Towards atomistic simulations of the electro-thermal properties of nanowire transistors

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Abstract—In this paper, the electronic and thermal properties of ultra-scaled nanowire transistors are investigated using a single, atomistic, quantum transport simulator based on the Nonequilibrium Green’s Function (NEGF) formalism and the tight-binding and valence force field methods to accurately describe the electron and phonon population, respectively. Although the length of the considered device structures does not exceed a few nanometers, dissipative scattering mechanisms such as electron-phonon and anharmonic phonon-phonon scattering still play an important role and should therefore be fully taken into account by the modeling approach. Hence, it will be shown here that these two effects strongly affect the performance of nanowire transistors, either by decreasing (backscattering) or increasing (opening of additional propagation channels) the electrical and thermal currents flowing through them.

Introduction

Heat dissipation and power consumption in integrated circuits (ICs) are becoming two major issues that the semiconductor industry has to deal with, especially now that the transistor size does not exceed a few nanometers and billions of devices are packed on a small area [1]. Multi-gate, three-dimensional transistor structures, as recently introduced by Intel [2], consume less power than their planar, single-gate counterparts, due to a better electrostatic control, a reduced sub-threshold slope, and therefore an increase (decrease) of the ON-(OFF-)current at constant supply voltage. However, FinFET-like devices might suffer from reduced thermal conductivity, being thus more difficult to cool down [3].

Device simulation can help reduce heat generation and manage power dissipation in nanostructures, provided that a computer aided design (CAD) tool containing the right physics is available. Drift-diffusion solvers, as widely used in industry and academia, and the Boltzmann Transport Equation solved with Monte Carlo approaches allow for coupled electro-thermal device simulations, but they are (semi-)classical and continuous approaches that lack of predictability at the nanometer scale where atomic fitting, energy quantization, geometrical confinement, and quantum mechanical tunneling play an important role.

Taking power dissipation into account while simulating nanoscale transistors requires a quantum transport approach going beyond the ballistic limit of transport. To deliver accurate electro-thermal results the electron and phonon populations must be simultaneously driven out-of-equilibrium and the energy exchange between them carefully described. However, coupling electro-thermal transport at a quantum mechanical level and within a full-band and atomistic simulation approach represents a real computational challenge. In this paper, the basic steps to achieve this goal in nanowires will be presented, first through the inclusion of electron-phonon scattering in a tight-binding basis, then through the consideration of anharmonic phonon decay in thermal simulations.

Approach

As CAD tool, a three-dimensional quantum transport simulator that self-consistently solves the Schrödinger and Poisson equations with open boundary conditions is employed [4]. It is based on different flavors of the nearest-neighbor tight-binding model (single-s, sp^3, sp^3d^5s^*, sp^3d^5s^*^, p_z, · · · ) to treat electrons [5], on a modified valence-force-field (VFF) method going beyond the Keating model to describe phonons and deal with thermal transport [6], and on the popular Nonequilibrium Green’s Function (NEGF) formalism to solve the Schrödinger equation for electrons

\[
\left\{\begin{array}{ll}
(E - H - \Sigma^{RB} - \Sigma^{RS}) \cdot G = I \\
G = G^R \cdot \left(\Sigma^{\bar{R}} + \Sigma^{\bar{S}}\right) \cdot G^A
\end{array}\right.\]

(1)

and for phonons

\[
\left\{\begin{array}{ll}
(\omega^2 - \Phi - \Pi^{RB} - \Pi^{RS}) \cdot D = I \\
D = D^R \cdot \left(\Pi^{\bar{R}} + \Pi^{\bar{S}}\right) \cdot D^A.
\end{array}\right.\]

(2)

In Eq. (1) and (2), \(G \ (D)\) refer to the electron (phonon) Green’s Functions, \(\Sigma \ (\Pi)\) to the corresponding self-energy, the index \(B\) stands for boundary and \(S\) for scattering. The main differences between the electron and phonon Green’s Function equations reside in the facts that the tight-binding Hamiltonian matrix \(H\) is replaced by a dynamical matrix \(\Psi\) constructed in the VFF models and that the electron energy \(E\) is replaced by the squared phonon frequency \(\omega^2\). Otherwise, exactly the same approach, usually a recursive Green’s Function (RGF) algorithm, can be used to solve both equations.

