Thermoelectric properties of β-$FeSi_2$ with Co and Ni addition

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β-$FeSi_2$ crystallized in orthorhombic structure with *Cmce* space group is an abundant and eco-friendly material. In addition, this compound is promising in thermoelectric applications because of its good thermal stability and strong oxidation resistance at high temperatures [1)]. However, at high temperatures, the bipolar effect occurs due to a low carrier density (n_H) with a narrow band gap of about 0.7 eV. The presence of the bipolar effect remarkably deteriorates the Seebeck coefficient (S). As a result, the power factor ($PF = S^2\rho^{-1}$, where S is the Seebeck coefficient and ρ is electrical resistivity) also significantly decreases. It was reported that the addition of Co to β-$FeSi_2$ effectively increases the n_H and stabilizes S with temperature [2)]. In addition, the ρ decreases with Co doping, but it is independent of temperature which is probably due to small carrier mobility (μ_H). Therefore, in this work, we attempt to improve the μ_H of Co-doped β-$FeSi_2$ by Ni addition. TE properties of β-$Fe_{0.97-x}Co_{0.03}Ni_x Si_2$ ($0 \le x \le 0.03$) are reported from 80 to 800 K. The bulk samples were prepared by arc melting method and followed by heat treatment at 1150 °C for 3 hours and 840 °C for 20 hours. The X-ray diffraction data were measured by a CuKα diffractometer (SmartLab, Rigaku). The elemental analysis was performed by a scanning electron microscope (SU8010, Hitachi High-Technologies) equipped with an EDS XFlash5060FQ detector. The ρ and S were measured by using ResiTest8300 (TOYO Co.) and homemade apparatus. The thermal conductivity (κ_{total}) was measured by using a power efficiency measurement (PEM-2, ULVAC, Inc.). Then, the ZT can be calculated by $ZT = S^2T / (\rho\kappa_{total})$. The result shows that the metallic ε-phase increases with Ni and the solubility of Ni for β-phase is 1%. The presence of the ε-phase decreases the solubility of both Co and Ni in the β-phase. As Ni is added, the $|S|$ decreases because of the formation of the ε-phase. Fig. 1 shows that the ρ decrease with Ni doping because of the improved μ_H as shown in the inset of Fig. 1. The κ_{total} slightly decreases with Ni probably due to the porosity. Consequently, the highest PF = 2400 $\mu Wm^{-1}K^{-2}$ and ZT = 0.31 is obtained in the 1% Ni-substituted sample.

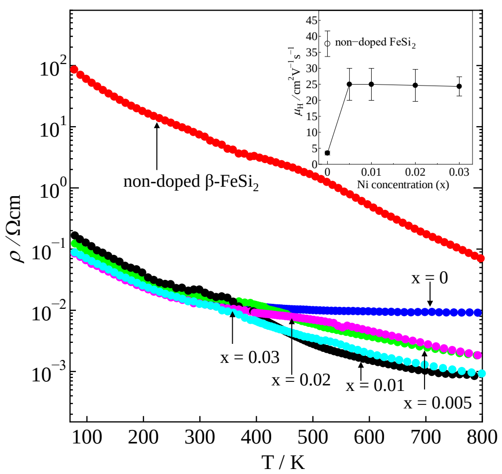

Fig. 1. Resistivity (ρ) of pure β-$FeSi_2$ and β-$Fe_{0.97-x}Co_{0.03}Ni_x Si_2$ ($0 \le x \le 0.03$). The mobility (μ_H) is plotted as the inset.

References

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2) S. Sam, H. Nakatsugawa and Y. Okamoto, Jpn. J. Appl. Phys. **61**, 111002 (2022).