Electro-Thermal Transport in Silicon and Carbon Nanotube Devices

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Summary. This work examines electro-thermal transport in silicon devices and in single-wall carbon nanotubes (SWNTs). Non-local transport is found to strongly affect heat generation in quasi-ballistic silicon devices. Under such conditions, Joule heat is mainly dissipated in the drain region, and increasing power densities may lead to phonon non-equilibrium. Significant current degradation is observed in suspended SWNTs, which is attributed to the presence of hot optical phonons and to a decrease in thermal conductivity (as ~$1/T$) at high temperature (T) under self-heating. The high temperature thermal conductivity can then be extracted by using the high bias characteristics of suspended SWNTs.

1 Introduction

Sharply increasing power densities are often considered the ultimate roadblock for the continued evolution of nanoscale electronics. As the dimensions and voltage of semiconductor devices are down-scaled linearly, the volume and area available for heat dissipation decrease cubically and quadratically. Three-dimensional integration and incorporating materials with lower thermal conductivities than silicon are accelerating such trends, while the thermal boundary resistance between materials also plays a role for designs with large surface-area-to-volume ratio [1]. Confined geometry devices (i.e. FinFET, ultra-thin body SOI, surround gate FETs, nanowires) will further limit the heat dissipation volume, leading to increased temperatures and the associated negative consequences on performance and reliability. Even carbon nanotubes, which have been shown to possess very high thermal conductivity [2], suffer from small thermal *conductance* owing to their small diameter. This combination may also yield power dissipation and self-heating issues under high bias current flow.

In this work, we examine the consequences of self-heating with emphasis on non-equilibrium effects in two types of nanometer scale devices. First, we describe Monte Carlo (MC) simulations which have been used to compute heat generation in bulk and strained silicon devices. We find that Joule heating occurs primarily in the drain of short devices when transport across the channel is quasi-ballistic. We show that non-equilibrium optical phonon (OP) effects may be important at power densities greater than 10^{12} W/cm^3, a range attainable in silicon devices with channel lengths below 20 nm under the current Technology Roadmap (ITRS) guidelines [3]. Second, we investigate electro-thermal transport in freely suspended single-wall carbon nanotubes (SWNTs), which represent the worst-case scenario of self-heating under high current flow. We find that the high bias electrical characteristics of suspended SWNTs exhibit Negative Differential Conductance (NDC) owed to non-equilibrium OPs and a decrease in thermal conductivity as ~1/*T* at high temperatures ($T > 400$ K).

2 Joule Heating in Bulk and Strained Silicon Devices

The physical mechanism through which self-heating occurs in silicon is that of electron scattering with phonons, and thus only a simulation approach which deliberately incorporates all such scattering events can capture the microscopic, detailed picture. We have studied heat generation using special-purpose Monte Carlo (MC) simulations. The conduction band is modeled with the analytic nonparabolic approximation, and each phonon mode is reproduced with a quadratic dispersion [4]. The heat generation rate is computed as a sum of all phonon emission events minus all phonon absorption events. Hence, complete phonon generation spectra can be obtained both for bulk silicon samples (e.g., as a function of electric field) and in various device geometries [5]. In particular we find that the heat

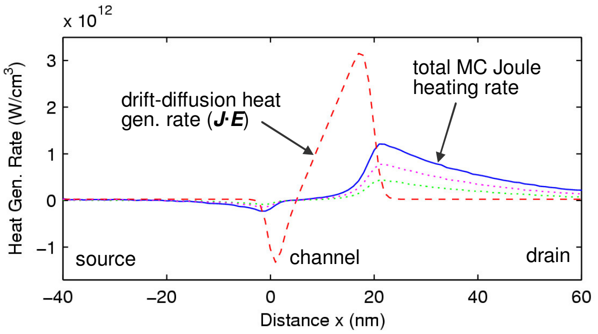

Fig. 1: Heat generation in a n+/n/n+ quasi-ballistic device with channel length *L* = 20 nm. The source and drain are doped to 10^{20} cm^{-3}, the applied voltage is 0.6 V. Unlike the classical (drift-diffusion) result, the MC simulation shows that heat is dissipated far into the device drain. The dotted lines represent the optical phonon (upper) and acoustic phonon (lower) heat generation profiles from the MC result.

generation region extends far into the drain of nanoscale devices (Fig. 1), since transport along the channel is quasi-ballistic. By contrast, the classical drift-diffusion approach is inadequate for computing heat generation within such scaled device geometries due to the highly non-local nature of transport. At the very least the hydrodynamic (carrier temperature dependent) approach ought to be used for calculating the location and magnitude of the heat generation term in TCAD device simulations [6].

