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Achieving high power factor and output power density in p-type half-Heuslers Nb$_{1-x}$Ti$_x$FeSb

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Improvements in thermoelectric material performance over the past two decades have largely been based on decreasing the phonon thermal conductivity. Enhancing the power factor has been less successful in comparison. In this work, a peak power factor of $\sim 16 \mu W \cdot cm^{-1} \cdot K^{-2}$ is achieved by increasing the hot pressing temperature up to 1,373 K in the p-type half-Heusler Nb$_{0.95}$Ti$_{0.05}$FeSb. The high power factor subsequently yields a record output power density of $\sim 22 \ W \cdot cm^{-2}$ based on a single-leg device operating at between 293 K and 868 K. Such a high-output power density can be beneficial for large-scale power generation applications.

The majority of industrial energy input is lost as waste heat. Converting some of the waste heat into useful electrical power will lead to the reduction of fossil fuel consumption and CO$_2$ emission. Thermoelectric (TE) technologies are unique in converting heat into electricity due to their solid-state nature. The ideal device conversion efficiency of TE materials is usually characterized by (1)

$$\eta = \frac{T_H - T_C}{T_H} \cdot \sqrt{\frac{1 + ZT}{1 + ZT + \frac{L}{\ell}}}$$

where $ZT$ is the average thermoelectric figure of merit (ZT) between the hot side temperature ($T_H$) and the cold side temperature ($T_C$) of a TE material and is defined as

$$ZT = \frac{PF \cdot T}{\kappa_{tot}}$$

$$PF = \frac{S^2 \sigma}{\kappa_{tot}}$$

$$\kappa_{tot} = \kappa_L + \kappa_e + \kappa_{harp}$$

where $PF$, $T$, $\kappa_{tot}$, $S$, $\sigma$, $\kappa_L$, $\kappa_e$, and $\kappa_{harp}$ are the power factor, absolute temperature, total thermal conductivity, Seebeck coefficient, electrical conductivity, lattice thermal conductivity, electronic thermal conductivity, and bipolar thermal conductivity, respectively. Higher $ZT$ corresponds to higher conversion efficiency.

One effective approach to enhance $ZT$ is through nanostructuring that can significantly enhance phonon scattering and consequently result in a much lower lattice thermal conductivity compared with that of the unmodified bulk counterpart (2). This approach works well for many inorganic TE materials, such as Bi$_2$Te$_3$ (2), IV–VI semiconductor compounds (3, 4), lead–antimony–silver–tellurium (LAST) (5), skutterudites (6), clathrates (7), CuSe$_2$ (8), Zintl phases (9), half-Heuslers (10–12), MgAgSb$_2$ (13, 14), Mg$_2$(Si, Ge, Sn) (15, 16), and others.

However, nanostructuring is effective only when the grain size is comparable to or smaller than the phonon mean free path (MFP). In compounds with a phonon MFP shorter than the nanosized grain diameters, nanostructuring might impair the electron transport more than the phonon transport, thus potentially decreasing the power factor and $ZT$. In contrast, improving $ZT$ by boosting the power factor has not yet been widely studied (17–20). To the best of our knowledge, there is no theoretical upper limit applied to the power factor. Additionally, the output power density $\omega$ of a device with hot side at $T_H$ and cold side at $T_C$ is directly related to the power factor by (21)

$$\omega = \frac{(T_H - T_C)^2 \cdot PF}{4L}$$

where $L$ is the leg length of the TE material and $PF$ is the averaged power factor over the leg. As contact resistance limits the reduction of length $L$, higher power factor favors higher power density when heat can be efficiently supplied and removed.

