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Strategies to Bulk Half-Heusler Nanocomposites with Simultaneously Enhanced Power Factor and Reduced Thermal Conductivity[1]

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Among promising thermoelectric materials for power generation, half-Heusler (HH) phases with general compositions TNiSn and TCoSb (T = Ti, Zr, Hf) have attracted tremendous attention not only because they involve abundant and environmentally friendly elements, but also due to their combination of large Seebeck coefficients with moderately low electrical resistivities. However, the ability to synthesize HH based materials with decent figures of merit (ZT>1) has been jeopardized by their very large thermal conductivities. Strategies to reduce the thermal conductivity of HH phases focusing on mass fluctuation phonon scattering via solid solution alloying or phonon scattering at grain boundaries and interfaces in HH phases with embedded pre-synthesized nanoparticles have failed to generate materials with high figures of merit due to simultaneous reductions in the power factor. Here, we introduce innovative approaches to revolutionary increases in the figure of merit of HH based materials through simultaneous large enhancement of the power factor and drastic reduction in the thermal conductivity. Our strategy is focused on atomic-scale structural engineering of the HH matrix through the confinement of full-Heusler (FH) inclusion phases on the lattice constant length-scale. Emphasis will be placed on the n-type $Zr_{0.25}Hf_{0.75}Ni_{1+x}Sn_{1-y}Pn_y$ and $Ti_{0.5}Zr_{0.5}Ni_{1+x}Sn_{1-y}Pn_y$ as well as the p-type $Ti_{0.5}Zr_{0.5}Co_{1+x}Pn_{1-y}Sn_y$, (Pn = Sb, Bi) nanocomposites. We will discuss the underlying mechanism for the formation of half-Heusler/full-Heusler (HH/FH) nanocomposites with coherent matrix/inclusion interfaces. The role of synthetic and processing methods; and size, dispersion and mole fraction of the FH inclusions on the thermoelectric performance of bulk HH/FH nanocomposites will be assessed by combining transmission electron microscopy studies with thermal and electronic charge transport data.

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