Examining the Effectiveness of Energy-Filtering in 1D vs. 2D Structures Using Quantum Mechanical Transport Simulations.

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Abstract

The energy filtering of carriers has been proposed as a promising means of improving the power factor, and thus, enhancing the ZT, figure of merit, of thermoelectric materials. In this talk we will review recent work, based on large-scale simulations using the fully quantum mechanical, non-equilibrium Green's functions (NEGF) method with electron-phonon scattering, which explores the relative potential for power factor enhancement in one-dimensional (1D) vs. two-dimensional (2D) channels.

We will demonstrate that the van Hove singularity in 1D channels (which has been suggested by Hicks and Dresselhaus[1] to provide larger Seebeck coefficients) makes more effective use of the energy filtering mechanism[2] as well, whether with a single filtering barrier structure or with many (i.e. a superlattice). In the most extreme case the relative advantage of 1D in utilizing energy filtering can be up to a factor of 3 compared to filtering in 2D channels. We show how the van Hove singularity of the 1D density of states plays in forcing carriers to flow at lower energies as well as producing a shorter energy relaxation length and discuss how these features allow 1D structures to receive a greater benefit from filtering.

We will also discuss the scenario where the thermal conductivity of the barrier material is less than that of the bulk and the direct effect that has on the power factor. Again we find that, although the power factor in 1D and 2D is benefited from variations in the thermal conductivity along the channel, the 1D channel sees 50% more benefit.

Our results demonstrate the higher potential of 1D materials in utilizing energy filtering, and could be particularly helpful in the design of low- dimensional nano-composite thermoelectrics.

References:

[1] Hicks, L. D., and M. S. Dresselhaus. "Thermoelectric figure of merit of a one-dimensional conductor." Physical review B 47.24 (1993): 16631.
[2] Vashaee, Daryoosh, and Ali Shakouri. "Improved thermoelectric power factor in metal-based superlattices." physical review letters 92.10 (2004): 106103.