Improved thermoelectric performance of *p*-type Si-Ge alloy

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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 level 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 of bulk nanocrystalline samples were investigated as a function of temperature 300 – 1000 K, respectively.

Experimental Procedure

High purity metal 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 973 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 366 $\mu V^{-1}K^{-1}$ at 1000 K was obtained presumably due to presence of sharp peaks near the valence band edge. The electrical resistivity was 3.78 mΩcm at 1000 K. As a consequence, a very large power factor reaching 3.54 $mWm^{-1}K^{-2}$ together with low thermal conductivity 1.49 $Wm^{-1}K^{-1}$ allow us to obtain high *ZT* = 2.4 at 1000 K, respectively as shown in Fig.1. The obtained *ZT* was approximately 50% higher than that of the previously reported Si-Ge-Au nanocomposites (*ZT* = 1.63) [2].

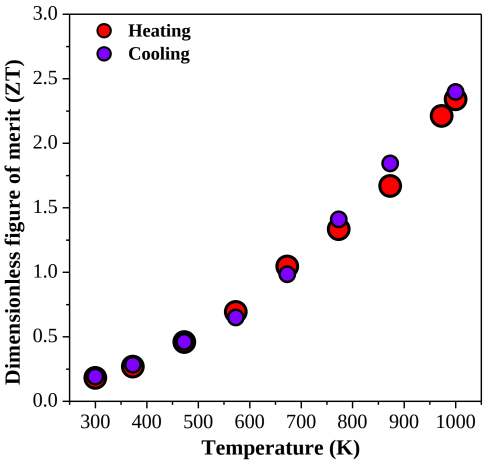

Figure 1 Figure of merit of B-doped Si-Ge with metal substituted nanocrystalline sample as a function of temperature.

References

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