Enhancing p-type thermoelectric performance in Mn doped β -FeSi₂

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Introduction

Thermoelectric materials offer a solution by converting this dissipated heat into electricity.¹⁾ Having both *p*-type and *n*-type semiconducting nature⁴⁾ Iron Silicide (FeSi₂) structured systems are the most investigated materials. This is because of their eco-friendly nature²⁾ and flexible crystal structure³⁾ that can be modified via various dopants to demonstrate the desired physical properties. They can exist in 3 phases: α -Fe₃Si₅, β -FeSi₂ and ε -FeSi.⁴⁾ Among them β -FeSi₂ is the semiconducting phase while the rest are metallic phases.⁴⁾ Various doping has been investigated to enhance the dimensionless figure of merit *ZT* for β -FeSi₂ like cobalt Co³⁾, nickel Ni⁵⁾, co-doping of Co and Ni²⁾ which resulted in *n*-type nature. This study deals with Manganese Mn doping at Iron Fe site that resulted in p-type semiconducting nature.¹⁾

Experimental Procedures

Pure Fe, Mn, and Si raw materials were weighed before being arc melting to make an ingot. NC wire cutting machine was used to cut the sample with specific dimensions. To convert the sample into single β -phase, the polished samples were heat-treated for 3 hours at 1150°C. They were then annealed for 20 hours at 840°C to improve their characteristics. Through Keyence VE-8800 SEM images of polished bulk samples were taken while Rigaku-SmartLab computed X-ray Diffraction (XRD) data of the powdered form sample. ResiTest8300 assessed thermoelectric properties such as resistivity ρ and the seebeck coefficient S between 80 and 395 K.





Results and Discussions

S was found to be in the positive range indicating that all Mn doping contributed to the *p*-type semiconducting nature. Moreover, in comparison to non-doped FeSi₂¹⁾, Mn doping also helped to lessen the bipolar effect. Until Fe_{0.95}Mn_{0.05}Si₂, the carrier concentration was responsible for decrease in *S* but from Fe_{0.96}Mn_{0.04}Si₂, the increase at low temperature side and suppression of *S* at high temperature side is due to the effective mass. This can be explained by Mott's formula. The Fe_{0.97}Mn_{0.03}Si₂ sample has the largest power factor (*PF*), which is why the maximum *ZT* for this research study is likewise for Fe_{0.97}Mn_{0.03}Si₂, as shown in Fig 1.

References

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