Realizing *p*-type NbCoSn half-Heusler compounds with enhanced thermoelectric performance via Sc substitution

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Abstract

N-type half-Heusler NbCoSn is a promising thermoelectric material due to favourable electronic properties. It has attracted much attention for thermoelectric applications while the desired *p*-type NbCoSn counterpart shows poor thermoelectric performance. In this work, *p*-type NbCoSn has been obtained using Sc substitution at the Nb site, and their thermoelectric properties were investigated. Of all samples, $Nb_{0.95}Sc_{0.05}CoSn$ compound shows a maximum power factor of 0.54 mW/mK^2 which is the highest among the previously reported values of *p*-type NbCoSn. With the suppression of thermal conductivity, *p*-type $Nb_{0.95}Sc_{0.05}CoSn$ compound shows the highest measured figure of merit ZT = 0.13 at 879 K.

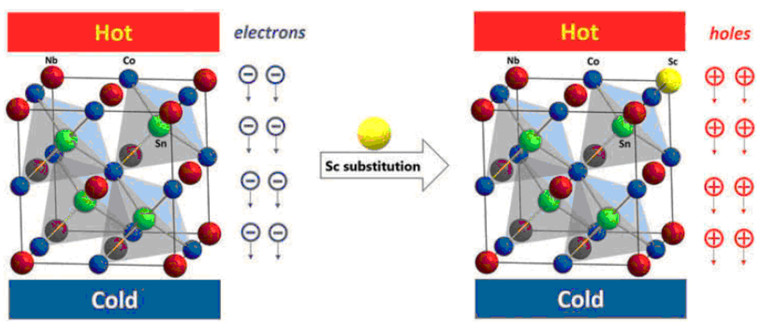

Figure 1 Crystal structure of NbCoSn and schematic illustration of Sc substitution

Phase characterization

➢ All samples show the cubic MgAgAs crystal structure with some minor Nb_3Sn impurities.

➢ The cell parameter increases with Sc concentration because of the ionic radius difference between Sc^{3+} (0.87 Å) and Nb^{5+} (0.74 Å).

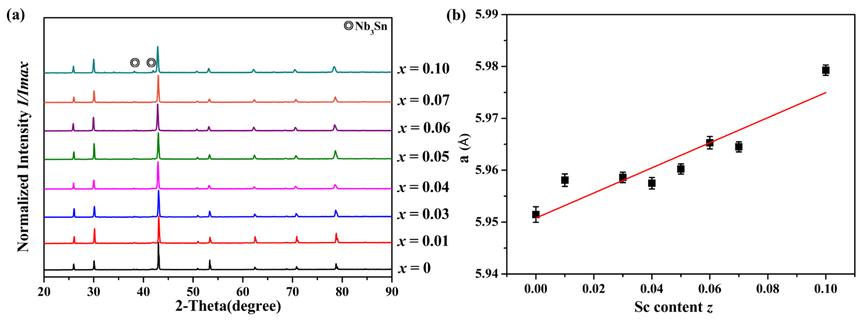

Figure 2 (a) PXRD patterns and (b) cell parameters of $Nb_{1-z}Sc_zCoSn$ samples.

There is no obvious phase segregation and the elements almost distribute uniformly in $Nb_{0.95}Sc_{0.05}CoSn$ sample.

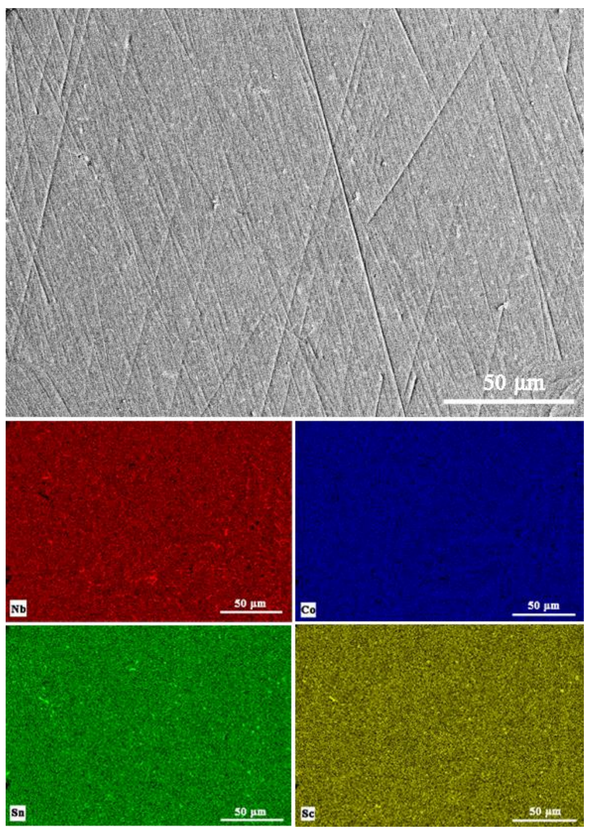

Figure 3 The secondary electron image and the elemental distribution mappings of $Nb_{0.95}Sc_{0.05}CoSn$.

