Role of defects in enhancing thermoelectric performance

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Abstract: Thermoelectric (TE) materials are capable of direct conversion of "waste" heat to electricity. Based on the Seebeck and Peltier effects, a thermoelectric module (consisting of *p*-type and *n*-type semiconductors) may be used for power generation and refrigeration applications, respectively. Power generation applications include Radioisotope Thermoelectric Generators (RTGs) by NASA in the deep space missions of the Voyager and the Cassini that supply electricity to the spacecraft. The efficiency of the state-of-the-art TE materials, however, needs to be further improved to maximize their performance over a broader range of temperature. The thermal-to-electrical energy conversion efficiency of a TE device is largely determined by the dimensionless figure-of-merit, $ZT = S^2\sigma T/\kappa$. The process of maximizing *ZT* involves the tuning of material parameters such as the Seebeck coefficient (*S*) and the electrical conductivity (σ) that exhibit an inversely-coupled relationship in most materials. We discuss the role of defects in enhancing the thermoelectric performance in two classic TE material systems, viz., PbTe and SnSe. Contrary to the general understanding about the detrimental effect of defects, the simultaneous incorporation of micro-, and nanostructures in a PbTe nanocube matrix enabled us to tune the grain boundary potential energy barrier that led to enhanced σ and *S* and a 10-fold increase in *ZT* compared to the host matrix. Furthermore, the effect of mass density on κ of SnSe and the role of 3D defects in enhancing *ZT* will be discussed.