ferrous metals [27] $B_0=163,4$ GPa, $B_0^{'}=5,38$.

DOI: 10.26459/hueunijns.v132i1B.6937

We present the impurity concentration dependence of the electrical resistivity of FeSi alloy at ambient pressures of 40 GPa and 80 GPa in Fig. 1. The experimental data on the electrical resistivity of FeSi alloy are also displayed for comparison. As can be seen in Fig. 1, when the Si doping concentration is less than 20%, our calculations are in close agreement with the experimental data reported by Matassov [28] as well as that of Gomi *et al.* [23]. In this Si impurity concentration range, the electrical resistivity of the FeSi alloy increases almost linearly with the increasing Si impurity concentration. This result is in good agreement with the prediction of Matthiesen's rule [14].



a)

b)

Fig. 1. Effect of Si-doped concentration on the resistivity of FeSi alloy. Experimental data of Gomi *et al.* by the DAC method [23] (solid square) and shock compression measurement by Matassov [28] (solid diamond shape). Calculation result from the original principle [23] (dotted lines and solid circles)

However, when the Si concentration is greater than 20%, previous experimental results show that the electrical resistivity of the alloy will no longer increase linearly but will decrease gradually. In this case, our calculation results do not explain the results of previous work. This is also consistent with the prediction of Gomi *et al.* [23, 24] that we made in section 2.

We now represent the pressure dependence of the electrical resistivity of FeSi alloys between 0 GPa and 100 GPa. As can be seen in Fig. 2, at pressures higher than 20 GPa, the electrical resistivity of FeSi alloy in the results of our theoretical calculations gradually decreases to saturation value in the high pressure region; his is in very good agreement with the ones of Ohta *et al.* [29]. This phenomenon is explained by Gunnarsson *et al.* [30]: the electrical resistivity depends on the interaction distance between atoms, so this value will decrease with pressure. The electrical resistivity tends to reach saturation value ρ_{sat} when the ean free path of an electron is equivalent to the interatomic interaction distance at high temperature and pressure.

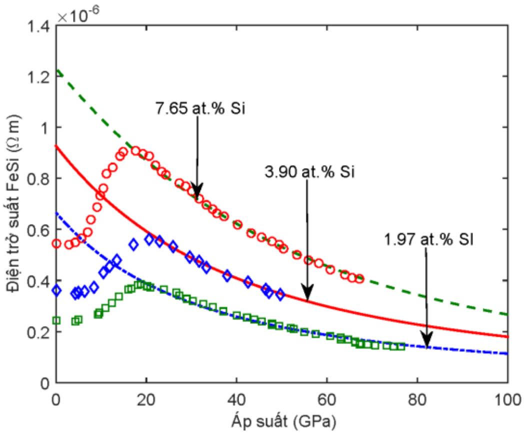


Fig. 2. Pressure dependence of the electrical resistivity of FeSi alloy. Experimental data of Gomi *et al.* by the DAC method [23]

However, our results have not yet described the variation of resistivity with pressure in the pressure region, which is less than 20 GPa. According to Gomi *et al.*, the resistivity of FeSi alloy initially increases rapidly with increasing pressure and reaches its maximum value at 20 Gpa pressure. It should be noted that the jump in resistivity around a pressure of 20 GPa is attributed to the structural phase transition of the alloy.

4 Conclusions

Matthiesen's rule and Cote and Meisel's saturation resistivity model were applied to investigate the dependence of the electrical resistivity of FeSi alloys on Si-doped concentration and pressure. Our numerical results for FeSi dilute alloys (where is the Si concentration is less than 20%) show that the electrical resistivity of FeSi alloys increases almost linearly with the Si doping concentration but gradually decreases to the saturation value as the pressure increases. The obtained results are consistent with experimental ones at pressure ranges higher than 20 GPa. It means that our theoretical model can be applied to study the resistivity of other alloys under the influence of pressure.

