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, \( \text{Nb}_{0.95}\text{Sc}_{0.05}\text{CoSn} \) 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.

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1. Introduction

Thermoelectric (TE) devices can directly convert waste heat into electricity via the Seebeck effect, which is a promising reliable alternative to mechanical converters if the efficiency can be improved [1]. This could become a pathway to more sustainable energy converters in times of energy consumption [2–5]. However, up to now the application of thermoelectric devices is limited by the low energy conversion efficiency \( \eta \), which is essentially decided by the materials’ dimensionless figure of merit \( ZT \): 

\[
ZT = S^2\sigma T/\kappa
\]

where \( S \) is the Seebeck coefficient, \( \sigma \) is the electrical conductivity, \( \kappa \) is the total thermal conductivity \( \kappa_c \) and \( \kappa_L \) are the carrier and lattice components of \( \kappa \), respectively, and \( T \) is the absolute temperature [6,7]. Thus, the combination of high \( S, \sigma \) and low \( \kappa \) is desirable for a large \( ZT \). Unfortunately, these thermoelectric parameters are strongly coupled via carrier concentration and mobility [8–10], making it difficult to optimize one single parameter without altering the others. Therefore, it has been quite challenging to develop highly efficient thermoelectric materials. The strategic goals of TE research are to discover new materials with high TE performance and/or improve the performance of the existing well-known materials, such as SiGe alloy [10], PbTe [11], chalcogenides [12], skutterudites [13,14], clathrates [15,16], Zintl phases [17] as well as full/half-Heusler compounds [18,19] by band engineering and carrier filtering effect [20–22], phonon engineering [23,24], reducing the dimension of materials [25], or spin fluctuation [26].

Due to the excellent electrical and mechanical properties, high-temperature stability, and possibility to use non-critical elements, half-Heusler (HH) compounds have become attractive candidates for thermoelectric...
application [27–31]. This compound has a general formula Xyz (X, Y = transition metals, Z = main group elements), crystallizing in cubic C1b structure, F43m space group [32,33]. An empirical rule proposed by Mahan and Sofo [34] states that the best thermoelectric performance is found with materials whose band gap is about 10kBT0, where kB is the Boltzmann constant and T0 is the operating temperature of the device. NbCoSn is one of HH thermolectric compounds with a band gap of 0.987 eV [35], and such a band gap fulfils the ‘10kBT0’ rule. In addition, the small electronegativity difference between Co (1.88) and Sn (1.96) ensures larger carrier mobility. Therefore, NbCoSn is a promising mid-high temperature thermoelectric material. Unsubstituted NbCoSn is an intrinsically n-type semiconductor. In 2006 Ono et al. [36] investigated the Sn and Ti substituted n-type NbCoSn and the highest ZT of 0.3 was achieved for the Nb0.99Ti0.01CoSn0.9Sn0.1, at 850 K. A decade later, He et al. [37] synthesized n-type NbCoSn1−xScx samples by arc melting combined with ball milling and hot-pressing processes, and the highest ZT reached ~0.6 at 1000 K for NbCoSn0.95Sn0.05. Generally, a TE device needs not only high ZT in n-type and p-type materials, but the n-type and p-type materials should have similar compositions and thus comparable mechanical properties and thermal expansion coefficient. For instance, n-type MnI (Sn,Sb) [38] and p-type MCoSn(Sb,Sn) [39,40] (M = Zr and Hf) compounds fulfill such criteria, and the thermoelectric module made of them reaches a record-high conversion efficiency of 12.4% with a temperature difference of 698 K [41]. To fabricate p-n NbCoSn couple, a p-type NbCoSn based compound is needed to match with the developed n-type NbCoSn compounds. However, few efforts have been devoted to investigating p-type NbCoSn. To the best of our knowledge, Ferluccio et al. [42] first realized p-type NbCoSn via substituting Ti and Zr at Nb site, and the maximum ZT value for p-type Nb0.8Zr0.2CoSn is only 0.03 at ~790 K. Obviously, the ZT value of p-type Nb0.8Zr0.2CoSn compounds is much inferior to those of n-type counterparts. Therefore, it is crucial to identify new p-type dopants and further improve the thermoelectric performance of p-type NbCoSn.

