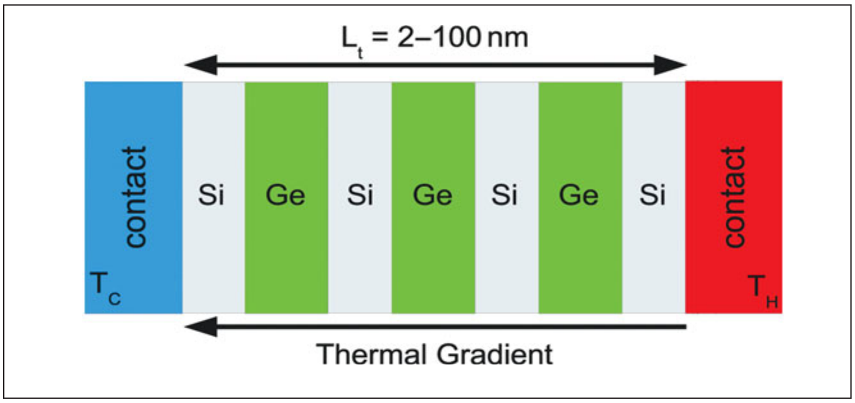
Nano Focus

Quantum model predicts thermoelectric figure of merit for superlattices

Thermoelectric devices could provide a new means for power generation by converting small thermal gradients into electricity. A proven method to increase the performance of bulk thermoelectric materials is through the incorporation of nanostructured superlattices, that is, periodic layers of two or more materials. Because layer composition, thickness, and doping affect the thermoelectric properties, a variety of parameters can be tuned to optimize device performance. It would be useful to have an accurate model that not only screens combinations of such parameters but also provides fundamental insights into the physics at hand. Terence Musho, professor of Mechanical and Aerospace Engineering at West Virginia University, has developed such a model to calculate the thermoelectric properties of superlattice devices. The work is published in a recent issue of the *Journal of Materials Research* (DOI: 10.1557/jmr.2015.256).

Thermoelectric properties arise from both electron and phonon contributions. The thermoelectric figure of merit, denoted *ZT*, describes both the thermal and electrical contributions to a thermoelectric system. The system's efficiency depends explicitly on its *ZT* value. "The novelty of the model is in calculating the full *ZT*," says Musho, the sole author of this work. "In much of the literature they're looking at enhancing one aspect, either the Seebeck coefficient or the electrical conductivity, or they're trying to decrease the thermal conductivity." In Musho's model, the problem is reduced to a single dimension of electron and phonon transport across the superlattice in order to calculate the full *ZT* for the system.

Musho's model is based on quantum mechanical descriptions of both electrons and phonons using a nonequilibrium Green's function. "One nice thing about using the nonequilibrium Green's function formalism is that it takes into account some of the wave effects of these species," says Jeffery Urban, Facility Director at the Molecular Foundry and Head of the Thermoelectrics Program at Lawrence Berkeley National Laboratory, who was not involved in this work. "Often in modeling thermoelectric devices, [phonons and electrons] are treated as particles. This model gets away from a strictly particle-based description, which is appealing particularly for these small feature sizes."



Schematic diagram of the thermoelectric device studied in this work to provide proof-of-concept validation for the combined phonon and electron quantum model. Source: *Journal of Materials Research*.

Because a quantum description is used, this model recovers contributions to *ZT* from quantum phenomena such as tunneling and electron confinement effects. To aid in reproducing such quantum effects, Musho's model calculates multiple phonon frequencies, rather than relying on the dominant phonon frequency. Calculating multiple phonon frequencies is important because electrons are scattered by phonons during transport. This phonon–electron interaction aids in generating electron tunneling through the layers, which in turn increases the electron conductivity of the system. "If you only have a single phonon frequency, you might underestimate the probability of the electron going through one of the layers. By having multiple phonons, you take into account that these electrons will have the required phonon to get through the thickness barrier," Musho says.

To demonstrate the proof of concept of his approach, Musho modeled a device consisting of alternating, nanosized layers of silicon and germanium. He calculated the Seebeck coefficient, electrical conductivity, thermal conductivity, and full *ZT* for a variety of devices of different layer thickness and doping concentrations. The values of his model along with those calculated using a simple ballistic model and a model using only a single phonon frequency were compared against experimental values found in the literature. Musho's model more closely matched experimental values, showing the importance of calculating multiple phonon frequencies, as well as using a quantum mechanical description to determine the thermoelectric properties of such devices.

This model represents a new method for designing high-performing thermoelectric devices. "The idea is to eventually apply this model in a high throughput fashion," Musho says. "In order to find the ideal material, first you need a good bulk material. On top of that you need to nanostructure. One of the advantages [of this model] is that you can account for this nanostructured effect." Because parameters such as layer thickness, doping, and temperature are included in the model, full devices can be engineered computationally, much in the same way of modern drug discovery.

Jenna Bilbrey