In addition, we find that optical phonons (OPs) account for nearly two thirds of the heat generation in bulk silicon at most applied electric fields, and in strained silicon at high electric fields [4]. Dissipation with the acoustic phonon (AC) modes accounts for the remaining one third. This observation contradicts the long-held (simplifying) assumption that heat dissipation occurs predominantly with the OP modes [7]. Nevertheless we find that significant non-equilibrium OP populations may build up, particularly for the *g*-type longitudinal optical (LO) mode. The generation rates for the other phonon modes are either smaller or their density of states (DOS) is larger (the DOS is proportional to the square of the phonon wave vector, which is largest at the edge of the Brillouin zone) and non-equilibrium effects are less significant. Assuming a 10 ps phonon lifetime [8] we find the occupation number of the *g*-type LO phonon to exceed $N_{LO} > 0.1$ and become comparable to unity for power densities greater than 10^{12} W/cm^3 [5]. Such power densities are attainable in the drain of 20 nm (or shorter) channel length devices at operating voltages from the current ITRS guidelines (Fig. 1). Non-equilibrium phonon populations will increase electron scattering in the drain, leading (at the very least) to a magnification of the drain series resistance. The full ramifications of such behavior are still under investigation.

3 Electro-Thermal Transport in Suspended SWNTs

We have also recently explored electro-thermal transport in metallic single-wall carbon nanotubes (SWNTs). While such nanotubes on substrates are known to exhibit very high (> 20 μA) current-carrying capability, we have found that freely *suspended* nanotubes carry much lower currents due to significant self-heating. The suspended nanotube resistance at high bias in Fig. 2 is greater than expected near $T \sim 800$ K (the burning temperature of SWNTs in air), suggesting a lower lattice temperature and a higher non-equilibrium, hot OP population [9]. This observation is consistent with recent studies indicating much longer phonon lifetimes in suspended SWNTs [10]. This is attributed to the lack of intimate coupling with a substrate, which would otherwise provide additional phonon relaxation channels. We

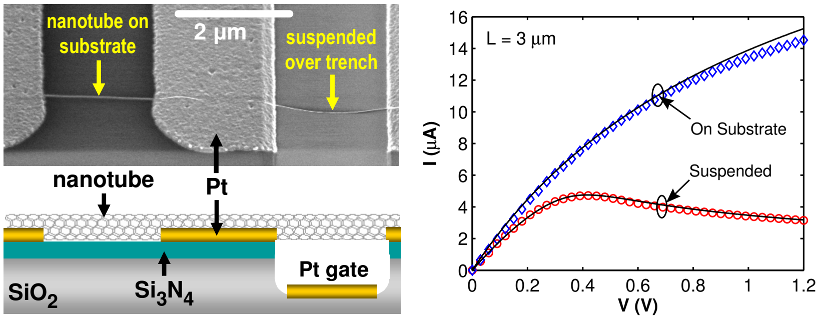

Fig. 2: SEM (top left) and diagram (bottom left) of a metallic SWNT with one portion grown across a substrate, the other suspended across a trench. The measured (symbols) and calculated (lines) *I-V* characteristics of the two nanotube segments are also plotted for a similar device with *L*~3 µm and *d*~2.4 nm (right) [9].

also observe Negative Differential Conductance (NDC) in our longest (10 µm) suspended SWNTs at much lower electric fields (~200 V/cm) than predicted by previous theoretical models which assume isothermal conditions (~5 kV/cm) [11]. This also indicates that the observed NDC is a thermal and not electrical (e.g. contact or field-related) effect.