In this work, the NbCoSn compound has been prepared through arc melting followed by annealing processes, and then Sc, chosen as a p-type dopant, is substituted at Nb site to obtain Nb1−xScxCoSn (x ≤ 0.1). There are two main reasons for choosing Sc as a p-type dopant: (1) The substitution of Nb (III B) by Sc (V B) can create more holes in this compound and further achieve a p-type NbCoSn. (2) The larger mass fluctuation between Nb (92.91 g/mol) and Sc (44.96 g/mol) can strengthen defect and alloying phonon scattering which can significantly suppress the lattice thermal conductivity. It is found that Nb1−xScxCoSn compound possesses p-type conducting behaviour when Sc = 0.05. The highest power factor of this p-type compound is 0.54 mW m−1 K−2, which is 230% higher than the reported value of Nb0.8Zr0.2CoSn [42]. As a result, a peak ZT of ~0.13 is achieved.

2. Experimental details

Nb1−xScxCoSn (x ≤ 0.1) compounds were prepared by arc-melting stoichiometric amounts of the elements Nb (wire, 99.999%), Sc (piece, 99.99%), Co (bulk, 99.999%), Sn (shot, 99.999%) in Ar atmosphere. The ingots were melted several times with flipping twice over each time to ensure homogeneity. The obtained ingots were sealed into evacuated quartz tubes, annealing at 1173 K for 7 days. And then the bars and pellets for measurements were prepared by cutting these annealed ingots.

The crystal structures of samples were investigated by powder X-ray diffraction (PXRD) on a Rigaku diffractometer (Rigaku, Japan) using Cu Kα radiation (λ0 = 1.5418 Å). The microstructures of polished samples were characterized by scanning electron microscopy (SEM; Zeiss Gemini, Germany), and the phase compositions were analyzed by energy-dispersive X-ray spectroscopy (EDX; Bruker, Germany). Electrical transport properties (Seebeck coefficient and electrical conductivity) were simultaneously measured by a ZEM-3 instrument (Ulvac-Riko, Japan) under He atmosphere from 300 to 900 K. The measurement errors for all samples are around ±3% (electrical conductivity) and ±5% (Seebeck coefficient). The Hall carrier concentration

\[ n_{H} = \frac{1}{eR_{H}} \text{ and mobility } \mu_{H} \text{ were calculated via } \]

\[ p_{H} = \frac{1}{eR_{H}} (n_{H} = -1/eR_{H}) \text{ and } \mu_{H} = \sigma R_{H}, \]

where e is unit charge and R_H is the Hall coefficient measured by commercial Physical Properties Measurement System (PPMS; Quantum Design, USA) under magnetic fields from −5.2 T to 5.2 T. The thermal conductivity was calculated by the formula \[ k = D\rho_{d} \text{, where } D \text{ is thermal diffusivity measured by laser flash instrument (NETZSCH, LFA457, Germany) by coating all samples with a thin layer of graphite to minimize emissivity errors (the actual measurement error is about 3%), } C_{p} \text{ is specific heat derived by temperature-dependent heat data using the differential thermal analyzer (NETZSCH, DSC204F1, Germany), and } d_{s} \text{ is the samples’ density estimated by the Archimedes method.} \]

The relative densities of these samples are about 95%.

3. Results and discussion

3.1. Phase and microstructure

The cubic NbCoSn crystal structure is shown in Figure 1. The element Nb (4a site) and Co (4b site) frame the NaCl sublattice with octahedral coordination, leaving the all tetrahedral central sites (4c site) to the element Sn, but only half of the 4c site is occupied by Sn, forming this half-Heusler compound. Simply, by applying the Zintl chemistry concept [43], this crystal structure can be
described into an anionic framework \([\text{CoSn}]^{5-}\) formed by the tetrahedral coordination of Co and Sn, and an electropositive \(\text{Nb}^{5+}\) filled in the octahedral voids formed by these tetrahedral frameworks.

