

Title: Improvement of thermoelectric properties of β -FeSi₂ by Ni substitution

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As a semiconducting material having an orthorhombic crystal structure with *Cmce* space group, β -FeSi₂ is considered as promising candidate for high temperature thermoelectric application owing its ability of strong oxidation resistance, good thermal stability, and low cost. However, due to the negative impact of its narrow band gap of about 0.73eV, the absolute value of Seebeck coefficient ($|S|$) significantly decreases at high temperature because of bipolar effect. This issue can be effectively solved by increasing carrier concentration (n_H) with impurities doping. In this study, we attempt to eliminate the bipolar effect by doping Ni into Fe site with activation rate (2 electrons per Ni) in order to increase n_H of β -Fe_{1-x}Ni_xSi₂. The samples were fabricated by using arc-melting in Ar atmosphere and the powder XRD data were measured using SmartLab. The S and electrical resistivity (ρ) were measured by ResiTest8300 and homemade apparatus, and thermal conductivity (κ) was measured using PEM-2. As a result, the addition of Ni significantly reduces the bipolar due to the increase in n_H and the S of β -Fe_{1-x}Ni_xSi₂ is remarkably more stable than that of β -FeSi₂ above 400 K. We observed that both $|S|$ and ρ remarkably decreases with increasing x , while κ is not significantly varied with x . Therefore, the highest $ZT = 0.01$ is obtained at 760 K for β -Fe_{0.99}Ni_{0.01}Si₂ with $n_H = 2.3(9) \times 10^{17} \text{ cm}^{-3}$ due to the stability in $|S|$, the significant reduction in ρ , and no remarkable effect in κ .

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