Power Factor Degradation Mechanisms in Energy-Filtering Thermoelectric Materials

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The efficiency of a thermoelectric material is dictated by its figure-of-merit: $ZT = \sigma S^2/\ \kappa$, where the numerator, which is dependent on the conductivity (σ) and the Seebeck coefficient (S), is referred to as the power factor and the denominator is the thermal conductivity. The use of nano-scaled structures, be they voids, grains, inclusions or superlattices, have been shown effective at enhancing ZT through the reduction of the thermal conductivity, without overly hindering the conductivity. [1,2] However, enhancement of the power factor has proven more difficult, for the conductivity and the Seebeck are often inversely related. It has been argued, [3] that a superlattice structure, like that shown in Figure 1, could enhance the thermoelectric power factor and that optical phonon scattering in the space between potential barriers [4] could offer even further gains. Experimental demonstration of such enhancement has, unfortunately, been lacking.

In this talk the results of numerical quantum transport studies in one and two dimensional superlattices using the fully quantum mechanical Non-Equilibrium Green's Function (NEGF) method will be discussed. The effect of superlattice properties, such as potential barrier width, height, shape and random statistical variation in shape will be explored. It is found that although enhancement of the thermoelectric power factor can be obtained within a certain range of design parameters, a number of non-ideal effects can completely destroy any improvements. Thus, this sensitivity of power factor gains to statistical variation and non-optimal potential barrier shape could be a potential justification for the notable lack of experimental evidence in superlattice systems. Thus, this talk will provide guidance to experimental efforts as to which non-idealities are most detrimental to power factor gains. [5]

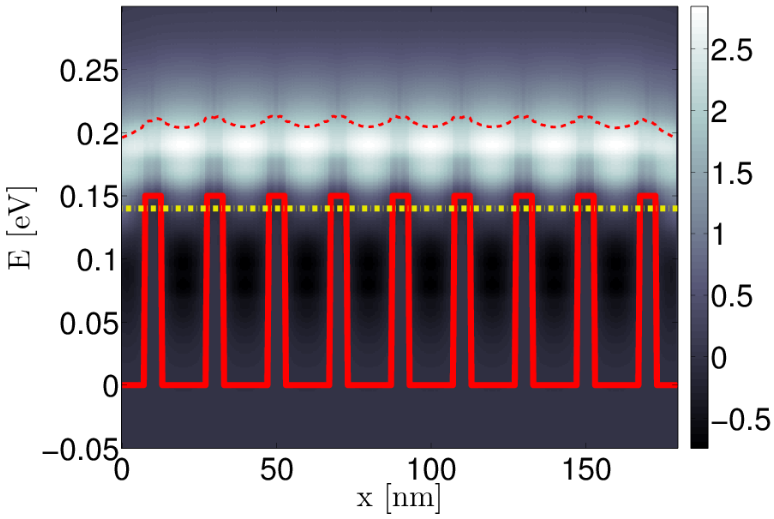

Fig1. Energy-resolved current vs. position within tyhe potential profile (solid red) of a superlattice system. The red dotted line refers to the average current energy and the yellow dotted line is the Fermi level.

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