PXRD patterns of \(\text{Nb}_{1-z}\text{Sc}_z\text{CoSn}\) (\(z = 0, 0.01, 0.03, 0.04, 0.05, 0.06, 0.07, 0.10\)) samples are shown in Figure 2(a). The diffraction peaks of all the samples can be indexed to MgAgAs cubic crystal structure despite some minor \(\text{Nb}_3\text{Sn}\) impurity phases, indicating all samples possess the HH phase. As it is visible from Figure 2(b), the unit cell parameter calculated via PowderCell [44] software increases with the increasing Sc content. Since the ionic radius of \(\text{Sc}^{3+}\) (0.87 Å) is larger than that of \(\text{Nb}^{5+}\) (0.74 Å) [45], the observed lattice expansion indicates \(\text{Nb}^{5+}\) is substituted by \(\text{Sc}^{3+}\).

The phase purity and elemental distribution were further examined by SEM combined with EDX mapping. Figure 3 shows the secondary electron image and the EDX maps of a polished \(\text{Nb}_{0.95}\text{Sc}_{0.05}\text{CoSn}\) sample, which indicates no obvious phase segregation and uniform elemental distribution on this scale. Table 1 summarizes the actual chemical compositions of all prepared samples analyzed by EDX, and it shows that the actual chemical compositions are close to the nominal compositions.

### 3.2. Electrical transport properties

Figure 4 shows the electrical transport properties of \(\text{Nb}_{1-z}\text{Sc}_z\text{CoSn}\) at different temperatures. For comparison, the literature data of \(\text{Nb}_{0.8}\text{Zr}_{0.2}\text{CoSn}\) [42] are also plotted (black line). As displayed in Figure 4(a), the electrical conductivity \(\sigma\) of unsubstituted \(\text{NbCoSn}\) compound decreases with the rise of temperature, showing a metal-like conducting behaviour. While, after substituting Sc at Nb site, the \(\sigma\) gradually increases with increasing temperature, indicating a semiconductor behaviour. Besides, with the Sc concentration up to 0.05, the \(\sigma\) significantly decreases from \(5.0 \times 10^4\) S/m (\(\text{NbCoSn}\)) to \(0.07 \times 10^4\) S/m (\(\text{Nb}_{0.95}\text{Sc}_{0.05}\text{CoSn}\)) at room temperature and then goes up to \(\sim 0.6 \times 10^4\) S/m with further increasing Sc concentration to 0.1 (\(\text{Nb}_{0.9}\text{Sc}_{0.1}\text{CoSn}\)). In addition, the band gap can be obtained from the slope of \(\ln\sigma\) vs. \(1000/T\) curve (shown in Figure 4(b)) using the Arrhenius equation

\[
\rho = \rho_0 \exp\left(\frac{E_g}{2k_B T}\right)
\]
where $\rho_0$ is a constant. The calculated band gap values are 0.35 eV, 0.33 eV, 0.29 eV and 0.20 eV for $p$-type Nb$_{0.95}$Sc$_{0.05}$CoSn, Nb$_{0.94}$Sc$_{0.06}$CoSn, Nb$_{0.93}$Sc$_{0.07}$CoSn and Nb$_{0.90}$Sc$_{0.10}$CoSn respectively. For the Nb$_{1-z}$Sc$_z$CoSn compounds with $z > 0.04$, the slope of $\sigma$-$T$ changes above 500 K and it can be explained by the impact of intrinsic conduction.

To further understand the conduction mechanism, the Hall coefficient at room temperature was measured and the calculated charge carriers concentration and mobility are presented in Figure 5 (a,b). The electron concentration $n_{H}$ for NbCoSn is $17 \times 10^{19}$ cm$^{-3}$, which is on the same order of magnitude as compared to the value reported by He et al. (~$24 \times 10^{19}$ cm$^{-3}$) [37]. Moreover, the $n_{H}$ decreases remarkably with the Sc content reaching 0.04. For $z = 0.05$, holes become the dominant carriers, and the hole concentration $p_{H}$ increases from $0.8 \times 10^{19}$ cm$^{-3}$ to $3.7 \times 10^{19}$ cm$^{-3}$ with the Sc content increasing from 0.05 to 0.10. Therefore, Sc is obviously an effective hole ($p$-type) dopant since it generates acceptor level near the top of the valence band and shifts the Fermi level toward the valence band, resulting in an increase of hole concentration. As for the carrier mobility $\mu_{H}$, the trend is similar to that of carrier concentration. Therefore,
the $\sigma$ decreases obviously and then increases slightly with increase of Sc content. The temperature dependence of Seebeck coefficient ($S$) in $\text{Nb}_{1-x}\text{Sc}_x\text{CoSn}$ is shown in Figure 6(a). The value of $S$ for unsubstituted $\text{NbCoSn}$ is $-185$ $\mu$V/K at room temperature, showing that $\text{NbCoSn}$ is apparently an $n$-type semiconductor. With Sc content increasing, the $S$ of $\text{Nb}_{1-x}\text{Sc}_x\text{CoSn}$ changes gradually from negative to positive with increasing of Sc content, which matches very well with the Hall measurements. The peak value of $S$ reaches $-306$ $\mu$V/K at 850 K for the $\text{Nb}_{0.95}\text{Sc}_{0.05}\text{CoSn}$ sample, and it is much higher than that (150 $\mu$V/K) of $\text{Nb}_{0.8}\text{Zr}_{0.2}\text{CoSn}$. The single parabolic band (SPB) model is usually used to analyze the transport properties of half-Heusler compounds [46]. Assuming electron conduction occurs within an SPB, the Seebeck coefficient of a non-degenerate