As indicated by the index \(S\) in the self-energies \(\Sigma^S\) and \(\Pi^S\), the CAD tool can go beyond the ballistic limit of transport and include different types of dissipative scattering. The electron-phonon scattering self-energy, for example, takes the following simplified forms [7]

\[
\Sigma^S(E) \approx \int d\omega’ |M_{e-ph}|^2 G(E - h\omega') \cdot D(\omega')
\]

(3)

\[
\Pi^S(\omega) \approx \int dE’ |M_{e-ph}|^2 G(E’ - \omega) \cdot G(E’)
\]

(4)

where it appears that the electron and phonon Green’s Functions are coupled to each other. Self-consistently solving Eq. (1) and (2) with (3) and (4) automatically accounts for heat dissipation and other self-heating effects, but is computationally very intensive. Hence, the electron and phonon equations...
Finally, the phonon scattering limited low field mobility $\mu_{\text{hole}}$ is obtained. This approach is known as the "dR/dL" method [10].

The holly grail in atomistic device modeling consists in solving either Eq. (1) to (3) or Eq. (2) and (5). This is out of the scope of this paper which focuses on solving either Eq. (1) to (3) or Eq. (2) and (5).

Results

The goal of this paper is to investigate the performance of gate-all-around nanowire transistors as depicted in Fig. 1 not only from an electrical, but also a thermal perspective. Apart from the current characteristics and the electron-(hole-)phonon scattering limited mobility of these nanowires, their thermal conductivity will be analyzed in the presence of anharmonic phonon-phonon scattering, indicating how efficiently heat can be removed from their active region.

The typical transfer characteristics of a Si nanowire field-effect transistor (FET) [7] and band-to-band tunneling transistor (TFET) [9] are given in Fig. 2. The presence of electron-phonon scattering produces different effects in both cases: in FETs, the current magnitude is decreased through the backscattering of electrons when phonons are emitted, while in TFETs, phonon-assisted tunneling processes increase the electron current, especially in indirect band gap semiconductors. There is another difference at the energy level: electrons usually loose energy when they emit phonons in FETs, but they can also gain energy in TFETs by absorbing phonons when the device is close to its OFF-state, as illustrated in Fig. 3. If only Eq. (1) to (3) are solved and not Eq. (4), the phonon population remains at equilibrium and the formation of hot spots or the local cooling of the crystal temperatures are not captured by the simulation approach.

The influence of phonon scattering on the performance of the nanowire FETs in Fig. 1 can be more precisely quantified by calculating their electron and hole phonon-limited mobility. To do that, nanowires with different lengths $L$ are simulated and the resulting channel resistance $R(L)$ extracted. Since transport is diffusive in these devices, $R$ increases linearly with $L$ so that the resistivity $\rho=\frac{dR}{dL}$, which is equal to the derivative of $R$ with respect to $L$, can be calculated. Finally, the phonon scattering limited low field mobility $\mu_{\text{ph}}$ is obtained. This approach is known as the “dR/dL” method [10]. Results are reported in Fig. 4 [10]. The transport direction that offers the best compromise between a high electron and hole mobility is $<110>$, $<100>$ performing badly for holes and $<111>$ for electrons. Hence, $<110>$-oriented nanowires are expected to deliver a higher ON-current at a given OFF-current in long channel devices.

To draw the whole picture, the thermal properties of the same nanowires should be considered now. After calibrating the anharmonic phonon decay so that it can reproduce the bulk lattice thermal conductivity of Si over a large range of temperatures (see Fig. 5(a)), the thermal current that flows through ultra-scaled nanowires with a small temperature difference across them can be computed. Results are plotted in Fig. 5(b) and compared to ballistic transport simulations, which significantly overestimate the currents at temperatures exceeding 200 K.