Electrical properties

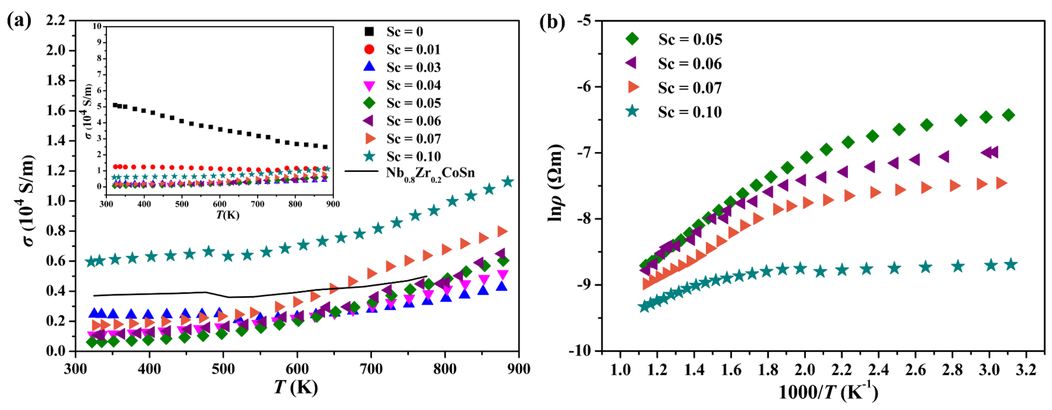

Figure 4 Temperature dependence of the electrical transport properties of $Nb_{1-z}Sc_zCoSn$ (a) electrical conductivity (b) lnσ *vs.* 1000/T plot.

➢NbCoSn shows a metal-like behavior.

➢ With Sc substitution, the electrical conductivity significantly decreases (Sc ＜ 0.05) and then goes up.

➢The values of the band gap decreases gradually with the Sc content for the *p*-type NbCoSn.

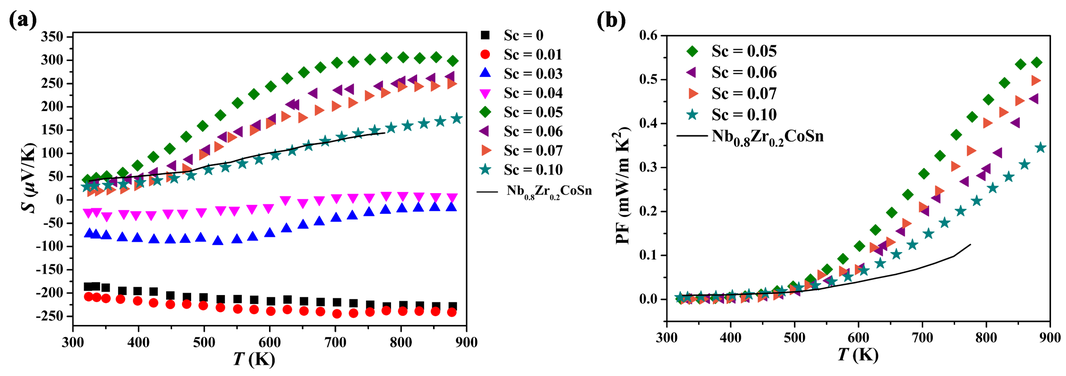

Figure 5 Temperature dependence of the Seebeck coefficient (a), power factor (*p*-type) (b) of $Nb_{1-z}Sc_zCoSn$ samples and the power factor of $Nb_{0.8}Zr_{0.2}CoSn$ as comparison [2].

➢When Sc = 0.05, NbCoSn becomes *p*-type semiconductor (positive *S*).

➢The highest PF is 0.54 mW/m K^2 in *p*-type $Nb_{0.95}Sc_{0.05}CoSn$, which is 77% higher than that of the reported *p*-type $Nb_{0.8}Zr_{0.2}CoSn$ (0.125 mW/mK^2).

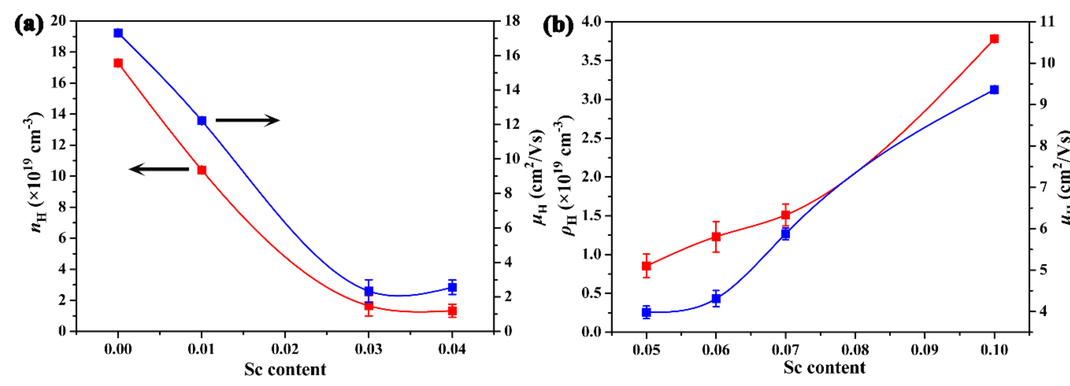

Figure 6 The carrier concentration and carrier mobility of $Nb_{1-z}Sc_zCoSn$ samples at room temperature (a) *n*-type, (b) *p*-type.