One group of thermoelectric materials that may have high power factor is half-Heusler (HH) compounds. Among the various HH compounds, ZnNiSb-based n-type and ZrCoSb-based p-type materials have been widely studied due to their satisfactory $ZT \sim 1$ at 873–1,073 K (10), low cost (11), excellent mechanical properties (22), and nontoxicity. Recently, the NbFeSb-based p-type materials were found to possess good TE properties. Joshi et al. (23) and Fu et al. (24) reported $ZT \sim 1$ with Ti substitution. Moreover, a record-high $ZT \sim 1.5$ at 1,200 K was reported with Hf substitution (12). These work mark HH compounds among the most promising candidates for thermoelectric conversion in the mid-to-high temperature range. As reported by Joshi et al. (23), a high power factor of $\sim 38 \ \mu W \cdot cm^{-1} \cdot K^{-2}$ was realized in the p-type half-Heusler Nb$_{0.95}$Ti$_{0.05}$FeSb.

**Significance**

Thermoelectric technology can boost energy consumption efficiency by converting some of the waste heat into useful electricity. Heat-to-power conversion efficiency optimization is mainly achieved by decreasing the thermal conductivity in many materials. In comparison, there has been much less success in increasing the power factor. We report successful power factor enhancement by improving the carrier mobility. Our successful approach could suggest methods to improve the power factor in other materials. Using our approach, the highest power factor reaches $\sim 16 \ \mu W \cdot cm^{-1} \cdot K^{-2}$ at room temperature. Such a high power factor further yields a record output power density in a single-leg device tested between 293 K and 868 K, thus demonstrating the importance of high power factor for power generation applications.
N\textsubscript{0.9}Ti\textsubscript{0.1}FeSb\textsubscript{0.95}Sn\textsubscript{0.05} at 973 K. However, the composition with 40% Ti substitution strongly scatters the electrons as well. A subsequent work by Fu et al. (24) reported a higher power factor of \( \sim 62 \mu W\cdot cm^{-1}\cdot K^{-2} \) at 400 K in Nb\textsubscript{0.9}Ti\textsubscript{0.1}FeSb that was attributed to less electron scattering. However, they studied only one sintering temperature at 1,123 K (12, 24). Because high-temperature heat treatment for TE materials can be beneficial to TE performance (25), further optimization may be achieved in the NbFeSb system. Here we report the thermoelectric properties of the Nb\textsubscript{0.9}Ti\textsubscript{0.1}FeSb system with Ti substitution up to \( x = 0.3 \) prepared by using arc melting, ball milling, and hot pressing (HP) at 1,123 K, 1,173 K, 1,273 K, and 1,373 K. We find that higher HP temperature enhances the carrier mobility, leading to a high power factor of \( \sim 106 \mu W\cdot cm^{-1}\cdot K^{-2} \) at 300 K in Nb\textsubscript{0.9}Ti\textsubscript{0.1}FeSb. Such an unusually high power factor has previously been observed only in metallic systems such as YbAl\textsubscript{3} and constantan (26, 27). Furthermore, a record output power density of \( \sim 22 \) W cm\(^{-2}\) with a leg length \( \sim 2 \) mm is experimentally obtained with \( T_C = 293 \) K and \( T_H = 868 \) K. We also observe that the lattice thermal conductivity hardly changes within the range of grain sizes studied in this work. Thus, by using a higher HP temperature of 1,373 K and changing the Ti concentration, we have achieved higher power factor and ZT than the previously reported results for the same compositions (24).

**Materials and Methods**

**Synthesis.** Fifteen grams of raw elements (Nb pieces, 99.9%, and Sb broken rods, 99.9%, Atlantic Metals & Alloy; Fe granules, 99.98%, and Ti foams, 99.9%, Alfa Aesar) are weighed according to stoichiometry. The elements are first arc melted multiple times to form uniform ingots. The ingots are ball milled (SPEX 8000M Mixer/Mill) for 3 h under Ar protection to produce nanopowders. The powders are then consolidated into disks via hot pressing at 80 MPa for 2 min at 1,123 K, 1,173 K, 1,273 K, or 1,373 K with an increasing temperature rate of \( \sim 100 \) K/min.

**Characterization.** An X-ray diffraction machine (PANalytical X'Pert Pro) is used to characterize the sample phases. Morphology and elemental ratios of the samples are characterized by a scanning electron microscope (SEM) (LEO 1525) and electron probe microanalysis (EPMA) (JXA-8600), respectively. A transmission electron microscope (TEM) (JEOL 2100F) is used to observe the detailed microstructures.

