Electro-Thermal Transport, Thermoelectric Devices, and NEEDS

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Background and goals

Thermal transport has become almost as important as electronic transport for electronic devices. Device downscaling has taken us to the nanometer regime where it has become important to clearly understand and effectively model both electrical and thermal. While self-heating is detrimental for devices, coupled electro-thermal transport can be used to realize solid-state refrigerators and energy harvesters. Recent progress in thermoelectric devices has been driven by various schemes for nanostructuring materials to degrade heat flow without degrading electron flow. The goal of this work is to bring the approaches and tools that have been developed over the years to treat nanoscale electron transport to the field of thermal and coupled electro-thermal transport. The starting point was a theory of thermoelectric [1] and thermal transport [2] at the nanoscale based on the well-known Landauer approach to electron transport. During the NEEDS program, we have further developed this approach, and we have developed both physically detailed simulations and compact SPICE models for thermoelectric devices. The work is guided by close connections with experimental work.

What was accomplished?

As discussed in [1-3], the thermo-electric transport parameters, conductivity, Seebeck coefficient, and electronic thermal conductivity, can be computed from the following equations:

$$G = \int_{-\infty}^{+\infty} G'(E)\,dE \qquad S = -\frac{1}{qT}\int_{-\infty}^{+\infty}(E - E_F)G'(E)\,dE \Big/ \int_{-\infty}^{+\infty} G'(E)\,dE$$

$$K_0 = \frac{1}{q^2T}\int_{-\infty}^{+\infty}(E - E_F)^2 G'(E)\,dE \qquad K_e = K_0 - TGS^2$$

where the differential conductance,

$$G'(E) = q^2\Sigma(E)\left(-\frac{\partial f_0}{\partial E}\right)$$

is given in terms of the so-called transport distribution,

$$\Sigma(E) = \frac{2}{h}M(E)\mathcal{T}(E),$$

where $M(E)$ is the number of Landauer channels per cross-sectional area, and $\mathcal{T}(E)$ is the electron transmission across the structure. Similar expressions can be developed for the lattice thermal transport. Reference [1] gave a prescription for extracting $M(E)$ from a numerically computed band structure**.** The value of the Landauer approach is that it expresses thermal and electrothermal transport in a form that is widely-used to described electron transport from the nano to macroscale, so that one approach can be used to treat electron and phonon transport. It also provides a clear physical interpretation of the transport distribution – it is simply proportional to the product of the number of channels and the transmission. In our first project in the NEEDS program, MSEE student Kyle Conrad worked with post-doc, Dr. Jesse Maassen, to develop and document a tool, LANTRAP, which takes a full, numerically computed

bandstructure, extracts $M(E)$, and calculates thermoelectric transport parameters [4]. This tool facilitates "first-principles informed" analysis of thermoelectric transport. Right now, these types of calculations are done by a few experts. Our goal is to broaden the use of first-principles analyses by experimentalists and device designers.

Under the NEEDS program, we have also been developing simple approaches (suitable for analyzing experimental results or for designing devices) to treat ballistic and quasi-ballistic phonon transport. The "breakdown" of Fourier's Law at the nanoscale is discussed in hundreds of paper, but 30 years ago, it was discovered that Fick's Law of diffusion could be used to treat ballistic to diffusive electron transport across the thin base of a bipolar transistor – if the boundary conditions are properly specified. Drawing on this analogy, we have shown that a surprisingly large number of problems in one-dimensional nanoscale heat transport can be solved with Fourier's Law [5, 6]. Although still new, these approaches are beginning to find use in the heat transfer community.

The work described above is at the fundamental level. To address the charter that NEEDS has "to connect fundamental research to applications", we have also developed two device models for thermoelectric devices. The first uses Sentaurus, which is widely used in the electronics industry. The basic electro-thermal models in Sentaurus were extended so that simulations of devices with realistic, temperature material parameters, and Joule heating at contacts could be treated. At the same time, we developed a compact SPICE model for thermoelectric devices to model the performance of devices in realistic applications. While many such models exist, the NEEDS model is the first to include the so-called Thomson effect, which arises from the temperature-dependent Seebeck coefficient. It is also the first SPICE model to be benchmarked against a physically detailed model. As the figure below shows, the results of the Sentaurus simulations can be reproduced with much less computational expense using the compact model. The first version of the compact model was deployed by Kyle Conrad as part of his MSEE thesis [7]. More recently, a new version that is MAPP compatible and that follows the new guidelines for "simulation-ready compact models" has been deployed [8].

Why was it important?

