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Decoupled phononic-electronic transport in multi-phase *n*-type half-Heusler nanocomposites enabling efficient high temperature power generation

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Strongly coupled electronic and thermal transport behavior in thermoelectric (TE) materials has limited their figure of merit (zT). Here we provide breakthrough in decoupling TE parameters in *n*-type $(Hf_{0.6}Zr_{0.4})NiSn_{0.99}Sb_{0.01}$ half-Heusler (hH) alloys through multi-scale nanocomposite architecture comprising of tungsten nanoinclusions. The tungsten nanoparticles not only assist electron injection, thereby improving electrical conductivity, but also enhance the Seebeck coefficient through energy filtering effect. The microstructure comprises of disordered phases with varying size of microstructural features, which assists in effective scattering of heat-carrying phonons over diverse mean-free-path ranges. Cumulatively, these effects are shown to result in outstanding thermoelectric performance of $zT_{max} \sim 1.4$ at 773 K and $zT_{avg} \sim 0.93$ between 300 and 973 K. Using this material, a TE generator is demonstrated, which exhibits high power density of 13.93 W cm^{-2} and conversion efficiency of 10.7% under $\Delta T = 674$ K. The fundamental material design principle for TE nanocomposites demonstrated here can be generalized and extended to other TE systems.

Introduction

A rapid increase in global energy demand and greenhouse-gas emissions has turned the spotlight on energy efficiency and waste energy recovery. It is well-known [1–3] that a substantial portion (20–50%) of the energy is lost as waste heat, resulting in total loss of 5–13 quadrillion Btu/yr [4] across US industry. According to Forman's estimation, the fraction of work potential (Carnot potential) for global heat lost with hot-side temperature above 100 °C is 79% and more than 55% waste heat has medium to high hot-side temperature of >300 °C [5]. The Carnot efficiency of the system (theoretical maximum for converting thermal energy into useful work) increases with hot-side temperature. This indicates the importance of developing waste heat recovery mechanisms that can operate over wide temperature ranges and provide easy integration with variety of industrial processes. In this respect, thermoelectric (TE) energy harvesting is promising as it can provide wide temperature operation through cascading. Further TE modules provide solid-state noiseless operation which is relevant for generator applications.

Half-Heusler (hH) compounds are an important class of TE materials for moderate to high temperature applications due to their excellent mechanical strength and in-air thermal stability [6]. In particular, hH alloys have potential for mass-scale thermoelectric power generation where not only high output power

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 https://doi.org/10.1016/j.mattod.2020.01.002