**Measurement.** The thermal conductivity is calculated as a product of the thermal diffusivity, specific heat, and mass density that are measured by laser flash (LFA457, Netzsch), a differential scanning calorimeter (OSC 404 C, Netzsch), and an Archimedes’ kit, respectively. Bar-shaped samples with sizes around 2 mm \( \times \) 2 mm \( \times \) 10 mm are used for measuring the electrical conductivity and the Seebeck coefficient in a ZEM-3 (ULVAC). Hall concentrations (\( n_H \)) are measured using the Van der Pauw method in a physical properties measurement system (PPMS) (Quantum Design) under \( \pm 3 \) Tesla magnetic induction. The uncertainties for electrical conductivity, Seebeck coefficient, and thermal conductivity are 4%, 5%, and 12%, respectively. In particular, the thermal conductivity uncertainty comprises 4% for thermal diffusivity, 6% for specific heat, and 2% for mass density. As a result, the combined uncertainties for power factor and ZT are 10% and 20%, respectively. To increase the readability of the figures presented, we add error bars only to some of the curves (Figs. 3 and 5B).

**Results and Discussion**

**Enhanced Power Factor with Higher Hot Pressing Temperature.** All of the compositions in this work possess pure half-Heusler phases (Fig. S1). Fig. 1 A–F shows the thermoelectric properties of Nb\textsubscript{0.9}Ti\textsubscript{0.1}FeSb with hot pressing temperatures of 1,123 K, 1,173 K, 1,273 K, and 1,373 K. As shown in Fig. 1L, the power factor (PF) improves significantly at below 573 K. The peak value reaches \( \sim 106 \mu W\cdot cm^{-1}\cdot K^{-2} \) at 300 K and is the highest measurement value in half-Heusler compounds. When the temperature is higher than 873 K, the power factor values converge.

Fig. 1B shows that the high power factor is mainly due to the improved electrical conductivity. Above 673 K, the electrical conductivity values converge and follow the \( T^{-3/2} \) law, suggesting that acoustic phonons dominate carrier scattering (28). In contrast, Fig. 1C shows that the Seebeck coefficient changes little regardless of the hot pressing temperature. The dashed line in Fig. 1C is the calculated Seebeck coefficient using the single parabolic band (SPB) model (29),

\[ S = + \left( \frac{k_B}{e} \right) \frac{2F_H(\eta)}{\frac{F_H}{F_0}(\eta) - \eta} \]  

\[ F_H(\eta) = \int_0^\infty \frac{x^2}{1 + e^{x-\eta}} dx, \]  

where \( \eta \) is related to \( n_H \) through

\[ n_H = 4\pi \left( \frac{2m^*_h k_B T}{\hbar^2} \right)^{3/2} 4F_H^2(\eta) 3F_1^{-1/2}(\eta), \]  

where \( \eta \), \( n_H \), \( m^*_h \), and \( k_B \) are the reduced Fermi energy, the Hall carrier concentration, the density of states (DOS) effective mass.
of holes, and the Boltzmann constant, respectively. The \( n_{\text{H}} \) values are obtained through the Hall measurement and are presented in Table 1. The DOS hole effective mass (\( m^*_{\text{H}} \)) is obtained by fitting the Pisarenko relation (as is shown in TE Properties of p-Type Nb\(_{1-x}\)Ti\(_x\)FeSb). \( F_n(\eta) \) is the Fermi integral of order \( n \). The good agreement between the calculated result and experimental data shows the adequacy of the SPB model in describing the hole transport.

