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Design of segmented high-performance thermoelectric generators with cost in consideration

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HIGHLIGHTS

- Segmentation of high-ZT TE materials can offer $< 1\,\$\,W^{-1}$ cost-performance ratio.
- And maintaining an efficiency of 17.8% and a power density of $3\,\text{Watt}\,\text{cm}^{-2}$.
- The ZT is the top benchmark for commercial feasibility of segmented TEGs.

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ABSTRACT

In this study, state-of-the-art thermoelectric (TE) materials working between 300 K and 1000 K are cautiously selected, including materials in categories of Chalcogenides, SiGe alloy, Skutterudites and Half-Heuslers. The selection principle is an overall reflection of the figure of merit (ZT), compatibility factors and power factors of TE materials. These chosen TE materials are divided into four groups for construction of two kinds of segmented p-type TEG legs and two kinds of segmented n-type TEG legs. Built on different combinations of these segmented TE groups, thermoelectric generators (TEGs) have been systematically modelled to find out the best cost-performance ratios and the corresponding efficiencies, output power densities and TEG geometries as well. All the TE material properties input in the simulation are temperature-dependent and the electrical & thermal contact resistances have been taken into account for every TE-TE and TE-electrode interfaces. The results demonstrate that the successful segmentation of high-ZT TE materials rather than their counterparts with large power factors can offer a cost-performance ratio of $\sim 0.86\,\$\,W^{-1}$, less than the commercially desired cost-effectiveness of $1\,\$\,W^{-1}$, while maintaining an efficiency of 17.8% and delivering a power density over $3\,\text{Watt}\,\text{cm}^{-2}$. These results not only confirm ZT as indeed the top criterion for choosing TE materials, but also predict the commercial feasibility and competitiveness of segmented TEGs in the same dollar per watt metrics as other renewable energy sources.

1. Introduction

Thermal energy is widely present in every aspect of the world and the majority of it goes to waste. Thermoelectric generators (TEGs) convert heat directly into electricity through Seebeck effect [1]. As a promising renewable energy source, TEGs hold the potential to power everything from small electronics to large grids without any emission of greenhouse gas to the environment. In addition, TEGs are able to operate quietly and stably for a long time (over 30 years) without maintenance, since they are solid-state devices without moving parts [2]. The huge amount of untamed heat, if properly utilized by TEGs, can help meet the ever-increasing energy demand around the globe. However, the thermoelectric (TE) technology has only found limited number of practical applications, the most well-known ones are powering the NASA space probes [3–6]. The major issue is the low thermal-to-electricity conversion efficiency, which depends directly on the dimensionless figure of merit (ZT) of TE materials and the Carnot efficiency, which caps the efficiency of any heat engine, including TEGs [7]. Generally speaking, $ZT \sim 1$ is an entry-level for a TE material to be practical [8]. Larger value is preferred and gives rise to higher efficiencies. The highest ZT of 2.6 ± 0.3 at 923 K has been demonstrated for p-type TE materials [9]. Though most of the TE materials, especially n-type ones, possess peak ZT value from 1 to 2.2 in different temperature ranges [10–18]. Enhancing ZT value is a hard task and usually not achievable at low temperature [19]. In contrast, it is comparatively easier to augment the Carnot efficiency, which is the ratio of

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temperature difference between hot stage and cold stage to the temperature of the hot stage. Increasing the Carnot efficiency is usually realized by enlarging the temperature difference, indicating that more than one TE material are needed since no single TE material currently possesses high *ZT* values over a broad enough temperature range.

There are two approaches to put various TE materials into cooperation for the same TEG device. One is using multi-stage design with different electrical circuits built for various TE materials working in different temperature stages [20–22]. This method places less restrictions on the selection of TE materials but introduces heat shunts from high temperature stages directly to the load [23]. The other strategy is segmenting TE materials continuously into the same electrical circuit [24]. This tactic doesn't have thermal energy loss through shunts but imposes relatively more stringent restraints on the selection of TE materials. Snyder et al. theoretically deduced a function called compatibility factor, through which feasibility of combining two or more TE materials can be quantified [25].

With prudent choice of compatible high-performance TE materials, segmented TEGs can be quite lucrative in terms of both efficiency and output power density. In a previous work, we have shown that efficiency of over 20% and aerial power density over 2 Watt cm^{-2} are possible at the temperature difference of 700 K, taking into account the effects of electrical and thermal contact resistances as well as the thermal radiation [26]. When choosing candidates for segmentation, compatibility is as important as high *ZT*. Although great effort has been made to increase *ZT*, the progress has stagnated [27,28]. A diverting part of the research passion in the field is to escalate the TE power factor, which can be simply viewed as the product of *Z* and the thermal conductivity. TE materials with larger power factor are expected to produce greater output power without necessarily higher efficiency. Compared with high-*ZT* Chalcogenides and SiGe, Skutterudites (SKDs) and Half-Heuslers (HHs) are representative TE materials of superior power factors but moderate *ZTs* [29,30]. SKDs and HHs are also promising candidates for segmented TEGs. Ngan et al. used a customized1D numerical model to estimate efficiencies of segmented TEGs with various combinations of TE materials, including HHs [31]. McEnaney et al. studied segmented model with Bi_2Te_3 and SKDs [32]. Zhang et al. have successfully built bismuth telluride/SKDs segmented TE modules with a current highest efficiency of 12% at a temperature difference of 541 K, matching results of their theoretical simulation [33]. In fact, most of the research projects in the TE field focus on improving the thermoelectric properties of TE materials or performance of TEG devices.

