Electrothermal simulation of ultra-scale MOSEFT

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***Abstract*— To investigate self-heating effects in double gate MOSFETs, a simulator solving self-consistently the Boltzmann transport equations (BTE) for both electrons and phonons has been developed. A Monte Carlo (MC) solver for electrons is coupled with a direct solver for the phonon transport. This method is particularly efficient to evaluate accurately the phonon emission and absorption spectra in both real and energy spaces. The resulting degradation of the I-V characteristics is estimated for a 20 nm-long Double-Gate MOSFET.**

***Keywords*— Keywords: phonon, electron, Boltzmann, Transport Equation, Silicon, MOS, DGMOS, transistors, self-heating.**

I. INTRODUCTION

Heat conduction/dissipation and self-heating effects are taking an increasing place in the design of solid-state devices and circuits. The mean free path (MFP) of phonons, the pseudo-particles associated with the lattice vibrations, is typically estimated to be 300 nm at room temperature in silicon [1]. On distance scales larger than the MFP, the phonon system remains close to thermal equilibrium and may be well described by the classical Fourier heat equation. However, in modern electronic devices the length of the active region is in the order of a few tens of nanometers and in the presence of a perturbation, phonon scattering events are too rare for the system to recover local thermodynamic equilibrium. Thus, in such devices the use of a macroscopic description of thermal transport as the Fourier heat equation is questionable. In this case, the phonon Boltzmann transport equation (pBTE) is much more relevant.

To capture out-of-equilibrium thermal phenomena, the Vasileska and Goodnick group solved the energy balance equations of thermal transport to describe the optical phonon bottleneck in ultra-short transistors[2] . Kamakura et al. have implemented a MC method to solve the BTE for both electrons and phonons for 1D Si diodes with simplified phonon scattering rates but this approach has not been extended to transistors yet [3]. Ni et al. have used the phonon generation spectrum extracted from eMC simulation as input for a pBTE solver with anisotropic relaxation times and Brillouin zone to evaluate the hotspot temperature in a MOSFET[4].

In this paper, we describe and make use of a computationally efficient approach to solving deterministically the steady-state 1D pBTE within the relaxation time approximation (RTA). This phonon transport solver has been self-consistently coupled to an eMC device simulation to study the electro-thermal effects in nanoelectronic devices. This model provides deep insight into the out-of-equilibrium phonon effects in small devices.

II. THERMAL SIMULATOR

A. Phonon dispersion

The phonon dispersion in silicon is composed of six phonon modes, i.e. two transverse acoustic (TA), one longitudinal acoustic (LA) acoustic, two transverse optical (TO) and one longitudinal optical (LO) modes. In this work, the TA and TO modes have been considered to be degenerate. As suggested in Ref. [5], the dispersion relation for each mode *s* has been assumed to follow an analytic and quadratic expression of the form

$$\omega_s(q) = \omega_{0,s} + v_{g,s}\, q + a_s\, q^2 \tag{1}$$

where q is the modulus of the phonon wave vector $\vec{q}$.

B. Thermal transport equation

Since the out-of-equilibrium character of phonon transport may be significant in nano-devices, the use of the Boltzmann transport formalism to study the heat diffusion is particularly relevant. The drift term is absent from the Boltzmann transport equation for phonons (pBTE), the steady-state form of which can be written for each mode *s* as

$$\vec{v}_{g,s}(\vec{q}).\vec{\nabla}_{\vec{r}}.N_s(\vec{r},\vec{q}) = \left.\frac{\partial N}{\partial t}\right|_{coll} + G_s(\vec{r},\vec{q}) \tag{2}$$

where $\vec{r}$ is the position vector, $\vec{v}_{g,s}$ is the group velocity, $N_s(\vec{r},\vec{q})$ is the phonon distribution, $\left.\frac{\partial N}{\partial t}\right|_{coll}$ is the scattering term and $G_s(\vec{r},\vec{q})$ is the generation term. The equilibrium phonon distribution $N_s(\vec{r},\vec{q})$ at a given temperature follows the Bose-Einstein statistics.

C. Heat generation

The generation term $G_s(\vec{r},\vec{q})$ in Eq. 2 derives from either an internal source, i.e. from the phonon bath itself, or from an external one. The internal source only affects the acoustic

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modes. Its origin is the anharmonic decay of optical phonons in excess into acoustic phonons of lower energy. This phenomenon gives rise to a significant energy transfer from optical to acoustic modes and has to be taken into account to ensure the energy conservation of the system. The external heat generation is related to the energy exchange between phonons and electrons. A difference between the phonon and electron temperatures induces a net increase of emitted (or absorbed) phonons. In the self-consistent electro-thermal loop of our model, these specific generation terms are extracted from the previous solution of electronic transport. More details about these generation terms can be found in Ref. [6], in particular about the computation of the anharmonic decay.

