Special issue: electrothermal and thermoelectric modeling of nanoscale devices

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The purpose of this special issue is to describe modeling of *thermal effects* in semiconductor devices. Thermal effects can be separated into two different but related categories: (1) *Electrothermal effects*, which are related to Joule heating and become more prominent as we scale semiconductor devices into the nanometer scale (which ultimately is followed by 3D integration), and (2) *Thermoelectric effects*, that are related to the direct conversion of temperature differences to electric voltage and vice versa. Simply said, a thermo-electric device creates a voltage when there is a different temperature on each side, and when a voltage is applied to it, it creates a temperature difference. Both modeling of electrothermal effects and thermoelectric effects requires development of sophisticated simulation tools and expertise in both the theoretical formulation of the problem at hand and its numerical implementation. Below, we give a brief description of both electrothermal and thermoelectric effects and how they relate to the work presented in the papers that follow this short introduction in the field.

1 Electrothermal effects

Technology advancements have made it possible for feature sizes to shrink continuously. Interconnects, unlike transistors, have not followed the same trend. Thus, in state-of-the-art nanodevices, a larger portion of the total chip capacitance comes from interconnects. Furthermore, with the introduction of vias and repeaters to compensate for the performance

loss of long wires, the interconnect power consumption rises dramatically. 3D integrated circuits are one of the recently proposed approaches to overcome the problems associated with interconnects. This is due to the fact that when components are placed on a 3D architecture, the length of interconnects, and the large power consumption associated with them, is drastically reduced. However, 3D integration introduces challenges due to the high power density resulting from the placement of computational units on top of each other. High power densities are already a major concern in 2D circuits, and in 3D systems the problem is even more severe.

It is well known that self-heating limits the performance of semiconductor devices such as high power transistors, high electron mobility transistors (HEMTs), or CMOS transistors. The presence of thermal hot spots increases cooling costs, negatively impacts reliability, and degrades performance. Hot spots also accelerate failure mechanisms such as electromigration, stress migration, and dielectric breakdown, which then cause permanent device failures. Also, it is important to point out that the leakage is exponentially related to the temperature, so that an incremental feedback-loop exists between temperature and leakage, which can cause dramatic increases in temperature and damage the circuit if left uncontrolled. High temperatures also adversely affect performance, as the effective operating speed of devices decreases as temperature increases.

Thermal management has become a crucial part of designing modern microelectronic components. Only after a careful study of thermal effects, we can predict their performance, reliability and yield. In integrated circuits, thermal management is important at all levels, starting from the transistor level, over the chip level, the package level, and the printed circuit board (PCB) level, to the system level. Self-heating of transistors changes their electric properties and this can affect the circuitry.

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Within the semiclassical limits, the most accurate way of addressing the problem of self-heating in nanoscale devices is by solving self-consistently the electron and the phonon Boltzmann transport equations (see paper 1 below by Jerome Saint Martin, Philippe Dollfus and T.T. Trang Nghiêm). Multi-scale modeling (not presented here) is a way of bridging the differences in the length-scales of electron charge transport and phonon heat conduction to include the effect of interconnects.

2 Thermoelectric effects

Traditionally, the term *thermoelectric effect* or *thermoelectricity* encompasses three separately identified but closely related effects: the Seebeck, Peltier, and Thomson effects. The Peltier and Seebeck effects are the most basic of the three and are essentially the inverses of one another, so that the thermoelectric effect may also be called the Peltier–Seebeck effect.

Thermoelectric materials take advantage of the coupling between thermal and electrical currents, and are used for the direct conversion between thermal (heat) and electrical energy. With these materials, electricity can be used to pump heat (thermoelectric coolers) or waste heat can be used to generate electricity (thermoelectric generators).

The ideal thermoelectric material is one which is an “Electron Crystal - Phonon Glass”, where high-mobility electrons are free to transport charge and heat but the phonons are disrupted at the atomic scale. Semiconductor materials exhibit highest conversion efficiency, which makes them the primary choice for thermoelectric applications. Si-based nanowires and nanoribbons have enhanced thermoelectric figure of merit and can be used for thermoelectric refrigeration in integrated circuits. SOI nano-membranes and membrane-based nanowires and ribbons can be used as efficient thermoelectrics.

The efficiency of thermoelectric devices is determined by the dimensionless figure of merit of the material ZT that quantifies the ability of a material to convert heat into electricity. The ZT figure of merit is calculated as $ZT = \sigma S^2 T / (\kappa_e + \kappa_l)$, where σ is the electrical conductivity, S is the Seebeck (thermo-power) coefficient, and κ_e and κ_l are the electronic and the lattice contributions to the thermal conductivity, respectively. The larger the value of ZT , the better is the thermoelectric efficiency of the material/structure under investigation. A material with a large thermoelectric power

factor and, therefore, ZT , needs to have a large Seebeck coefficient (found in low carrier concentration semiconductors or insulators) and a large electrical conductivity (found in high carrier concentration metals). Therefore, the thermoelectric power factor σS^2 is maximized somewhere between a metal and semiconductors. Good thermoelectric materials are typically heavily-doped semiconductors with carrier concentration of 10^{19} to 10^{21} carriers/cm³. To ensure that the net Seebeck effect is large, there should be only a single type of carrier. Mixed n-type and p-type conduction will lead to an opposing Seebeck effect and low thermopower (defined as the absolute value of the Seebeck coefficient).

A good thermoelectric material also needs to have low thermal conductivity. Thermal conductivity in such materials comes from two sources of heat transport. Phonons travelling through the crystal transport heat and lead to lattice thermal conductivity. The electrons (or holes) also transport heat and lead to the electronic contribution to the thermal conductivity. The electronic term is related to the electrical conductivity through the Wiedeman-Franz law $\kappa_E = L\sigma T$, where L is the Lorenz factor. Thus, the best option to enhance ZT is to minimize the lattice thermal conductivity. This can be done by increasing phonon scattering by introducing heavy atoms, disorder, large unit cells, clusters and rattling atoms, etc.

For a very long time, the thermoelectric figure of merit ZT has been constrained to a value of $ZT \sim 1$ or below. With the revolution of nanostructures, large improvements in the ZT (up to values of $ZT \sim 2.2$) have been demonstrated. Much of this enhancement is due to a large reduction of the thermal conductivity (the lattice part of the thermal conductivity) compared to bulk materials. However, the benefits obtained from reducing the thermal conductivity are reaching their limits, and further increase of ZT can only be achieved through improvements of the power factor σS^2 . (paper 2 by Neophytos Neophytou and Mischa Thesberg)

According to early work of Hicks and Dresselhaus, there is the possibility of improving ZT when moving from higher to lower dimensional materials using the change of the shape of the density-of-states function. They concluded that the sharp features in reduced-dimensional materials provide energy-filtering and push the electron energies upward relative to their bulk counterparts. This results in enhanced thermopower. (paper 3 by Adithya Kommini and Zlatan Aksamija)

As a final note, we again want to use the opportunity to thank the three research groups that contributed excellent papers to this special issue.