Figure 4. Temperature dependence of the electrical transport properties of $\text{Nb}_{1-x}\text{Sc}_x\text{CoSn}$ (a) electrical conductivity (b) $\ln\sigma$ vs. $1000/T$ plot.

Figure 5. The carrier concentration and carrier mobility of $\text{Nb}_{1-x}\text{Sc}_x\text{CoSn}$ samples at room temperature (a) $n$-type, (b) $p$-type.

Figure 6. Temperature dependence of the Seebeck coefficient (a) and the Seebeck coefficient versus the carrier concentration ($p$-type) (b) of $\text{Nb}_{1-x}\text{Sc}_x\text{CoSn}$ samples.
semiconductor is related to the effective mass \( m^* \), carrier concentration \( p_H \) and scattering parameter \( \lambda \) via

\[
S = \frac{k_B}{e} \left\{ 2 + \lambda + \ln \left[ \frac{2(2\pi m^* k_B T / h^2)^{3/2}}{p_H} \right] \right\}
\]

where \( e \) is the elementary charge and \( h \) is the Planck constant \([47]\). For the NbCoSn compound, we assume that acoustic phonon scattering is the predominant scattering mechanism, thus \( \lambda = 0 \). According to the measured \( S \) and \( p_H \), the \( m^* = 0.11 m_e \) is obtained. With the \( m^* = 0.11 m_e \) and the Equation (2), we can plot \( S \) at 300 K as a function of \( p_H \), a plot well-known as a ‘Pisarenko relation’. As shown in Figure 6(b), the red line is the calculated Pisarenko plot, and the blue dots represent measured data of Nb\(_{1-z}\)Sc\(_z\)CoSn compounds. Most of the data lie on the calculated line, except for that of Nb\(_{0.93}\)Sc\(_{0.07}\)CoSn compound. The reason for such an exception is not clear yet. It is suspected that the second phase or/and the deviation of the composition may be responsible for such an exception.

![Figure 7. Temperature dependence of the power factor of Nb\(_{1-z}\)Sc\(_z\)CoSn.](image)

Accordingly, the power factor (PF) was calculated via \( PF = S^2 \sigma \) and is shown in Figure 7. The highest PF of 0.54 mW/mK\(^2\) is achieved for Nb\(_{0.99}\)Sc\(_{0.05}\)CoSn compound mainly due to its high \( S \), and it is 3 times higher than that of p-type Nb\(_{0.99}\)Zr\(_{0.01}\)CoSn (0.125 mW/mK\(^2\)) \([42]\). However, the PF of Nb\(_{0.99}\)Sc\(_{0.05}\)CoSn is still much lower than the state of the art p-type HH compounds, such as (Ti/Hf)Co(SbSn) \([39]\) and NbFeSb \([48]\). Therefore, much more effort must be devoted to optimizing the carrier concentration of p-type NbCoSn compounds.

