Investigation of p-type thermoelectric properties for Mn doped *β*-$FeSi_2$

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Introduction

According to scientists, over 60% of global energy consumption losses occur due to waste heat released into the environment without utilization. Thermoelectric materials offer a solution by converting this dissipated heat into electricity.[1)] Iron Silicide ($FeSi_2$) structured systems are the most investigated materials. This is because of their eco-friendly nature[2)] and flexible crystal structure[3)] that can be modified via various dopants to demonstrate the desired physical properties. They can exist in 3 phases: α-Fe_3Si_5, β-$FeSi_2$ & ε-FeSi.[4)] Among them β-$FeSi_2$ is the semiconducting phase while the rest are metallic phases.[4)]

Experimental Procedures

After weighting pure Fe, Mn & Si raw materials were proceeded to the Arc Melting in Argon (Ar) environment to fabricate an ingot. Bulk samples were cut by NC wire cutting apparatus. The polished samples were fabricated by Heat Treatment with a maximum temperature of 1150°C for 3h to make it single β-phase from peritectoid reaction of ε and α-phase and then Annealed at 840°C for 20h to enhance their properties. Rigaku-SmartLab calculated X-ray Diffraction (XRD) data of powdered form sample while SEM images of polished bulk samples were taken by Keyence VE-8800 to understand the microstructure of the sample. ResiTest8300 measured Thermoelectric Properties like Seebeck Coefficient and Resistivity from 80-395K in Helium atmosphere. Thermal Conductivity κ was measured by PEM-2.

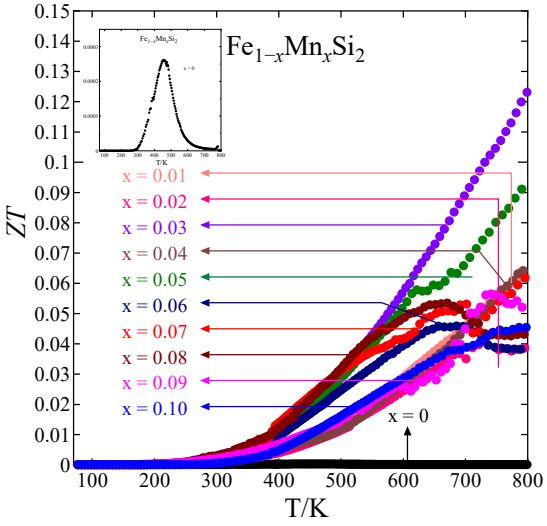

Fig 1. *ZT* of *β*-$Fe_{1-x}Mn_xSi_2$ ($0 \leq x \leq 1$)

Results & Discussions

For all Mn doped samples, the Seebeck coefficient *S* is positive indicating that all Mn doping contributed to the p-type nature of $FeSi_2$. Furthermore, Mn doping also contributed to the reduction of bipolar effect as compared to non-doped $FeSi_2$[1)]. The carrier concentration effect was dominant until $Fe_{0.95}Mn_{0.05}Si_2$ while the effect of effective mass gets dominant from $Fe_{0.96}Mn_{0.04}Si_2$. The maximum Power factor *PF* was availed for $Fe_{0.97}Mn_{0.03}Si_2$ sample because of which the maximum *ZT* that is achieved during this research study is also for $Fe_{0.97}Mn_{0.03}Si_2$ as shown in Fig 1.

References

1) S.Sam, F.Umar, M.Namba, K.Yamazaki, H.Nakatsugawa, Journal of Alloys and Compounds, **989**, 174367 (2024).

2) S.Sam, H.Nakatsugawa, and Y.Okamoto, Materials Advances, **4**, 2821 (2023).

3) S.Sam, H.Nakatsugawa, and Y.Okamoto Japanese Journal of Applied Physics, **61**, 111002 (2022).

4) S.Sam, K.Yamazaki, H.Nakatsugawa, Solid State Communications, **371**, 115287 (2023).