The total thermal conductivity is a multiplication of bulk density, thermal diffusivity, and specific heat (Fig. S2). The total thermal conductivity is slightly lower for samples hot pressed at lower temperature (Fig. 1D). This is mainly due to the difference in the electronic thermal conductivity originating from the difference in the electrical conductivity

\[
\kappa_e = L \sigma T, \tag{9}
\]

where \( L \) is the Lorenz number evaluated using the SPB model (29). By subtracting the \( \kappa_e \) from \( \kappa_{\text{tot}} \), we plot the sum \( \kappa_L + \kappa_{\text{bip}} \) in Fig. 1E. The sums of \( \kappa_L + \kappa_{\text{bip}} \) are barely affected by the hot pressing temperature. Furthermore, at temperatures above 773 K, the thermal conductivity trend deviates slightly from the \( T^{-1} \) behavior, indicating some minor bipolar effects even though the Seebeck coefficient seems not to show such an effect. The \( \kappa_{\text{bip}} \) is calculated using a three-band model (Fig. 1F, Fig. S3, and Table S1). The peak \( \kappa_{\text{bip}} \) reaches \( \sim 0.4 \text{ W m}^{-1} \text{ K}^{-1} \) at 973 K, a small value compared with the \( \kappa_L \).

Because of the enhanced power factor and the almost unaffected thermal conductivity, the \( ZT \) improves with elevated hot pressing temperatures (Fig. 1G). This is especially obvious at temperatures below 573 K, as shown in Fig. 1H, where the power factor shows larger differences (Fig. L1).

SEM images show significant enlargement of the grains with higher hot pressing temperatures (Fig. 2 A–D). The average grain sizes are found to be \( \sim 0.3 \mu m, \sim 0.5 \mu m, \sim 3.0 \mu m, \) and \( \sim 4.5 \mu m \) for samples pressed at 1,123 K, 1,173 K, 1,273 K, and 1,373 K, respectively (Fig. S4). Meanwhile, the room temperature (RT) Hall measurement (Table 1) shows an \( \sim 73\% \) enhancement of Hall mobility (\( \mu_H \)) of samples pressed at 1,373 K over those pressed at 1,123 K. Because the lattice thermal conductivity changes little with the grain size (Fig. 1E), it is very interesting to investigate why the enlarged grain size affects the electron transport so differently.

**Effect of Grain Size on Lattice Thermal Conductivity and Carrier Mobility.** The lattice thermal conductivity (\( \kappa_L \)) of sample pressed at 1,373 K is obtained by subtracting \( \kappa_e \) and \( \kappa_{\text{bip}} \) from \( \kappa_{\text{tot}} \). To describe the lattice thermal conductivity, we use the Klemens (30) model and split the phonon scattering into four different sources: three-phonon (3P) processes, grain boundary (GB) scattering, point defects (PD) scattering, and electron–phonon (EP) interaction. The calculation details and the fitting parameters are given in Supporting Information, Klemens Model. The complete table 1. RT Hall carrier concentration (\( n_{\text{H}} \)), Hall mobility (\( \mu_H \)), deformation potential (\( E_{\text{def}} \)), relative density, and EPMA composition of Nb\(_{1-x}\)Ti\(_x\)FeSb at different Ti concentrations and hot pressing temperatures.

