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RESEARCH DEVELOPMENTS IN THERMOELECTRIC MATERIALS: MOVING FORWARD WHILE REFLECTING ON THE PAST

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Abstract

The core of thermoelectrics, the most straightforward method for direct thermal-to-electrical energy conversion, is high-performance thermoelectric materials. The subject of thermoelectric materials research has halted multiple times in the last 60 years, but new paradigms have revitalized it each time. A number of potentially revolutionary mechanisms made possible by defects, size effects, critical phenomena, anharmonicity, and the spin degree of freedom are reviewed in this article. In order to improve material performance, these mechanisms separate the normally negatively correlated physical quantities. A variety of promising materials, sophisticated methods for material synthesis and preparation, and fresh prospects are also briefly discussed. If the current trend in thermoelectric materials development continues into the near future, the landscape of renewable energy will change.

Key words

thermoelectric materials, Seebeck, solid state, efficiency, ZT, materials research.

Introduction

Since the second Industrial Revolution, the globe has been burning an increasing amount of fossil fuels to meet the growing demand for power. Fossil fuels are not renewable, though, and burning them poses a threat to both natural and human systems due to the world's critical reliance on them. Conversely, heat might be regarded as renewable due to its widespread and unavoidable nature: More than 90% of the energy we use is produced by thermal processes, whereas the majority of the energy we waste eventually takes the form of heat [1]. The most straightforward method for direct heat-to-electricity energy conversion is thermoelectrics [2-4].

Thermoelectrics found specialized uses in the 20th century, particularly "where cost and efficiency were not as important as energy availability, reliability, and predictability," based on the Seebeck, Peltier, and Thomson effects observed in the 19th century [5]. A thermoelectric (TE) device can be used in conjunction with other energy-conversion technologies since it is solid state, free of moving parts, sounds, and greenhouse emissions, and it can be made smaller [6]. Additionally, it is a top option for distributed spot-size active heat control [7]. Examples include μW to mW wristwatch and pacemaker batteries, 10- to 100-W radioisotope TE power generators (RTGs) for NASA's deep-space probes, 10- to 100-W microelectronics and wine coolers, 100-W car seat climate control systems, and kW-level waste-heat harvesting for cars [8]. The NASA RTG helped astronaut Mark Watney live for several months when stranded on Mars in the 2015 20th Century Fox film The Martian.

Due to the poor performance of TE material, thermoelectrics now have a lower efficiency than other energy-conversion methods (Fig.1) [9]. Therefore, the development of higher-performance materials is crucial to the wider (beyond niche) application of thermoelectrics in the twenty-first century. One of the authors of this paper authored a Science Perspective [10] about filled skutterudites [11], one of the fascinating new TE materials of the time. This was more than 20 years ago. Since then, there have been numerous advancements in material performance, which has led to a continuous improvement in the state of thermoelectrics (Fig. 1). If the current

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trend in TE materials development continues for the foreseeable future, the landscape of renewable energy could very well change.

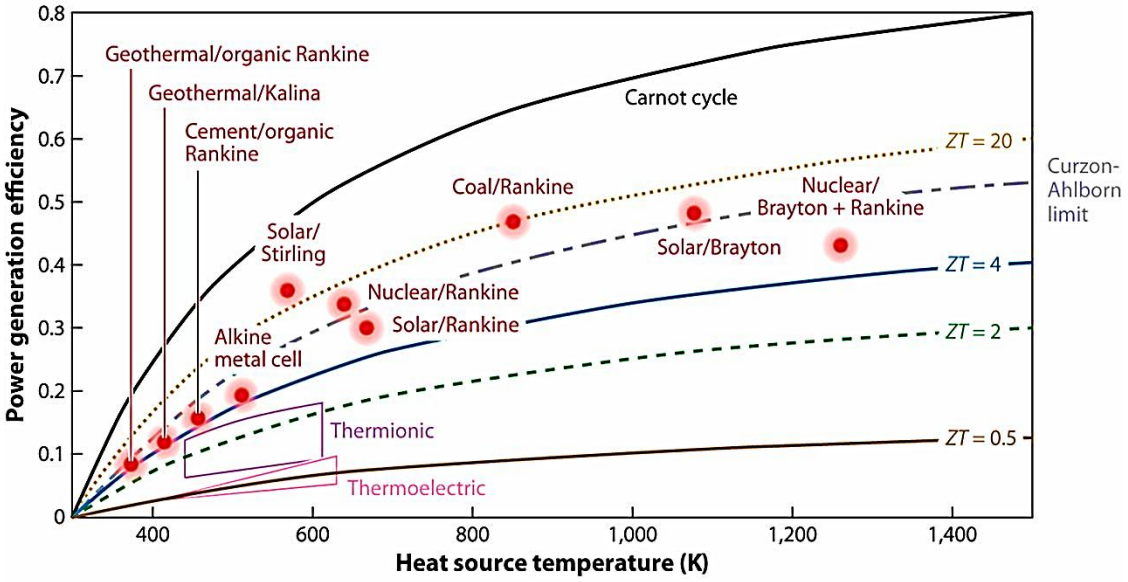

Fig. 1 Thermoelectric in the global landscape of energy conversion.