Applying the same “dR/dL” procedure as for electrons [10], the diffusive thermal currents flowing through nanowires of different lengths are simulated, the corresponding thermal resistance extracted, and finally the thermal conductivity calculated. The results are shown in Fig. 6 and summarized in Fig. 7. It turns out that the $<110>$-oriented Si nanowire does not only provide the best electrical characteristics, but also the highest thermal conductivity, which makes it a very promising candidate as next-generation ultra-scaled field-effect transistor.

Conclusion

To analyze the performance of nano-scale transistors, it is necessary to go beyond the realm of ON/OFF current ratios and also look at thermal properties. Here, a first step in this direction is demonstrated with the electronic and thermal properties of nanowires treated independently. Next, as already mentioned in the Approach Section, the electron and phonon populations should be self-consistently coupled to improve the quality of the results.

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References

Fig. 1. (a) Schematic view of a gate-all-around nanowire (GAA NW) transistor with a gate length $L_g$. The transport direction $x$ is aligned with the $<100>$, $<110>$, and $<111>$ crystal axis corresponding to the cross section shown in subplot (b), (c), and (d), respectively. The $y$ and $z$ axis are directions of confinement. All the devices considered in this paper are made of Si and have a diameter $d=3$ nm.

Fig. 2. (a) Transfer characteristics $I_d$-$V_{gs}$ of a $n$-type Si GAA NW field-effect transistor at $V_{ds}=0.6$ V with $L_g=15$ nm, a source and drain doping concentration $N_D=1e20$ cm$^{-3}$, with (solid line with circles) and without (dashed gray line) electron-phonon scattering. The left y-axis is on a logarithmic scale, the right one on a linear scale. (b) Same as (a), but for a Si band-to-band tunneling transistor (TFET) at $V_{gs}=1$ V. The gate length $L_g$ is set to 15 nm, the $p$-type ($n$-type) doping concentration in the source (drain) amounts to $N_A=2e20$ cm$^{-3}$ ($N_D=1e20$ cm$^{-3}$), and the channel is intrinsic.

Fig. 3. (a) Spectral current of a $<110>$-oriented Si GAA NW transistor with $L_g=15$ nm at $V_{ds}=V_{gs}=0.6$ V. Dark regions indicates high current concentrations. The dashed line represents the conduction band edge. It can be seen that electrons lose energy while flowing from the source to the drain of the transistor. (b) Spectral current of the TFET in Fig. 2(b) at $V_{gs}=0$ V and $V_{ds}=1$ V close to the source-channel interface. The conduction and valence band edges are reported. Due to phonon absorption, electrons can gain energy and flow from source to channel although the transistor is in its OFF-state.
Fig. 4. Phonon-limited $\mu_{ph}$ (a) and effective mobility $\mu_{eff}$ (b) of electrons in Si nanowire transistors with $L_D=15$ nm as function of the electron concentration and extracted with the $dR/dL$ method [11] after a self-consistent quantum transport simulation. The lines with circles refer to $<100>$-oriented nanowires, the lines with stars to $<110>$, and the dashed lines with triangles to $<111>$. Subplots (c) and (d) are the same as (a) and (b), respectively, but for holes.

Fig. 5. (a) Si bulk thermal conductivity as measured experimentally (dashed line) and simulated with a valence force field model including anharmonic phonon decay (phonon-phonon scattering), boundary, and impurity scattering (solid line with stars). (b) Thermal current flowing through 40nm-long Si nanowires as function of the temperature and transport direction with (solid lines) and without (dashed gray lines) anharmonic phonon decay.

Fig. 6. Anharmonic phonon decay limited lattice thermal conductivity $\kappa_{th}$ of Si nanowires with $<100>$ (solid line with circles) and $<110>$ (dashed line with crosses) as transport directions as function of the temperature. The conductivities are computed with the $dR/dL$ method [11].

Fig. 7. Phonon limited ($\mu_{ph}$) and effective ($\mu_{eff}$) electron and hole mobility at a given electron and hole carrier concentration as well as anharmonic phonon decay limited thermal conductivity $\kappa_{th}$ at room temperature in Si nanowires with $<100>$, $<110>$, and $<111>$ as transport directions.