### 3.3. Thermal transport properties

The temperature dependence of total thermal conductivity (\( \kappa \)) and lattice thermal conductivity (\( \kappa_L \)) are displayed in Figure 8. The \( \kappa_c \) is calculated by using the Wiedemann-Franz law: \( \kappa_c = L \sigma T \), where \( L \) is Lorenz number estimated by Fermi integral, and then \( \kappa_L \) is derived from the value subtracting the carrier component \( \kappa_c \) from the total thermal conductivity. Because of the low electrical conductivity, the calculated \( \kappa_c \) is much lower than \( \kappa_L \). In other words, for Nb\(_{1-z}\)Sc\(_z\)CoSn compounds \( \kappa_L \approx \kappa \). As shown in Figure 8(b), the \( \kappa_L \) of unsubstituted NbCoSn is ~10.8 W/mK at room temperature, and this value is similar as compared to the result reported by Ferluccio et al. \([42]\). After substituting Sc, the room temperature \( \kappa_L \) decreases dramatically to 4.2 W/mK for Nb\(_{0.9}\)Sc\(_{0.1}\)CoSn, where a reduction of 60% is achieved after Sc substitution. Such a significant reduction mainly ascribes to the point defect scattering due to the substantial atomic mass difference (mass fluctuation) and interatomic coupling force differences (strain field fluctuation) between Nb and Sc, thereby giving rise to the reduction of \( \kappa_L \), especially at room temperature.

To explain the reduction of \( \kappa_L \) in terms of the phonon scattering mechanisms, the lattice thermal conductivity of Nb\(_{1-z}\)Sc\(_z\)CoSn can be evaluated via Debye-Callaway model \([49]\):

![Figure 8. The temperature dependence of total thermal conductivity \( \kappa \) (a) and lattice thermal conductivity \( \kappa_L \) (b).](image)
can be formulated in terms of the lattice thermal conductivity \(\kappa\). The combined phonon relaxation time \(\tau_{PD}\) is the relaxation time of the phonon-point-defect scattering processes due to strain and mass field fluctuations. The volume per atom \(V\) is the sound speed, \(\nu\) is the Debye temperature, and \(\tau_{C}\) is the combined phonon relaxation time. The literature data for NbCoSn are used in Nb_{0.8}Sc_{0.2}CoSn compounds as a good approximation. We assume all phonon scattering processes, including point-defect scattering, boundary scattering, Umklapp scattering, and phonon-free-electron scattering, occur in parallel and thus each adds to the process according to the Matthiessen’s rule, then the \(\tau_{C}\) can be formulated in Equation (4)

\[
\tau_{C}^{-1} = \tau_{PD}^{-1} + \tau_{B}^{-1} + \tau_{U}^{-1} + \tau_{pe}^{-1}
\]

where \(\tau_{PD}\), \(\tau_{B}\), \(\tau_{U}\), and \(\tau_{pe}\) are phonon-point-defect scattering, phonon-boundary scattering, phonon-Umklapp scattering, and phonon-free-electron scattering relaxation times, respectively. The \(\tau_{PD}\) can be obtained through:

\[
\tau_{PD}^{-1} = \tau_{S}^{-1} + \tau_{M}^{-1} = \frac{V\omega^{4}}{4\pi

\]

where \(\tau_{S}\) and \(\tau_{M}\) are relaxation times of the phonon-point-defect scattering processes due to strain and mass field fluctuations, \(V\) is the volume per atom, \(\theta_{D}\) and \(\Gamma_{M}\) are the disorder scattering parameters due to and strain and mass field fluctuations [50]. The experimental disorder scattering parameters \(\Gamma_{exp}\) (\(\Gamma_{exp} = \Gamma_{S} + \Gamma_{M}\)) can be obtained by

\[
\Gamma_{exp} = \frac{hv^{2}u^{2}}{\pi^{2}\theta_{D}V} \times \frac{1}{k_{f}^{v}} \text{ and } \frac{\kappa_{LO}}{\kappa_{FLO}} = \frac{tan^{-1}(u)}{u}
\]

where \(u\) is the disorder scattering parameter, \(\kappa_{LO}\) is the lattice thermal conductivity of the crystal with the disorder, and \(\kappa_{FLO}\) is the lattice thermal conductivity of the crystal without disorder [51]. The disorder scattering parameters of Nb_{1-x}Sc_{x}CoSn compounds calculated according to Equation (6) are listed in Table 2.