References

1. Ouyang G, Chen X, Liang YF, Macziewski JC. Review of Fe-6.5 wt%Si high silicon steel-A promising soft magnetic material for sub-kHz application. Journal of Magnetism and Magnetic Materials. 2019;481:234-250.
2. Liang YF, Wang S, Li H, Jiang YM, Ye F, et al. Fabrication of Fe-6.5wt%Si Ribbons by Melt Spinning Method on Large Scale. Advances in Materials Science and Engineering. 2015;2015:1-5.
3. Zhanga Y, Luob K, Hou, M, Driscollb P, Salkee NP, Minar J, et al. Thermal conductivity of Fe-Si alloys and thermal stratification in Earth's core. Proceedings of the National Academy of Sciences. 2021;119:1-8.
4. Wicks JK, Smith RF, Fratanduono DE, Coppari F, Kraus RG, Newman MG, et al. Crystal structure and equation of state of Fe-Si alloys at super-Earth core conditions. Science Advances. 2018;4:1-10.
5. Litasov KD, Shatskiy A. Composition of the Earth's core: A review. Russian Geology and Geophysics. 2016;57:22-46.
6. McDonough WF. Compositional Model for the Earth's Core. Treatise and Geochemistry. 2014;547-568.
7. Fei Y, Murphy C, Shibazaki Y, Shahar A, Huang H. Thermal equation of state of hcp-iron: Constraint on the density deficit of Earth's solid inner core. Geophysical Research Letters. 2016;43 (13):6837-6843.
8. Lin JF, Sturhahn W, Zhao J, Shen G, Mao HK, Hemley RJ. Sound Velocities of Hot Dense Iron: Birch's Law Revisited. Science. 2005;308:1892-1894.
9. Williams Q. The Thermal Conductivity of Earth's Core: A Key Geophysical Parameter's Constraints and Uncertainties. Annu Rev Earth Planet Sci. 2018;46:47-66.
10. Davies C, Pozzo M, Gubbins D, Alfè D. Constraints from material properties on the dynamics and evolution of Earth's core. Nature Geoscience. 2015;8 (9):678-685.
11. Cayman U, Wendy P. Scaling the Earth: A Sensitivity Analysis of Terrestrial Exoplanetary Interior Models. The Astrophysical Journal. 2016; 819:1-8.
12. Mohri T, Chen Y, Kohyama M, Ogata S, Saengdeejing A, Bhattacharya SK, et al. Mechanical properties of Fe-rich Si alloy from Hamiltonian. Computational Materials. 2017;3(1):1-14.
13. Cote PJ, Meisel LV. Origin of Saturation Effects in Electron Transport. Physical Review Letters. 1978; 40 (24):1586-1589.
14. Matthiessen A, Vogt C. Ueber den Einfluss der Temperatur auf die elektrische Leitungsfähigkeit der Legirungen. Annalen Der Physik. 1864;198(5): 19-78.
15. Gomi H, Ohta K, Hirose K, Labrosse S, Caracas R, Verstraete MJ, et al. The high conductivity of iron and thermal evolution of the Earth's core. Physics of the Earth and Planetary Interiors. 2013;224:88-103.

16. Stacey FD, Anderson OL. Electrical and thermal conductivities of Fe-Ni-Si alloy under core conditions. Physics of the Earth and Planetary Interiors. 2001;124(3-4):153-162.

17. Sata N, Hirose K, Shen G, Nakajima Y, Ohishi Y, Hirao N. Compression of FeSi, Fe3C, Fe0.95O, and FeS under the core pressures and implication for light element in the Earth's core. J Geophys Res. 2010;115:B09204.

18. Xu J, Zhang P, Haule K, Minar J, Wimmer S, Ebert H, et al. Thermal Conductivity and Electrical Resistivity of Solid Iron at Earth's Core Conditions from First Principles. Phys Rev Lett. 2018;121: 096601

19. Zhang Y, Hou M, Liu G, Zhan C, Prakapenka VB, Greenberg E, et al. Reconciliation of Experiments and Theory on Transport Properties of Iron and the Geodynamo. Phys Rev Lett. 2020;125:078501.

20. Zhang Y, Luo K, Hou M, Driscoll P, Salkee NP, Minar J, et al. Thermal conductivity of Fe-Si alloys and thermal stratification in Earth's core. PNAS. 2022;119(1):1-8.

21. Zhang Y, Hou M, Driscoll P, Salke NP, Liu J, et al. Transport properties of Fe-Ni-Si alloys at Earth's core conditions: Insight into the viability of thermal and compositional convection. Earth and Planetary Science Letters. 2021;553:116614.

22. Bass J. Deviations from Matthiessen's Rule. Advances in Physics. 1972;21(91):431-604.

23. Gomi H, Hirose K, Akai H, Fei Y. Electrical resistivity of substitutionally disordered hcp Fe–Si and Fe–Ni alloys: Chemically-induced resistivity saturation in the Earth's core. Earth and Planetary Science Letters. 2016;451:51-61.

24. Gomi H, Yoshino T. Impurity Resistivity of fcc and hcp Fe-Based Alloys: Thermal Stratification at the Top of the Core of Super-Earths. 2018;6:1-22.

25. Bohnenkamp U, Sandström R, Grimvall G. Electrical resistivity of steels and face-centered-cubic iron. Journal of Applied Physics. 2002;92 (8):4402-4407.

26. Vinet P, Ferrante J, Rose JH, Smith JR. Compressibility of solids. Journal of Geophysical Research Geophys Res. 1987;92(B9):9319-9325.

27. Dewaele A, Loubeyre P, Occelli F, Mezouar M, Dorogokupets PI, Torrent M. Quasihydrostatic equation of state of Iron above 2 Mbar. Physical Review Letters. 2006;97(21):29-32.

28. Matassov G. The electrical conductivity of iron–silicon alloys at high pressures and the Earth's core. publishing house of United States; 1977.

29. Ohta K, Kuwayama Y, Hirose K, Shimizu K, Ohishi Y. Experimental determination of the electrical resistivity of iron at Earth's core conditions. Nature. 2016;534(7605):95-98.

30. Gunnarsson O, Calandra M, Han JE. Colloquium: Saturation of electrical resistivity. Reviews of Modern Physics. 2003;75(4):1085-1099.