D. Scattering term

The scattering term has been implemented within the relaxation time approximation (RTA), i.e. in the form

$$\left.\frac{\partial N}{\partial t}\right|_{coll} = -\frac{N_s(\vec{r},\vec{q}) - N_s^0\left(T_{Fourier}(\vec{r}),\vec{q}\right)}{\tau_s\left(T_{Fourier}(\vec{r}),\vec{q}\right)} \quad (3)$$

where τ_s refers to the total relaxation time at the temperature $T_{Fourier}$.

The main issue in such description of the scattering term that provides a linear and tractable expression is to determine the temperature $T_{Fourier}$ to describe locally the temperature-dependence of the relaxation time. This temperature is basically an unknown variable that could be rigorously determined via a self-consistent solution. However to simplify the iterative process, in our model this temperature is directly estimated from a preliminary solution of a simple 1D Fourier heat equation. The input parameter $T_{Fourier}$, is inserted in the scattering term (Eq. 3) and then Eq. (2) can be solved.

In this work, the total relaxation time is computed via the Mathiessen's rule and includes the Normal and Umklapp types of three-phonon scattering [4], phonon-impurity scattering [7] and phonon-boundary scattering [8]. Using adjusted parameters of the Holland's model for phonon scattering, our model reproduces the thermal conductivity in silicon in the full 100–600 K temperature range (not shown here).

The optical decay into acoustic phonon modes is also considered within the approach developed in [9].

E. Boundary conditions

We consider the thermal transport to be 1D. For 2D or 3D devices, that means that the spatial phonon distribution is assumed to be uniform and the thermal fluxes to be zero along the transverse direction(s) perpendicular to the transport. It is relevant in the case of quasi-infinite transverse dimensions or in the presence of quasi thermal insulator such as SiO_2 surrounding the active region, like in FD-SOI transistors. Along the transport direction, the two thermal contacts are assumed to be in equilibrium with two ideal reservoirs at temperatures T_1 and T_2, respectively. Thus, the distribution of phonons entering the device at a given contact follows the corresponding Bose-Einstein distribution. Phonons hitting the contact interfaces are free to leave the device and their related energy disappear [10].

F. Effective temperature

In the context of non-equilibrium phonon distributions which is often encountered at the nanoscale, the concept of (standard) temperature is meaningless. An "equivalent temperature" field called the effective temperature T_{eff}, defined from the total energy of the local phonon bath resulting from the actual phonon distribution (which may be out-of-equilibrium), naturally extends the common temperature concept [11, p. 2006]. According to this definition, an effective temperature can be evaluated for each mode.

III. Electro-thermal Simulator

To investigate self-heating effects in electronic devices, the thermal solver presented in the previous section has been coupled to an electron transport simulator. The resulting electro-thermal simulator is described in this section.

A. Electron Monte Carlo simulation

To solve the electron transport equation we have used a homemade Ensemble Monte Carlo simulation for electrons (eMC). In this approach the Boltzmann equation is solved using a stochastic calculation of particle trajectories self-consistently coupled with the Poisson equation. In this version of the code the conduction band of electrons in silicon is described through an analytical non-parabolic model for the six ellipsoidal Δ valleys. All details of the band structure and the scattering parameters used for acoustic phonon, inter valley phonon, ionized impurity and oxide interface roughness scattering mechanisms can be found in Ref. [12].

B. Heat generation and phonon dispersion

The cartography of the phonon temperature is an input to the eMC simulation that provides the heat generation term needed in Eq. 2 via the local counting of electron-phonon scattering events. In contrast to macroscopic approaches assuming local equilibrium, this method includes an accurate description of the energy transfers between phonons and hot electrons and gives access to their exact location [6].

As in most common eMC models, the phonon dispersions used to conveniently compute the intervalley scattering rates are assumed to be wave vector-independent. Fortunately, the simulator provides information about the wave vector of the phonon selected to be involved in the electron-phonon scattering event. Then, the angular frequency of an interacting phonon is computed afterward via the quadratic dispersion of Eq. 1. (see more details in Ref. [6]).

C. Self-consistent alogorithm

The coupled simulation starts with an isothermal (300 K) eMC simulation (referred as "open loop" simulation). Then, the net phonon generation rates, which are functions of both the position and the phonon frequency, are extracted from eMC outputs and used as inputs for both the Fourier heat equation and the pBTE solver described in Section 2. The resulting local effective temperature is then re-injected in the eMC simulator.