Thermoelectrics and other energy-conversion technologies are compared for efficiency in relation to the temperature of the heat source. The heat-sink temperature is fixed at room temperature, and it is assumed that the ZT values are independent of temperature.

Material performance

Three combinatorial material metrics are used to assess a material's TE promise. The primary parameter is the dimensionless figure of merit, *ZT*, which helps us determine the "efficiency." The maximum power-generation efficiency of a TE material, η, is

$$\eta = \left(\frac{T_{\text{hot}} - T_{\text{cold}}}{T_{\text{hot}}}\right)\left[\frac{\sqrt{1+ZT_{\text{m}}}-1}{\sqrt{1+ZT_{\text{m}}}+\left(\frac{T_{\text{cold}}}{T_{\text{hot}}}\right)}\right]$$

where the Carnot efficiency is the ratio of the temperature difference between the hot end and the cold end ($T_{\text{hot}} - T_{\text{cold}}$) to T_{hot}. The coefficient of performance for TE refrigeration adopts a slightly different expression, but in the same spirit.

General aspects of the TE process

The TE process that each TE material embodies can be generalized within the framework of linear nonequilibrium thermodynamics of coupled dissipative processes, despite the fact that each TE material is unique. Using electrons and holes as the working medium, a TE process is nothing more than a heat engine. The entropy and entropy production of the TE process within a material determine the magnitude of α and ZT, respectively.

The average entropy carried by a charge carrier divided by its charge in the limit of thermal equilibrium determines the magnitude of the Seebeck coefficient. We offer an approximation formula derived from the Bethe-Sommerfeld expansion of the Mott relation for degenerate statistics and single-band conduction to assist demonstrate the relationship between the Seebeck coefficient and the microscopic band structure and transport parameters.

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$$\alpha = \frac{\pi^2}{3}\frac{{k_B}^2 T}{e}\left[\frac{\mathrm{DOS}(E)}{n(E)} + \frac{1}{\mu(E)}\frac{d\mu(E)}{dE}\right]$$

where e is the carrier charge, DOS(E) is the energy-dependent electronic density of states, $n(E)$ is the energy-dependent number of states, k_B is the Boltzmann constant, and μ is the energy-dependent carrier mobility. Despite a limited applicability, clearly shows that the larger the DOS(E_F), the stronger the energy dependence of μ, and the higher the $|\alpha|$. These arguments hold in more-complex materials and act as the guideline for band structure and transport engineering.

The ZT value of a material reflects how reversible the TE process is in the material. In the case of zero entropy production, the TE process is reversible, the ZT of the material $\rightarrow\infty$, and the Carnot efficiency is reached. The Carnot efficiency is the upper efficiency limit of a TE process cycle, as with any heat-engine cycle. The entropy production in a TE process is the fundamental cause of irreversibility. The irreversible factor, derived from the compatibility factor S, gauges the sensitivity of the efficiency to the working condition. Generally, the higher the ZT value, the higher the sensitivity to the variation of working conditions. Enhancing the ZT of a material is thus tied to minimizing the entropy production of the TE process therein. According to Callen, the entropy production in a TE process arises from the heat flow from the hot end to the cold end and also from the degradation of electrochemical potential into heat (i.e., the dissipation effect, such as Joule heating).

Recent advances in TE materials research

Innovative transport mechanisms are the fountain of youth of TE materials research. This article reviews several potentially paradigm-shifting mechanisms enabled by defects, size effects, critical phenomena, anharmonicity, and the spin degree of freedom. These mechanisms embody the latest state of understanding and manipulating the interplay among charge, lattice, orbital, and spin degrees of freedom in TE materials. We use these mechanisms to guide the discussion of materials. Because of page limitations, the coverage of promising materials or synthesis and preparation techniques is purposely limited.

Identifying the correct causal chain is crucial in defect engineering, otherwise one risks getting the right result for the wrong reason. Taking the benchmark material Bi_2Te_3 as an example, doping Sb on the Bi site and Se on the Te site led to high p-type and n-type performance, respectively. The dopants (extrinsic point defects) first facilitate the formation of intrinsic point defects (antisites, interstitials, and vacancies), and then the intrinsic point defects directly determine the carrier concentration, thereby enhancing the material performance. Zhu *et al*. reviewed the role of intrinsic point defects in V_2VI_3 compounds and showed that intrinsic point defects could be manipulated compositionally, mechanically, and thermally. In particular, the electronegativity difference and the covalent radius difference between the cation and the anion effectively regulate the formation of cation antisites and anion vacancies. Intrinsic point defects are ubiquitous; a better understanding of intrinsic point defects and the interplay with other types of defects will enable more innovative defect engineering efforts.