A simple two-temperature (acoustic and optical) model is used to calculate the theoretical *I-V* characteristics (solid lines) in Fig. 2 [9]. The optical phonons are assumed to be stationary, and the acoustic phonons are solely responsible for thermal transport. The approach self-consistently computes the nanotube resistance, Joule heating and temperature along its length. A key feature is the temperature dependence of the SWNT thermal conductivity, which is found to be essential for reproducing the high bias behavior of the electrical characteristics. The ~1/*V* shape of the suspended SWNT *I-V* characteristics at high bias is found to be a reflection of the ~1/*T* dependence of the thermal conductivity at high temperatures due to Umklapp phonon scattering. This provides an indirect way to measure the thermal conductivity (k) of individual suspended SWNTs in the high temperature regime, and we find that $k \sim 3600(300/T)$ Wm^{-1}K^{-1} from $400 < T < 700$ K. This value is sensibly consistent with other recent measurements of the SWNT thermal conductivity [2].

4 Conclusions

This work briefly describes recent advances in the understanding of electro-thermal transport in nanoscale silicon devices and carbon nanotubes. Non-local transport is shown to strongly affect heat generation in quasi-ballistic silicon devices. Non-equilibrium phonon populations affect transport in suspended carbon nanotubes, which do not benefit from an intimate vibrational and thermal coupling with a substrate. A signature of the temperature dependence of the SWNT thermal conductivity ($\sim 1/T$ at high T) is observed in the measured high-bias current-voltage curves ($I \sim 1/V$). Aside from their fundamental importance, the "extreme" cases studied here may suggest ideas for the optimization of future nano-electronics (from SOI to nanotubes) through geometry, interface and materials design from an electro-thermal point of view.

References

1. E. Pop, C. O. Chui, S. Sinha, R. W. Dutton and K. E. Goodson, "Electro-thermal comparison and performance optimization of thin-body SOI and GOI MOSFETs," *Proc. IEDM*, p. 411, San Francisco CA (2004).
2. C. Yu, L. Shi, Z. Yao, D. Li and A. Majumdar, "Thermal conductance and thermopower of an individual single-wall carbon nanotube," *Nano Letters* **5**, 1842 (2005).
3. International Technology Roadmap for Semiconductors (ITRS). Online at http://public.itrs.net
4. E. Pop, R. W. Dutton and K. E. Goodson, "Monte Carlo simulation of Joule heating in bulk and strained silicon," *Appl. Phys. Lett*. **86**, 82101 (2005).
5. E. Pop, J. Rowlette, R. W. Dutton and K. E. Goodson, "Joule heating under quasi-ballistic transport conditions in bulk and strained silicon devices," *IEEE SISPAD*, Tokyo Japan (2005).
6. J.-H. Chun, B. Kim, Y. Liu, O. Tornblad, and R. W. Dutton, "Electro-thermal simulations of nanoscale transistors with optical and acoustic phonon heat conduction," *IEEE SISPAD*, Tokyo Japan (2005).
7. J. Lai and A. Majumdar, "Concurrent thermal and electrical modeling of sub-micrometer silicon devices," *J. Appl. Phys.* **79**, 7353 (1996).
8. S. Sinha, E. Pop and K. E. Goodson, "A split-flux model for phonon transport near hotspots," *Proc. IMECE*, Anaheim CA (2004) and *J. Heat Transfer* in press (2005).
9. E. Pop, D. Mann, J. Cao, Q. Wang, K. E. Goodson and H. Dai, "Negative differential conductance and hot phonons in suspended nanotube molecular wires," *Phys. Rev. Lett.* **95**, 155505 (2005).
10. B. J. LeRoy, S. G. Lemay, J. Kong and C. Dekker, "Electrical generation and absorption of phonons in carbon nanotubes," *Nature* **432**, 371 (2004).
11. V. Perebeinos, J. Tersoff and P. Avouris, "Electron-phonon interaction and transport in semiconducting carbon nanotubes," *Phys. Rev. Lett.* **94**, 086802 (2005).