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It should be mentioned that only the effective temperature fields are exchanged between steps because in standard situations the phonon occupations do not significantly differ from their equilibrium distribution [6]. Next, all electron scattering rates, as electron-phonon and electron-impurity scattering rates, are re-calculated in each cell according to the position-dependent T_{eff}. Then, the eMC simulation is performed again with this new field of temperature. This three-step process, that successively includes an electron and a phonon transport simulation, is called a loop. The convergence is reached when the difference of effective temperature between two consecutive loops is smaller than the target value. It should be noted that the convergence is commonly reached after only three loops.

IV. Self-heating effects in DG-MOS

The electro-thermal simulator was used to investigate the self-heating in a 20 nm long DGMOS transistor. As presented later, hot electrons play a significant role in this device; thus the optical modes and the related LTO decay have to be included in the pBTE solver.

A 2D cross-section of the studied Si DG-MOSFET is schematized in Fig. 1. The device consists of three regions: the highly N-doped (5×10^{19} cm^{-3}) source and drain regions and the 20 nm long and non-intentionally doped (10^{15} cm^{-3}) channel. The source length is 50 nm, while the drain length is 150 nm to be larger than the relaxation length of hot electrons. The thickness of the Si-film is 20 nm.

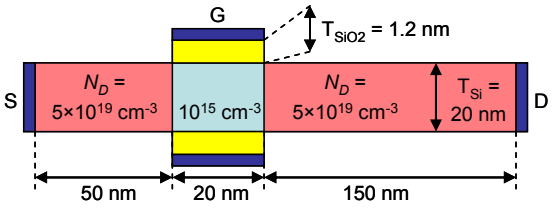

Fig. 1. Schematic cross-section of the simulated device.

The profile of heat power density resulting from the initial isothermal (300 K) eMC simulation (the 'open loop') is plotted in Fig 1.a. This MC result (solid line) indicates that hot electrons heated in the channel, i.e. the high electric field region, transfer their energy to the phonon bath mainly in the drain region, and for a significant part of them far into the drain extension. This result considerably diverges from the prediction based on local equilibrium (dashed line) which estimates the heat power as the product of the local electric field (**E**) and the local current density (**J**). This macroscopic approach, that neglects the strong out-of-equilibrium effects occurring in this DGMOS, predicts that the maximum of dissipated heat occurs in the gated part of the channel where the field is high.

In Fig. 2 the phonon generation rates computed for each phonon mode is plotted along the source-drain direction. In the source region where electrons remain close to equilibrium (see [6]) the emitted phonons belong mainly to the LA and TO branches while the other modes have no noticeable effect. In the channel, where the transit time of electrons is very short compared to the scattering times, the net phonon generation is almost zero for all modes. In the drain, where the phonon generation rate is clearly the strongest, the main emission processes are once again due the LA and TO modes. However a significant contribution of TA phonons can be observed near the channel, with a shorter decay length. From the channel-drain junction the decaying of the total phonon generation rate is characterized by a decay length of about 28 nm for V_{ds} = 1.0 V, which is much shorter than the length of the drain extension. Thus, near the drain contact the heat generation rate of each mode reaches a local equilibrium state very similar to that in the source. This long drain extension of 200 nm is thus necessary to make consistent the boundary conditions at thermal contact.

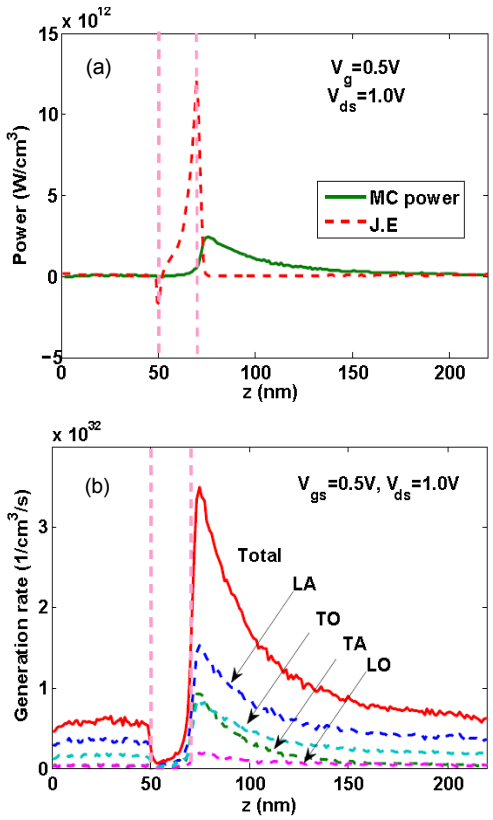

Fig. 2. . At Vgs = 0.5 V and Vds = 1.0 V. (a) Heat power density extracted from eMC simulation (green solid line) and from the product (dashed red line). (b) Net phonon generation rate per mode (dashed lines) and total generation rate (continous line) due to electron-phonon scattering, from eMC simulation.