$Nb^{5+}=Sc^{3+}+2h^+$

➢The carrier concentration trend matches with the σ variation.

➢The electrons are dominant (Sc ＜0.05) and with increasing Sc content, n decreases.

➢When Sc ≥ 0.05, the dominant carriers are holes and the content gradually increases.

Thermal properties

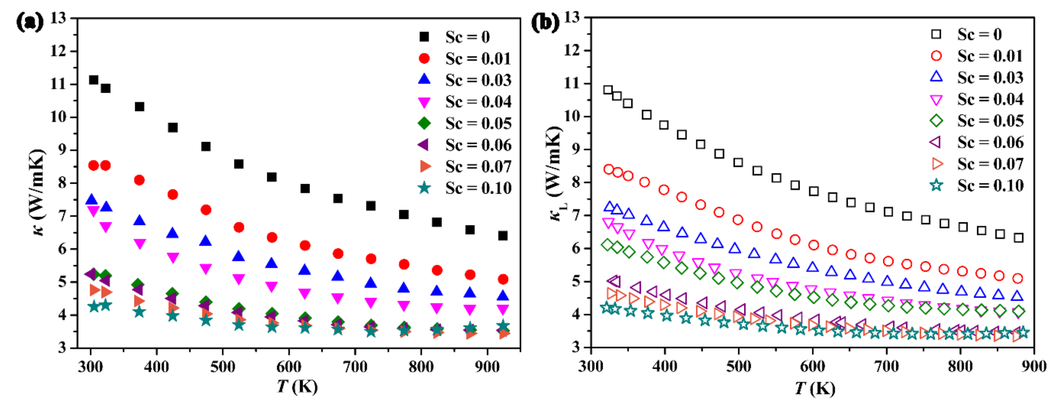

Figure 7 The temperature dependence of total thermal conductivity κ (a) and lattice thermal conductivity κ_L (b).

➢After substituting Sc, the κ decreases dramatically from 11.14 W/mK to 4.25 W/mK at room temperature due to the reduction of κ_L, which originates from the intensive point defect scattering (mass fluctuation and strain field fluctuation).

ZT

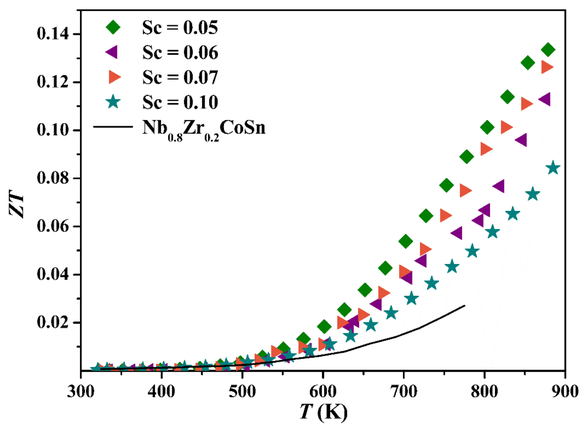

Figure 8 The figure of merit *ZT* for *p*-type NbCoSn and $Nb_{0.8}Zr_{0.2}CoSn$ and $Nb_{0.8}Zr_{0.2}CoSn$ as comparison [2].

➢The value of *ZT* improved to 0.13 at 879K in *p*-type $Nb_{0.95}Sc_{0.05}CoSn$ sample, which is much higher than that of $Nb_{0.8}Zr_{0.2}CoSn$.

Conclusions

➢ Sc is substituted at Nb site successfully and changes the original *n*-type NbCoSn to *p*-type semiconductor, indicating Sc is an efficient *p*-type dopant.

➢ Substituting Sc generates point defects and reduces lattice thermal conductivity.

➢ The highest *ZT* value of 0.13 is achieved in *p*-type $Nb_{0.95}Sc_{0.05}CoSn$.

References

[1] He R, Huang L, Wang Y, et al. Enhanced thermoelectric properties of *n*-type NbCoSn half-Heusler by improving phase purity. APL Mater. 2016;4:104804.

[2] Ferluccio DA, Smith RI, Buckman J, et al. Impact of Nb vacancies and *p*-type doping of the NbCoSn-NbCoSb half-Heusler thermoelectrics. Phys Chem Chem Phys. 2018;20:3979–3987.

Acknowledgement

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