In reality, it is the cost-performance ratio rather than the high performance alone that will lead to the widespread employment of a technology. For example, photovoltaic (PV) cells have established their competence and taken large market share with their ~1 dollar per watt ($\$\ \text{watt}^{-1}$) cost-effectiveness. TEGs should be judged with the same metrics in order to compete with other energy sources. Yee et al. have formulated an instructive method to apply the $ per W metrics to the TEG power generation [34]. In their ensuing work, cost-performance with optimal fill factors (active cross-sectional area of TEG to area of heat exchangers) and leg lengths of 30 different TE materials has been assessed on the level of a unicouple, i.e. one pair of n-leg and p-leg, assuming same magnitude of temperature-independent Seebeck coefficients, electrical conductivity and thermal conductivity for both n- and p-type legs [35]. Due to the strong temperature-dependence of these TE material properties and the possible differences between the n- and p-type legs, the more complicated numerical approaches such as finite element method (FEM) should be implemented to more accurately evaluate the TEG performance and associated cost-effectiveness. Rezania et al. have utilized finite element analysis solver ANSYS to appraise the power per price for a unicouple system consisting of Zn_4Sb_3 as p-leg and $Mg_2Si_{1-x}Sn_x$ as n-leg, but their analysis does not take the cost-contribution from the heat exchanger system into account [36]. Kim et al. proposed a design with spacer inserted inside TE legs and claimed that the cost drop outpaces the reduction of the output power by performing ANSYS simulation [37]. Benday et al. analyzed the performance and economic possibility of 4 TE materials utilizing ANSYS modelling, finding out that heat sources of higher temperature are desired for improvement of financial feasibility of TEGs [38]. However, all of the above-mentioned cost-performance evaluations have not taken electrical and thermal resistances into account. More importantly, no work has been done on the cost-effectiveness of segmented TEG systems with compatible state-of-the-art TE materials to fully study their potential in practical applications.

In this study, we carefully select 10 high-performance TE materials, with 5 p-types and 5 n-types, in the category of Chalcogenides, SiGe alloy, Skutterudites and Half-Heuslers. The selecting criteria are based on an overall consideration of the TE materials for segmentation, including figure of merit (*ZT*), compatibility factors and power factors. Two p-type and two n-type segmented TEG legs are formed by the selected TE materials to generate four combinations of TEG modules. Systematical modelling of these segmented TEG modules are carried out by the 3D finite element analysis (FEA) with ANSYS. All the thermoelectric properties of the TE materials are temperature dependent, spanning a temperature range from 300 K to 1000 K, extracted directly from the published experimental data [9–18]. Contact effects at the TE-TE and TE-electrode interfaces have also been taken into account, including both the electrical and thermal contact resistances. Optimum cross-sectional area ratios (A_n/A_p) of TEG n-leg to p-leg have been identified for the maximal device performance, by applying the type I boundary conditions (BCs), which are the fixed temperature at hot sides (1000 K) and four different temperatures at cold sides (300 K, 323 K, 348 K, 373 K) of the TEG modules. Based on the discovered cross-sectional area ratios, optimal TEG leg lengths for the best cost-performance ratio have been found by employing type II BCs with constant temperature at hot sides (1000 K) while altering the heat transfer coefficients of cold sides. The results show that the output power density of TEGs can be enhanced conditionally by SKDs and HHs, indicating that TE materials with high power factors but relatively low *ZTs* might be preferred for applications in which cost is less important. When costs are taken into consideration, including materials, heat transfer and manufacturing cost, TE materials of higher *ZTs* demonstrate notable advantages over their counterparts with higher power factors. The successful segmentation of high-*ZT* TE materials is able to offer a cost-performance ratio of ~0.86 $\$\ \text{W}^{-1}$, while maintaining an efficiency of 17.8% and delivering a power density of over 3.0 Watt cm^{-2}. On the other hand, segmented TE modules involving TE materials with larger power factors can only provide a cost-performance ratio of ~1.11 $\$\ \text{W}^{-1}$, corresponding efficiency of 16.2% and power density of ~2.4 Watt cm^{-2}. These results confirm that *ZT* is indeed the top benchmark for selecting TE materials. More importantly, the low dollar-per-watt values along with the high efficiencies and power densities make it possible for segmented TEGs to be competitive with other renewable energy sources such as photovoltaic cells.

2. Method

2.1. Governing equations of TEG physics

When the system arrives at a steady state, the heat flux $\overrightarrow{q}$ ($\text{W}\cdot\text{cm}^{-2}$) absorbed at the hot side of the TEG module and the current density $\overrightarrow{J}$ ($\text{A}\cdot\text{cm}^{-2}$) flows in the TEG legs can be expressed as follows [1],

$$\overrightarrow{q} = T\alpha\overrightarrow{J} + \kappa\overrightarrow{\nabla}T \tag{1}$$

$$\overrightarrow{J} = \frac{1}{\rho}(\overrightarrow{E} + \alpha\overrightarrow{\nabla}T) \tag{2}$$

where α, ρ, κ, $\overrightarrow{E}$ and T are the Seebeck coefficient, electrical resistivity, thermal conductivity, electrical field and absolute temperature,