A. Self-heating effect

The heat generation computed from the initial eMC simulation presented above has been included in the phonon transport equation (p-BTE) to initiate the iterative algorithm of an electrothermal simulation.

We plot in Fig. 3 the profile of the effective temperature T_{eff} at V_{gs} = 0.5 V and V_{ds} = 1.0 V after each loop. It confirms that the convergence is obtained after only three loops. The

feedback due to the iterative process induces a slight reduction of the hotspot temperature from 441 K in the 1st loop to 433 K after convergence. Besides, near the two contacts with the thermal reservoirs, a temperature drop can be observed. This drop is higher near the drain contact because the phonon transport is further from equilibrium than in the source side.

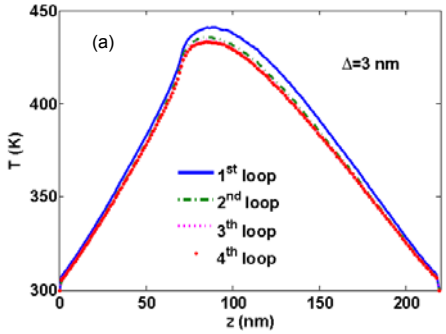

Fig. 1. At V_g = 0.5 V and V_{ds} = 1.0 V. (a) Evolution of the effective temperature T_{eff} along the device for several loop numbers.

V. Conclusion

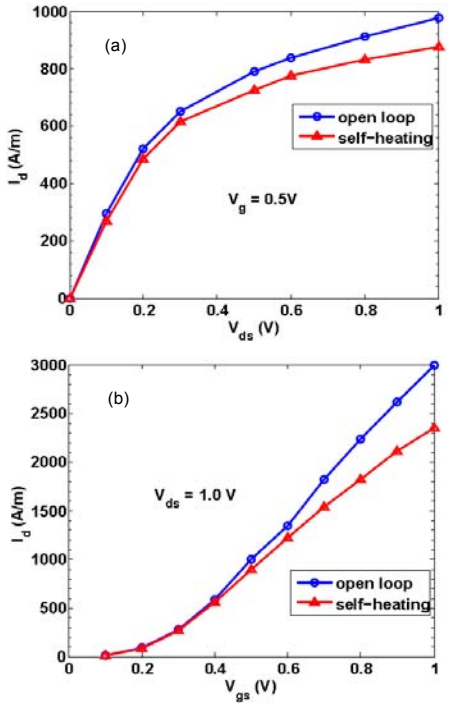

Fig. 2. (a) I_d-V_{ds} at V_g = 0.5 V and (b) I_d-V_{gs} at V_{ds} = 1.0 V. Open loop (blue lines with circular symbols) vs. electro-thermal simulations (red lines with triangular symbols). Roughness parameter Δ = 3 nm.

A. I-V characteristics

The drain current (I_d) characteristics as a function of the drain voltage (V_{ds}) at a gate voltage V_{gs} = 0.5 V and the I_d-V_{gs} curve at V_{ds} = 1.0 V are shown in Fig. 4.a and b, respectively. To highlight the effect of self-heating, the isothermal open loop simulations have been compared with electro-thermal simulations. As expected, the impact of self-heating manifests itself mainly at high drain current, when the enhancement of channel temperature is sufficient to induce a significant increase of the number of scattering events in the active region. It induces a drain current degradation of 6.9% and 20% for V_{ds} = 0.5 V and 1.0 V, respectively. Moreover, the maximum value of transconductance g_m is also degraded.

In conclusion, we have presented a numerical method to solve the stationary Boltzmann transport equation for phonons (pBTE) in the relaxation time approximation, considering quadratic phonon dispersions. A specificity of our approach is to evaluate the equilibrium temperature to be considered in the expressions of scattering relaxation times via a preliminary solution of the Fourier heat equation This pBTE simulator has been coupled with our home-made Ensemble Monte Carlo simulation for electrons to study the self-heating effects in a 20 nm -long DG-MOSFET. The convergence is quickly reached, i.e. usually after only three loops. In simulations with contacts perfectly thermalized at 300K, the effective temperature can exceed 400 K in the hot spot of the transistor in open-channel regime. Besides, it has been shown that the heat Fourier equation is not able to catch accurately the exact location and value of this temperature overshoot. The self-heating increases the detrimental effects of the access resistances and finally, the drain current can be reduced by a factor of 20% at high applied voltage.

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