For the phonon-boundary scattering, \(\tau_{B}\) is independent of temperature and phonon frequency, and it can be described as \(\tau_{B}^{-1} = \nu/d\), where \(d\) is the grain size of the bulk sample. For the Umklapp scattering, \(\tau_{U}\) is dependent on temperature and phonon frequency and can be described as [52]

\[
\tau_{U}^{-1} \approx \frac{h\gamma^{2}}{2\pi^{2}MV^{2}\theta_{D}^{2} \omega^{2} T exp(-\theta_{D}/3T)}
\]

where \(\gamma\) is the Grüneisen constant and \(M\) is the average atomic mass of the crystal. For the phonon-free-electron scattering process [53], in the case of high carrier concentration \(\tau_{pe}\) can be described as

\[
\tau_{pe}^{-1} = \frac{4\pi^{2}E_{def}^{2}m^{2}\omega}{h^{3}d_{s}\nu_{l}}
\]

where \(E_{def}\) is the deformation potential, \(d_{s}\) is the sample’s density, and \(\nu_{l}\) is the longitudinal sound velocity. With the reference values of physics parameters (Table S1 in Supplementary Information), the lattice thermal conductivity of Nb_{1-x}Sc_{x}CoSn can be calculated by Equation (3) and the results are presented in Figure 9. In the

**Table 2.** The lattice thermal conductivity \(\kappa\), disorder scattering parameter \(u\), disorder scattering parameters \(\Gamma_{exp}\),

| Composition          | \(\kappa\) | \(u\) | \(\Gamma_{exp}\) |
|----------------------|------------|-------|-----------------|
| NbCoSn               | 10.8       | 1.03  | 0.0025(4)       |
| Nb_{0.8}Sc_{0.2}CoSn | 8.4        | 1.44  | 0.0049(8)       |
| Nb_{0.6}Sc_{0.4}CoSn | 7.2        | 1.61  | 0.0062(7)       |
| Nb_{0.4}Sc_{0.6}CoSn | 6.8        | 1.93  | 0.0089(6)       |
| Nb_{0.2}Sc_{0.8}CoSn | 5.0        | 2.59  | 0.016(1)        |
| Nb_{0.0}Sc_{1.0}CoSn | 4.6        | 2.88  | 0.019(9)        |
| Nb_{0.0}Sc_{1.0}CoSn | 4.2        | 3.27  | 0.025(6)        |
calculation, we assume that Sc substitution does not significantly affect the basic physics parameters, such as $\theta_D$, $v_f$, $E_{df}$ and $\nu_s$, so the major variable parameter is $\Gamma_{\text{exp}}$. In such a case, Sc substitution mainly alters the $\tau_{PD}$. Generally, the calculated $\kappa_1$ matches with the experimental values, implying that calculations based on Callaway-Deybe model can give a rough prediction to the $\kappa_1$ of NbCoSn system. In short, at room temperature the reduction of $\kappa_1$ of Nb$_{1-x}$Sc$_x$CoSn compounds is mainly due to that the Sc substitution induces strong point defect phonon scattering.

3.4. Figure of merit

Figure 10 shows the dimensionless figure of merit $ZT$ of $p$-type samples. Due to the dramatic enhancement of power factor compared with $p$-type Nb$_{0.8}$Zr$_{0.2}$CoSn, and the significant suppression of thermal conductivity, the highest $ZT$ of $p$-type Nb$_{0.95}$Sc$_{0.05}$CoSn achieves 0.13 at 879 K. It is much higher than that of Nb$_{0.8}$Zr$_{0.2}$CoSn [42], indicating Sc is an efficient $p$-type dopant for NbCoSn as compared to Zr.

4. Conclusions

In this work, homogenous Nb$_{1-x}$Sc$_x$CoSn compounds were prepared by an arc-melting process followed by an annealing treatment. The $p$-type NbCoSn compounds were obtained by substituting iso-electronic Sc at the Nb site and the effects on the electrical and thermal properties were investigated. Generally, the substitution of Sc at Nb site can change the $n$-type NbCoSn to a $p$-type semiconductor by adjusting the Fermi level, indicating Sc is an appropriate $p$-type dopant. Also, the thermal conductivity is reduced. As a result, the highest $ZT$ is 0.13 at 879 K in $p$-type Nb$_{0.95}$Sc$_{0.05}$CoSn sample, which is roughly 5 times higher than that of $p$-type Nb$_{0.8}$Zr$_{0.2}$CoSn.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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