# High improvement of the figure of merit *ZT* in bulk amorphous-nanocrystalline $Si_{0.55}Ge_{0.35}(Fe_1,P_{0.10})$

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## Introduction

The SiGe alloys are a cheap and non-toxic thermoelectric materials for high temperature applications. In order to improve its figure of merit $ZT = S^2\sigma/\kappa$, Omprakash et al. decreased the thermal conductivity of the amorphous-nanocrystalline $Si_{0.55}Ge_{0.35}$ with a stable value of $\kappa$ = 1.35 W m$^{-1}$ K$^{-1}$ at T < 700 K [(1)]. However, the *ZT* value wasn't improved because of its low power factor. Takeuchi demonstrated that large transport properties $S^2\sigma$ can be obtained by the presence of two overlapping tight-bindings bands localized at the band edge of selected electrical band[(2)]. By the use of calculations, we determined that Fe created some impurity states near the conduction band edge of SiGe, fitting well the precious cited conditions.

Therefore in this study, we investigated the thermoelectric properties of the Fe-doped bulk amorphous-nanocrystalline $Si_{0.55}Ge_{0.35}(Fe_1,P_{0.10})$, with P as electron carrier dopant.

## Experimental Procedure

Several samples of $Si_{0.55}Ge_{0.35}(Fe_1,P_{0.10})$ composition were prepared by ball milling at 600 rpm for 6 h and then alternatively at 300 rpm for 125 h using a stainless pot container in a hydrogen/argon atmosphere. The nano-powder was then collected and load into a stainless die inside an argon chamber and finally sintered into bulk by means of SPS with an applied pressure of 400 MPa at 550 ºC for 6 hours at vacuum atmosphere. The thermal conductivity $\kappa$ was measured by laser flash method, the Seebeck coefficient *S* by a hand-made apparatus, and the electrical resistivity $\rho$ by four-probes method in the temperature range of 300-1100 K.

## Results and discussion

All the prepared bulk samples showed an amorphous structure together with 10 nm-size crystalline nano-grains measured by XRD and TEM.

The thermal conductivity $\kappa$ showed a stable value of $\kappa$ < 0.92 ± 0.05 W m$^{-1}$ K$^{-1}$ at T < 773 K together with a large magnitude of the Seebeck coefficient value about |S| > 500 ± 20 μV K$^{-1}$ at n-type condition, with a good reproducibility between each prepared samples. However, the crystallization at T > 900 K increased the thermal conductivity $\kappa$ > 1.5 ± 0.05 W m$^{-1}$ K$^{-1}$ at 1100 K with decreasing the Seebeck coefficient at the same temperatures. Nevertheless, the grain growth of crystallised nano-particles kept decreasing the electrical resistivity to less than $\rho$ = 3.13 ± 0.50 mΩ cm at 1100 K.

As a result, we succeeded to improved the transport properties of amorphous-nanocrystalline $Si_{0.55}Ge_{0.35}(Fe_1,P_{0.10})$ with low values of thermal conductivity. The figure of merit *ZT* showed a exponential increased exceeding 1.98 ± 0.3 at 1100 K for crystallised samples.

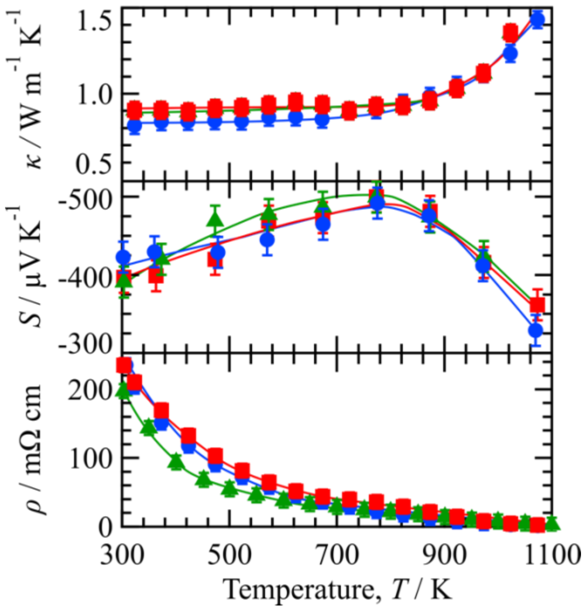


**Figure 1 :** Thermal conductivity $\kappa$, Seebeck coefficient *S*, and electrical resistivity $\rho$ of $Si_{0.55}Ge_{0.35}(Fe_1,P_{0.10})$ samples.

## References

[1] M. Omprakash et al., *J. Electron. Mater* **47**, (2018).
[2] T. Takeuchi, *Mater. Trans*. **50**, 2359 (2009).