<table>
<thead>
<tr>
<th>Composition and hot pressing temperature</th>
<th>( n_{\text{H}} ) ( 10^{20} ) cm(^{-3} )</th>
<th>( \mu_H ) ( \text{cm}^2\text{V}^{-1}\text{s}^{-1} )</th>
<th>( E_{\text{def}} ) eV</th>
<th>Relative density, %</th>
<th>EPMA composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x = 0.04 ) 1,373 K</td>
<td>6.3</td>
<td>25.2</td>
<td>12.5</td>
<td>99.1</td>
<td>Nb(<em>{0.95})Ti(</em>{0.05})Fe(<em>{1.03})Sb(</em>{0.98})</td>
</tr>
<tr>
<td>( x = 0.05 ) 1,123 K</td>
<td>7.2</td>
<td>15.2</td>
<td>( \sim)</td>
<td>99.4</td>
<td>—</td>
</tr>
<tr>
<td>( x = 0.05 ) 1,73 K</td>
<td>7.7</td>
<td>20.2</td>
<td>( \sim)</td>
<td>98.9</td>
<td>—</td>
</tr>
<tr>
<td>( x = 0.05 ) 1,273 K</td>
<td>7.7</td>
<td>24.3</td>
<td>11.8</td>
<td>98.6</td>
<td>—</td>
</tr>
<tr>
<td>( x = 0.05 ) 1,373 K</td>
<td>8.1</td>
<td>26.3</td>
<td>11.5</td>
<td>99.0</td>
<td>Nb(<em>{0.94})Ti(</em>{0.06})Fe(<em>{1.01})Sb(</em>{0.99})</td>
</tr>
<tr>
<td>( x = 0.06 ) 1,373 K</td>
<td>9.3</td>
<td>27.3</td>
<td>11.6</td>
<td>99.3</td>
<td>Nb(<em>{0.93})Ti(</em>{0.07})Fe(<em>{1.01})Sb(</em>{0.99})</td>
</tr>
<tr>
<td>( x = 0.07 ) 1,373 K</td>
<td>10.7</td>
<td>26.7</td>
<td>11.6</td>
<td>98.9</td>
<td>Nb(<em>{0.92})Ti(</em>{0.08})Fe(<em>{0.99})Sb(</em>{0.01})</td>
</tr>
<tr>
<td>( x = 0.10 ) 1,373 K</td>
<td>15.2</td>
<td>24.0</td>
<td>12.7</td>
<td>99.3</td>
<td>Nb(<em>{0.89})Ti(</em>{0.11})Fe(<em>{0.00})Sb(</em>{0.99})</td>
</tr>
<tr>
<td>( x = 0.20 ) 1,373 K</td>
<td>25.7</td>
<td>15.2</td>
<td>13.7</td>
<td>99.1</td>
<td>Nb(<em>{0.8})Ti(</em>{0.2})Fe(<em>{1.02})Sb(</em>{0.99})</td>
</tr>
<tr>
<td>( x = 0.30 ) 1,373 K</td>
<td>30.3</td>
<td>9.3</td>
<td>17.6</td>
<td>98.9</td>
<td>Nb(<em>{0.69})Ti(</em>{0.3})Fe(<em>{1.02})Sb(</em>{0.98})</td>
</tr>
</tbody>
</table>

*Data are not shown because the mobility is strongly affected by GB scattering.

![SEM images of Nb\(_{0.95}\)Ti\(_{0.05}\)FeSb hot pressed at 1,123 K, 1,173 K, 1,273 K, and 1,373 K.](image)

![Effects of grain size on Nb\(_{1-x}\)Ti\(_x\)FeSb Lattice Thermal Conductivity.](image)
results combining 3P, GB, PD, and EP are shown. For GB, the grain size is set at 4.5 μm. The error bars show 12% relative error.

\[ \mu_H = \sigma R_{H,300K} = \sigma (q n_{H,300K})^{-1}, \]

where \( q \) is the carrier charge, and \( R_{H,300K} \) and \( n_{H,300K} \) are the Hall coefficient and carrier concentration at 300 K, respectively.

At high temperatures, the dominant electron scattering is from acoustic phonons (AP), and thus the mobility is expressed as

\[ \mu_{AP} = \frac{F_0(q)}{2F_1(q)^{1/2}} v_0^2 d(N_e)^{1/3} E_{def}^{2/3}(m_h^{*})^{1/2}, \]

where \( v_0 \) is the longitudinal phonon velocity and calculated from the elastic constants (37), \( d \) is the mass density, and \( N_e \) is the valley degeneracy. \( E_{def} \) is the deformation potential that is obtained by extrapolating the high-temperature mobility back to room temperature, using the \( T^{-3/2} \) law. \( E_{def} \) is found to be \( \sim 12 \) eV for Nb_{0.05}Ti_{0.05}FeSb, a relatively smaller value compared with other TE systems like InSb (\( \sim 33 \) eV) (38), PbTe (\( \sim 22.5 \) eV) (39), and Bi_{2}Te_{3} (\( \sim 20 \) eV) (40), suggesting a weaker EP in the HH systems (29) that can benefit the electron transport and the power factor.

