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Viewpoint Paper

Importance of high power factor in thermoelectric materials for power generation application: A perspective

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ABSTRACT

The figure of merit (ZT) has been used for more than half a century to guide the research of thermoelectric materials. In this perspective viewpoint, we emphasize that the power factor (PF) is more important than the thermal conductivity for thermoelectric power generation for a given ZT. We also propose the newly defined engineering parameters $(ZT)_{eng}$ and $(PF)_{eng}$ are the more practical indicators to show the temperature dependent efficiency and output power, as compared with conventional ZT and PF.

Thermoelectric energy conversion has the advantage to harvest widely distributed waste heat, and is also proved as an alternative route to convert solar energy into electric power economically. Thermoelectric phenomena were discovered in metals in 1821, however, it did not attract enough scientific interests for energy conversion until the 1950s due to the low conversion efficiency [1–4]. After the pioneering efforts, semiconductors such as Bi_2Te_3, PbTe, and SiGe based thermoelectric materials were developed as good thermoelectric materials due to the reduced thermal conductivity by the alloying effect. However, the dimensionless thermoelectric figure of merit (ZT) of these materials has been limited to the benchmark value of $ZT = 1$ for a long time. Here, ZT is defined as $ZT = (S^2\sigma/\kappa)T$, where S, σ, κ, and T are the Seebeck coefficient, electrical conductivity, thermal conductivity, and absolute temperature, respectively. Although the benefits of the solid state thermoelectric devices are notable, the ineffective energy conversion (<5%) resulted in only niche market, such as power supply for the space exploring mission and portable refrigerator. After the huge declining in research during 1970s–1990s, thermoelectrics get revived in 1990s under the influence of fossil fuel energy crisis. The main activity in the 1990s was to explore the next generation of thermoelectric materials through two approaches: new materials with low thermal conductivity, and low-dimensional systems for improved power factor (PF) [5–7]. After 2000s, these two approaches started to merge [8]. The low dimensional structures are artificially introduced into the host matrix to form the nanostructured materials, or nanocomposite, which significantly reduces the lattice thermal conductivity resulting in enhanced ZT values [9–11]. One of the remarkable examples is the p-type $Bi_{0.4}Sb_{1.6}Te_3$ material, where 40% enhancement in ZT value from 1.0 to 1.4 was observed by applying a ball milling and hot pressing process to an ingot [11]. The new $Bi_{0.4}Sb_{1.6}Te_3$ nanocomposite characterized with the multi-size scale phonon scattering centers, includes fine grains of 50 nm–2 μm, nano inclusions of 5–20 nm, and atomic defects less than 5 nm, which successfully reduced the lattice thermal conductivity [12].

Pursuing high ZT has been the focus of the entire thermoelectric community by applying various phonon engineering via nano approaches to reduce the thermal conductivity [13–25], or by exploring new compounds with intrinsically low thermal conductivity, such as compounds having a complex crystalline structure, local rattlers, liquid like sub-lattice, and highly distorted lattice [26–37]. However, we recently realized that efficiency controlled by ZT is not the only concern for practical applications. In contrast, the output power is in fact equivalently as important as the efficiency, or more important when the heat source is unlimited (such as solar heat), or heat source is free (such as waste heat from automobiles, steel industry, etc.) [38]. In this perspective, we will discuss the importance of high PF in thermoelectric materials for a power generation application, and also suggest that seeking high PF for the high output power has an advantage in terms of thermo-mechanical reliability for a given efficiency.

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Theoretically, the efficiency η of thermoelectric power generation is determined by the figure of merit $Z = S^2\sigma/\kappa$ while the output power density ω is related to power factor $PF = S^2\sigma$ as following,

$$\eta_{\max} = \frac{T_h - T_c}{T_h}\left(\frac{\sqrt{1+Z(T_h+T_c)/2}-1}{\sqrt{1+Z(T_h+T_c)/2}+T_c/T_h}\right), \quad (1)$$

$$w_{\max} = \frac{1}{4}\frac{(T_h - T_c)^2}{L}PF, \quad (2)$$

where T_h, T_c, and L are the hot side temperature, cold side temperature, and thermoelectric leg length, respectively. In Eq. (2), there are three parts: temperature difference $(T_h - T_c)$, temperature gradient $(T_h - T_c)/L$, and power factor PF. The temperature difference $(T_h - T_c)$ and temperature gradient $(T_h - T_c)/L$ are the working boundary conditions and the power factor $S^2\sigma$ is the material parameter. For given boundary conditions, ω is only governed by PF. It is noted that Eqs. (1) and (2) are derived from constant transport property model, in which all the thermoelectric parameters S, σ, and κ are assumed to be temperature independent. Practically, most materials show strong temperature dependent thermoelectric transport properties. The ZT is commonly used as an index to evaluate the thermoelectric performance. We recently pointed out that the efficiency predicted by Eq. (1) based on prevailing averaging methods is often misleading and gives rise to a very large overestimation in some situations [39,40]. One of the reasons is the measured ZT represents a local at a given temperature, *i.e.*, $T_h = T + \delta$ and $T_c = T - \delta$ where δ is an infinitely small temperature. In other words, Eq. (1) is only effective in a small temperature range due to heavy temperature dependent thermoelectric properties of materials. To account for the temperature dependence of S, σ, and κ for more accurate efficiency and output power predictions, a numerical calculation based on the energy balance equation for one-dimensional heat flow is required [41].