Over the course of the NEEDS program we have developed new analysis techniques for thermal and electro-thermal transport at the nanoscale. These techniques provide a unified framework for modeling electron, phonon, and coupled electro-thermal transport from the nanoscale to the macroscale. We have also developed physically detailed and compact models for thermoelectric devices. We are currently working closely with two experimental teams – one led by Dr. Rama Venkatasubramanium at Johns Hopkins Applied Physics Lab and another led by Prof. Luna Lu at Purdue. As this work progresses, these partnerships will help us develop the tools that experimentalists need to analyze data and to design devices and systems. We plan to use nanoHUB cyberinfrastructure capabilities to deploy these models in a way that facilities easy access and use by experimentalists.

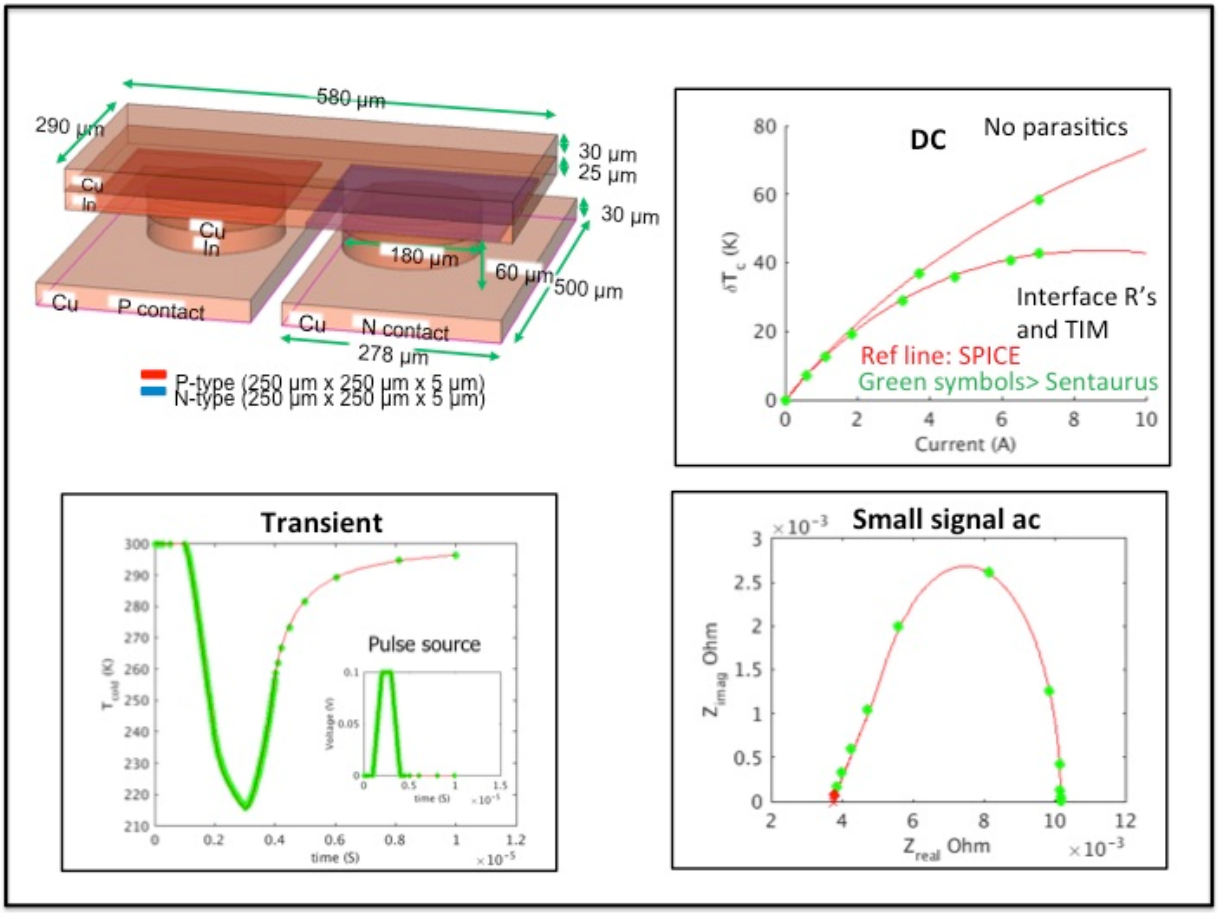

Figure 1. Comparison of Sentaurus thermoelectric device simulations with compact model results. Sentaurus simulations typically take 1-5 hours and the SPICE model simulation 1-10 minutes. **Upper left:** Device structure modeled after Bulman, Siivola, Shen, and Venkatasubramanian, "Large external Delta T and cooling power densities in thin-film Bi_2Te_3-superlattice thermoelectric cooling devices," *Appl. Phys. Lett*., 2006. **Upper right:** DC current vs.. temperature difference produced across the device. **Lower left**: Small signal simulation. **Lower right**: Transient response.

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