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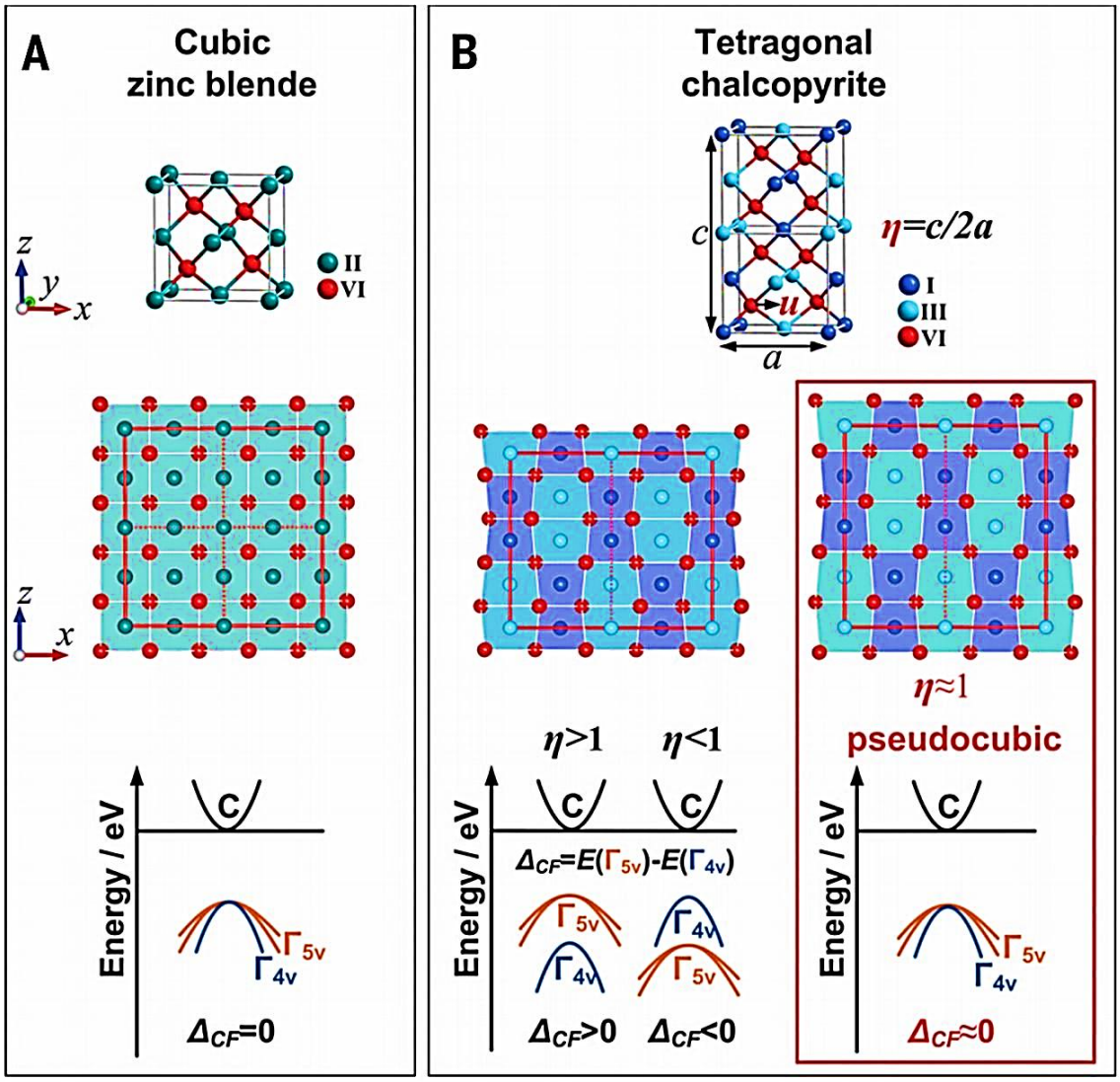

Fig. 2. The pseudocubic band-convergence scheme.

Conclusion

TE materials research is an application-driven fundamental research field bridging the disciplines of physics, chemistry, materials science, and mechanical engineering. High material performance builds on a delicate concert of hierarchical trade-offs, e.g., structural order and disorder, phase stability and instability, band convergence and splitting, effective mass and mobility, bond covalency, and ionicity. Although the TE materials research is application driven, it is the rich fundamental physics, chemistry, and materials science that actually drives the research. Today, emerging concepts such as topological states, the Rashba effect, the spin Seebeck effect, resonant levels, resonant bonding, and anharmonicity are keeping the field of TE materials research at the cutting edge of science.

After 60 years of fruitful work, the maximum *ZT* values have doubled, and, some might argue, essentially tripled. It may not sound that impressive, but in our opinion it is, given that a four-fold increase would have changed the renewable energy landscape. Thermoelectrics has specific technical advantages in distributed power generation and active spot-size heat management. Given the ubiquity of heat, thermoelectrics has secured a position in our total-package solution to global energy needs and environmental crisis. In the years to come, we expect scientists will look for more outliers of the current material-selection criteria; develop more high-performance TE materials out of nontoxic and earth-abundant elements; shift

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attention from power generation to refrigeration, as cooling is less cost-sensitive than power generation; and conduct high-throughput calculations and experiments in higher multinary compounds. Cross-checking the high *ZT* values of emerging materials by international round-robin studies is also crucial. The outcome of these efforts will shape the future of thermoelectrics over the next 20 years or more and, in turn, reshape the renewable energy landscape.

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