# High thermoelectric performance of Si-Ge alloy by modifying the electronic structure

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## Introduction

In order to improve the figure of merit *ZT*, many strategies have been reported. For example, nano-structuring and modulation doping approach has been utilized to improve the thermoelectric properties of Si-Ge alloy by decreasing thermal conductivity without degrading the power factor [1].

Our previous studies revealed that B-doped Si-Ge-Au thin film and bulk sample possessed *ZT* value of 1.38 and 1.63 at 1000K. We found that the electron transport properties were constructively improved using Au-doping to form an impurity states near the valence band top, and B-doping to control the Fermi level. Very small thermal conductivity ~ 1.5 $Wm^{-1}K^{-1}$ was obtained due to nanograins. However, Au is an expensive element and more than *ZT* = 1.63 is required for improving efficiency. In the present study, we synthesized bulk noncrystalline B-doped Si-Ge alloy with other metal substitution, which is a cheap and non-toxic element. Thermoelectric properties (TE) of bulk nanocrystalline samples were investigated as a function of temperature 300 – 1000 K, respectively.

## Experimental Procedure

High purity metal (3 at.%) substituted Ge mother ingot was crushed into powders and sealed with the high purity Si (5N) and 3 at.% of boron in a Zirconia container with Zirconia balls in the glove box under pressurized Ar gas atmosphere. The mixed powders were milled at a speed of 600 rpm for 6 h. Afterwards, the powders were subsequently sintered with a relatively high pressure of 400 MPa at 1003 K for 4 h.

## Results and discussion

The powder XRD indicated that the single phase of diamond structure was obtained after the ball-milling. The size of nano-crystals in the bulk sample was estimated to be 30 nm from the XRD peaks and the Scherrer equation. The large Seebeck coefficient of 360 $\mu V^{-1}K^{-1}$ at 1000 K was obtained presumably due to presence of sharp peaks near the valence band edge. The electrical resistivity was 4.5 mΩcm at 1000 K. As a consequence, a very large power factor reaching 2.6 $mWm^{-1}K^{-2}$ together with low thermal conductivity 1.47 $Wm^{-1}K^{-1}$ allow us to obtain high *ZT* = 1.8 at 1000 K, respectively as shown in Fig.1. The obtained *ZT* was higher than that of the previously reported Si-Ge-Au nanocomposites (*ZT* = 1.63) [2]. The TE properties of different at.% metal substituted *p*-type Si-Ge will be discussed.

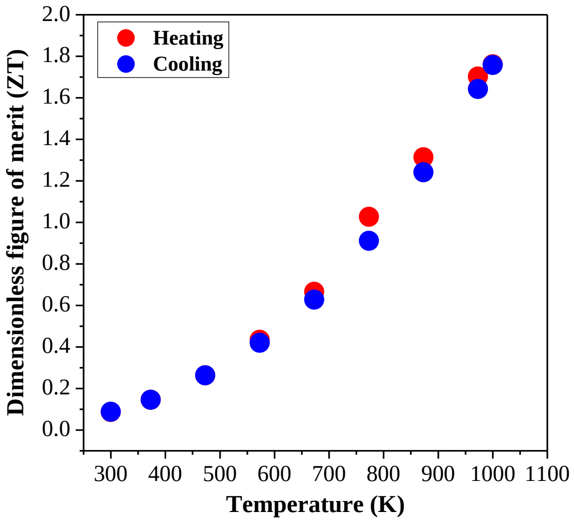


**Figure 1** Figure of merit of B-doped Si-Ge with 3 at.% metal substituted nanocrystalline sample as a function of temperature.

## References

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