Thermoelectric properties of bulk Ni-doped β -FeSi₂

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 β -FeSi₂ is considered a potential thermoelectric material for high-temperature applications due to strong oxidation resistance, good thermal stability, environmental friendliness, and low cost. However, with a narrow band gap of around 0.7 eV and low carrier density ($n_{\rm H}$), the bipolar effect that deteriorates the Seebeck coefficient |S| usually occurs as temperature increases. To solve this issue, doping with impurities having larger valences electron to either site of Fe or Si is considered an effective technique for improving ($n_{\rm H}$), and simultaneously enhancing |S| and decreasing electrical resistivity (ρ) [1]. Since Ni has two valence electrons larger than that of Fe, doping with Ni on the Fe site should effectively increase the $n_{\rm H}$. Tani and Kido [2] reported that the $n_{\rm H}$ of β -FeSi₂ can be increased by Ni substitution and its ρ simultaneously decreases. Therefore, the reduction in bipolar effect can possibly be also obtained by Ni substitution. In addition, Nagai *et al.* [3] reported that the |S| of β -FeSi₂ can also be improved with a small amount of Ni addition, resulting in an improvement in power factor ($PF=S^2 \rho^{-1}$). In this study, we are trying to optimize the Ni doping level to improve the TE performance of β -Fe_{1-x}Ni_xSi₂ ($0 \le x \le 0.03$) fabricated by the conventional arc-melting method. The elemental analysis was performed by a scanning electron microscope (SU8010, Hitachi High-Technologies) equipped with a Bruker EDS XFlash5060FQ detector. The *S* and ρ 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.). The ZT then can be calculated by $ZT = S^2T / (\rho \kappa_{total})$. The result shows that the ρ can be effectively decreased with x due to the increase in $n_{\rm H}$ as shown in the inset of Fig. 1. The | S | of all Ni-doped samples is higher and more stable than that of non-doped ones due to the reduction in bipolar effect; however, it becomes decreasing as x increases due to the high $n_{\rm H}$ and metallic ε -phase. The solid solution limit of Ni into the β -phase can be obtained at below x = 0.01. As a result, the highest *PF* of around 200 μ Wm⁻¹K⁻² is obtained in x = 0.001, leading to the improved ZT value of 0.019 at 600 K as shown in Fig. 1.



Fig. 1 ZT values of β -Fe_{1-x}Ni_xSi₂ with temperature dependence, where $n_{\rm H}$ is plotted in the inset.

References

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