The mobility with the GB scattering is written as (41, 42)

\[ \mu_{GB} = D e \left( \frac{1}{2\pi m_h^{*} k_BT} \right)^{1/2} \exp \left( \frac{E_B}{k_BT} \right), \]

where \( D \) is the grain size and \( E_B \) is a commonly fitted barrier energy of the GB. Combining the two scattering mechanisms according to Matthiessen’s rule yields the expression for Hall mobility:

\[ \mu_H^{-1} = \mu_{AP}^{-1} + \mu_{GB}^{-1}. \]

The calculated mobility (\( \mu_H \)) with \( E_B \sim 0.1 \) eV and the measured quantity \( \sigma R_{H,300K} \) are shown in Fig. 3B. The good fitting demonstrates the importance of the grain boundaries in scattering carriers below 573 K. At temperatures higher than 573 K the charge carriers are mainly scattered by the acoustic phonons, and thus the mobility curves converge. In addition, Fig. 3B shows that the GB scattering becomes stronger when the grain size is smaller. For decreasing size from 0.5 μm to 0.3 μm, the mobility decreases by ~30%, but for decreasing size from 4.5 μm to 3 μm, the mobility drops by only 5%.

**TE Properties of p-Type Nb_{1-x}Ti_{x}FeSb.** Fig. 4 shows the TE properties of Nb_{1-x}Ti_{x}FeSb pressed at 1,373 K with x = 0, 0.04, 0.05, 0.06, 0.07, 0.1, 0.2, and 0.3 as a function of temperature. The electrical conductivity (\( \sigma \)) of undoped NbFeSb (i.e., x = 0) increases with temperature, consistent with typical semiconductor behavior (Fig. 4A, Inset). For the highly doped samples, \( \sigma \) obeys the \( T^{-3/2} \) law, suggesting the dominant acoustic phonon scattering of charge carriers (28). Meanwhile, \( \sigma \) increases with increasing x up to 0.2 because of the increased \( n_H \). Upon further increase of x to

![Fig. 4. Thermolectric property dependence on temperature for Nb_{1-x}Ti_{x}FeSb with x = 0, 0.04, 0.05, 0.06, 0.07, 0.1, 0.2, and 0.3. (A) Electrical conductivity, (B) Seebeck coefficient, (C) power factor, (D) total thermal conductivity, (E) lattice and bipolar thermal conductivity, and (F) ZT. In A, the purple dashed line and Inset show the ~T^{-3/2} relation and the measured conductivity of undoped NbFeSb, respectively.](image-url)
0.3, $\sigma$ decreases due to the decreased $\mu_H$ because of the stronger alloy scattering (Table 1). The Seebeck coefficient varies with $n_H$ in good agreement with the Pisarenko relation using a DOS effective mass $m^*_{\|} = 7.5 \, m_0$ at 300 K (Fig. 4A) (43),

$$S = \frac{8\pi k_B^2}{5\hbar^2} m^*_{\|} T \left( \frac{\pi}{3n_H} \right)^{2/3}. \quad [14]$$

The power factors of the p-type Nb$_{0.95}$Ti$_{0.05}$FeSb are very high at a wide temperature range (Fig. 4C). These values are much higher than those reported by Fu et al. (24), where a temperature of 1,123 K was used for sintering. As shown in Fig. 6A, higher pressing temperature accounts for the higher power factor. Moreover, even when comparing the samples pressed at 1,123 K, our work also shows higher power factor, with the probable reason being the higher sample densities (~99%) in the current work compared with those reported by Fu et al. (24) (~95%).

The total thermal conductivities ($\kappa_{tot}$) are shown in Fig. 4D. With increased Ti doping, the lattice thermal conductivity decreases significantly (Fig. 4E). As a result, the peak ZT reaches 1.1 for Nb$_{0.95}$Ti$_{0.05}$FeSb (Fig. 4F) at 973 K with a linear upward trend suggesting even higher ZT at higher operating temperatures (Figs. 4F and 6B).

