Study of optimisation of Al addition amount to enhance thermoelectric properties of β-$FeSi_2$

Muhammad Ibrar [1, *], Sopheap Sam [2], Kosuke Yamazaki [1], Rio Oshita [1], Hiroshi Nakatsugawa [1]

Yokohama National University [1] and National Institute for Material Science[2]

E-mail: ibrar-muhammad-kw@ynu.jp

Thermoelectric devices (TEDs) offer a promising solution for harvesting waste heat and converting it directly into electrical energy via the Seabeck effect, featuring no moving parts, exhaust emissions, or mechanical pollution, thereby posing no harm to the environment. A highly efficient TED relies on top-quality thermoelectric (TE) materials. The performance of these materials is measured by the dimensionless figure of merit, ZT, which is calculated using the formula $ZT = S^2\rho^{-1}\kappa^{-1}T$. where $|S|$ represents the Seebeck coefficient, ρ is the electrical resistivity, κ denotes the thermal conductivity, and T stands for temperature in Kelvin. A higher *ZT* value indicates better TE performance, making it a crucial factor in designing and optimizing TEDs. Respectfully, materials exhibiting good *ZT* values, such as PbTe and Bi_2Te_3 are pose environmental hazards. Consequently, our goal is to enhance the TE performance of the non-toxic, abundant β-$FeSi_2$. Despite its promising properties, including a narrow band gap of approximately 0.7 eV, β-$FeSi_2$ suffers from a low carrier density (n_H). This makes it highly susceptible to the bipolar effect at elevated temperatures, resulting in a significant reduction in both the absolute Seebeck coefficient $|S|$ and the figure of merit (*ZT* value). Hence, Isoda *et al*. have attempted to enhance the carrier density (n_H) of β-$FeSi_2$ through doping with various impurities [1]. Notably, our Previous research has shown that Ni doping at the Fe site can significantly improve the TE performance of pure β-$FeSi_2$, increasing its *ZT* value from 2.6×10^{-4} to 0.019 at 600 K [2]. Therefore, we have recently investigated the doping of Al, which possesses 3 valence electrons, one less than Si, into p-type β-$FeSi_{2-x}Al_x$ ($0 \leq x \leq 0.1$). The samples were synthesized using the conventional arc-melting method, followed by a heat treatment process to convert the ε and α-phase into the β-phase. X-ray diffraction analysis was performed using a (Smart-Lab Rigaku diffractometer). The Seebeck coefficient $|S|$ and electrical resistivity ρ were measured using a (Resitest8300) and a custom-built apparatus, respectively. Meanwhile, the thermal conductivity (κ) was determined using a power efficiency measurement system (PEM-2) [3]. In this study, we explore the impact of aluminum (Al) doping on the scattering mechanisms in β-$FeSi_2$ with the ultimate goal of identifying the optimal Al concentration to enhance the p-type TE performance of the material. By introducing Al atoms into the β-$FeSi_2$ lattice, we can tailor the electronic and thermal transport properties, potentially yielding improved electrical conductivity, reduced thermal conductivity, or an enhanced Seebeck coefficient. Understanding the intricate relationship between Al doping levels and scattering effects is crucial for optimizing the materials efficiency in converting heat into electricity, a critical factor for TE application.

[1] Y. Isoda and H. Udono, in *Handbook of Thermoelectrics and Its Energy Harvesting, Preparation, and Characterization in Thermoelectrics*, e.d. D. M. Rowe, (Taylor & Francis, Abingdon, 2017) Chap. 18.

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

[3] S. Sam, S. Odagawa, H. Nakatsugawa, and Y. Okamoto, *Materials*. **16**, 927 (2023).