Calculating the power factor of nano-composite materials from fully quantum-mechanical large-scale simulations.

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Abstract

Nanostructuring of materials is commonly put forward as a means of improving thermoelectric efficiency above their bulk values. Such structures either act to scatter phonons, create quantum confinement effects or filter carrier energies to maximize the power factor [1]. Thus, their fundamental mechanism of enhancement is often quantum mechanical and non-equilibrium in nature. In addition, their nanoscale feature sizes lie in the regime where transport is neither totally diffusive, nor ballistic. Despite the fact that advanced simulation packages exist for phonon transport in these materials (mostly based on molecular dynamics), no such framework exists for electronic transport. In this work we present a non-equilibrium Green's function (NEGF) based simulation framework which captures all effects for electronic transport, from quantum mechanical to semiclassical, and from ballistic to diffusive, all within the same theoretical framework, and is tailored for 1D and 2D nanostructured geometries.

Such a solver allows for the inclusion of nanostructures of many different shapes and types, whether superlattices, nanovoids or more complex structures, and calculation of the energies of carriers, the Seebeck coefficient, charge densities and current anywhere within the channel. The ability to attain such thorough spatially resolved data from a non-equilibrium, two-dimensional, quantum mechanical channel allows for great insights into the nature of thermoelectric power factor enhancement in such systems.

Using this simulator, we will present example studies for the thermoelectric power factor in different geometries: superlattices [2], channels with nano-inclusions and other nano-engineered structures. We illustrate visualizations of the nature of carrier energy flow in such structures and discuss strategies for optimal power factor enhancement.

References:

[1] Snyder, G. Jeffrey, and Eric S. Toberer. "Complex thermoelectric materials." Nature materials 7.2 (2008): 105-114.
[2] Thesberg, M., Pourfath, M., Kosina, H., and Neophytou, N. (2015). The influence of non-idealities on the thermoelectric power factor of nanostructured superlattices. Journal of Applied Physics, 118(22), 224301.