Analysis of Advanced Thermoelectric Materials and Their Functional Limits

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The world’s demand for energy is increasing dramatically, but the best energy conversion systems operate at approximately 30% efficiency. One way to decrease energy loss is in the recovery of waste heat using thermoelectric (TE) generators. A TE generator is device that generates electricity by exploiting heat flow across a thermal gradient.

The efficiency of a TE material for power generation and cooling is determined by the dimensionless Figure of Merit (ZT): \( ZT = S^2\sigma T/\kappa \): where \( S \) is the Seebeck coefficient, \( \sigma \) is the electrical conductivity, \( T \) is the absolute temperature, and \( \kappa \) is the thermal conductivity. The parameters are not physically independent, but intrinsically coupled since they are a function of the transport properties of electrons. Traditional research on TE materials has focused on synthesizing bulk semiconductor-type materials that have low thermal conductivity and high electrical conductivity affording ZT values of 1. The optimization of the \( \sigma/\kappa \) ratio is difficult to achieve using current material formats, as these material constants are complementary.

Recent areas of research are focusing on using nanostructural artifacts that introduce specific dislocations and boundary conditions that scatter the phonons. This disrupts the physical link between thermal (phonon) and electrical (electron) transport. The result is that \( \kappa \) is decreased without decreasing \( \sigma \). These material formats give ZT values of up to 2 which represent approximately 18% energy gain from waste heat recovery.

The next challenge in developing the next generation of TE materials with superior performance is to tailor the interconnected thermoelectric physical parameters of the material system. In order to approach this problem, the fundamental physics of each parameter \( S, \sigma, \) and \( \kappa \) need to be physically understood in their context of electron/phonon interaction for the construction of new high ZT thermoelectric devices. Is it possible to overcome the physical limit imposed by of the effect of phonon lattice oscillation and energetic electrons towards thermal conductivity? Is the Seebeck coefficient, based on the difference in voltage over temperature gradient \( (\Delta V/\Delta T) \), an intrinsic parameter of each material? All these parameters were manipulated using nano-bridge and twin-lattice structural concepts at the NASA Langley Research Center. This talk will review the current trend of TE research to optimize the ZT and discuss about new approaches on increasing ZT within functional limits of each parameter.