CHAPTER 6

CONCLUSION

Electronic structure of Sc, Zr, Hf, Nb, V, Mn, As, Sb, and Bi dope TiNiSn

Doping Sc, Zr, Hf, Nb, V and Mn at Ti–site affected to change lattice parameter of TiNiSn. Codoping Sc, Zr, Hf, Nb, V and Mn at Ti–site induced the electron pocket in the conduction band, which is electron–doping. Doping As, Sb, and Bi at Sn–site shows electron pocket in the conduction band. The electron pocket increased with increasing by doping concentration.

Thermoelectric properties of Sc, Zr, Hf, Nb, V, Mn, As, Sb, and Bi dope TiNiSn

Doping Sc, Zr, Hf, Nb, V and Mn at Ti–site induced Debye temperature and lattice thermal conductivity. The lattice thermal conductivity reduced by 17.65 – 27.19% for $Ti_{0.75}Zr_{0.25}NiSn$, $Ti_{0.75}Hf_{0.25}NiSn$, and $Ti_{0.50}Mn_{0.50}NiSn$. Codoping Sc, Zr, Hf, Nb, V and Mn at Ti–site reduced the lattice thermal conductivity from 4.8 W m^{-1} K^{-1} (TiNiSn) to 2.42 W m^{-1} K^{-1}. The high power factor appeared in ScV, ScNb, and ZrHf codoped Ti–site and increased the dimensionless figure of merit from ~0.24 (TiNiSn) to 0.42 at Fermi level and 300 K. Doping As, Sb, and Bi at Sn–site obtained high power factor at low doping concentration <0.0625. As, Sb and Bi reduced the lattice thermal conductivity by 45%. So that, As, Sb, and Bi increased the dimensionless figure of merit for TiNiSn by 50% at 800 – 1000 K.