To analyze the RT lattice thermal conductivity, we use the Clemens model incorporating the 3P, GB, PD, and EP processes, as mentioned in the previous section (30). The fitting parameters are listed in Supporting Information (Table S2). As shown in Fig. 5B, the GB scattering is much weaker compared with the other scattering processes. Note that the EP interaction is quite important in this system. Similar results were also reported by Fu et al. (12) with Zr and Hf doping.

Fig. 6 C and D compares the power factor and ZT, respectively, of a few materials with very high power factor, including YbAl$_3$ single crystal (26), Nb$_{0.95}$Ti$_{0.05}$FeSb (this work), and constantan (27). These materials possess peak power factors of at least 100 $\mu$W cm$^{-1}$ K$^{-2}$. It should be noted that YbAl$_3$ and constantan are essentially metals where the anomalous Seebeck coefficients are due to Kondo resonance (44) and virtual bound states (45), respectively. To the best of our knowledge, such high power factor above RT has never been realized before in semiconductor-based TE materials. Despite similar power factors, the other two materials possess very high thermal conductivity because they are essentially metals, and thus their ZT are much lower than Nb$_{0.95}$Ti$_{0.05}$FeSb.

**Power Output.** Due to the higher power factor, higher power output is expected. Following the approach of Kim et al. (46), the output power density ($\omega$) and efficiency ($\eta_{max}$) under a large temperature gradient are calculated. With $T_C=293$ K and a leg length $L=2$ mm, the calculated $\omega$ and $\eta_{max}$ are $\sim 28$ W cm$^{-2}$ and 8.8%, respectively, for Nb$_{0.95}$Ti$_{0.05}$FeSb when $T_H$ is 868 K (Fig. 7A and B). The corresponding experimental measured values are $\sim 22$ W cm$^{-2}$ and 5.6%, respectively, which are lower than the calculated results, probably due to imperfect device fabrication and possible parasitic heat losses during device measurement (see Supporting Information for details, Fig. S6). To the best of our knowledge, this work obtains the highest power density for bulk thermoelectric materials, which can be important for power generation applications (12, 23, 47, 48).

For power generation applications, the hot side temperature could be easily maintained at about 873 K as long as enough heat is supplied. However, maintaining the cold side temperature at 293 K could be challenging, and it would be more practical to maintain the cold side temperature at around ~320–340 K by convection heat removal. Thus, we calculate the cold side temperature ($T_C$)-dependent output power density ($\omega$) and efficiency ($\eta_{max}$) with fixed $T_H$ at 873 K, as shown in Fig. 7C and D, respectively. Clearly, the cold side temperature is very important to both the output power density and conversion efficiency.

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**Fig. 6.** TE property comparison. (A) Power factor and (B) ZT of the Nb$_{0.95}$Ti$_{0.05}$FeSb systems from different reports (23, 24). (C) Power factor and (D) ZT among Nb$_{0.95}$Ti$_{0.05}$FeSb, constantan (27), and YbAl$_3$ (26), with peak power factor exceeding 100 $\mu$W cm$^{-1}$ K$^{-2}$. 3.2 mm, the calculated and measured ($\omega$) output power density and ZT of Nb$_{0.95}$Ti$_{0.05}$FeSb. (x = 0.05 and 0.2) samples with the cold side temperature at ~293 K and the leg length ~2 mm, calculated (C) output power density and (D) conversation efficiency of Nb$_{0.95}$Ti$_{0.05}$FeSb (x = 0.05 and 0.2) samples with hot side temperature at ~873 K and the leg length ~2 mm but varying the cold side temperature, and comparison of (E) power factor and (F) ZT of Nb$_{0.95}$Ti$_{0.05}$FeSb and Nb$_{0.9}$Ti$_{0.1}$FeSb.
Conclusions

A higher hot pressing temperature up to 1337 °K is found to be beneficial for higher carrier mobility due to larger grain size. The resulting increase in electrical conductivity leads to a much higher power factor of ~106 µW cm⁻¹ K⁻² in the p-type half-Heusler Nb₀.₉₅Te₀.₅₅FeSb. With the high power factor, a record output power density of ~22 W cm⁻² is experimentally achieved, which can be important for power generation applications.

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