$$\frac{d}{dx}\left(\kappa(x)\frac{dT(x)}{dx}\right) + J^2\rho(x) - JT(x)\frac{dS(x)}{dx} = 0, \quad (3)$$

where J is the current density. These equations are solved iteratively to match the temperature boundary conditions at a given current density. In order to solve the nonlinear differential equation, a finite difference method is used. A TE leg is segmented along the heat flow direction for 1-D analysis, and approximated temperature and TE properties at each segment elements are calculated, which yields a linear relation between infinitesimal elements as [42],

$$\frac{\kappa_{i+1}-\kappa_{i-1}}{2\delta x}\frac{T_{i+1}-T_{i-1}}{2\delta x} + \kappa_i\frac{T_{i+1}-2T_i+T_{i-1}}{(\delta x)^2} + J^2\rho_i - JT_i\frac{S_{i+1}-S_{i-1}}{2\delta x} = 0, \quad (4)$$

where $i = 1, 2, 3, \ldots, n-1$, n is the number of segments, and δx is length of each segment. By iterating until the temperature distribution T_i and electric current I are converged, the output power, input heat, and efficiency are obtained as,

$$P_{out} = I^2R_L, \quad (5)$$

$$Q_h = IT_1S_1 + A\kappa_1\frac{T_1 - T_2}{\delta x} - \frac{1}{2}\rho_1\frac{\delta x}{A} - \frac{1}{2}IT_1(S_1 - S_2), \quad (6)$$

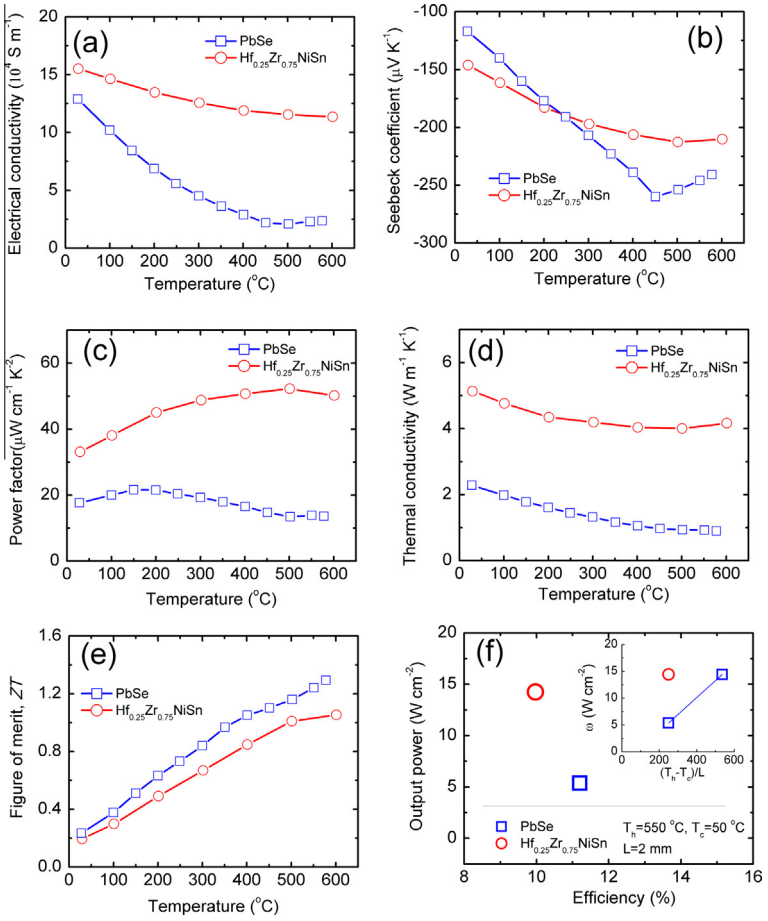

Fig. 1. Comparison of thermoelectric properties between two reported thermoelectric materials PbSe [43] and $Hf_{0.25}Zr_{0.75}NiSn$ [44]: (a) electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) thermal conductivity, (e) figure of merit (ZT), (f) leg output power by numerical calculation.