New self-consistent phonon-electron BTE solver for the simulation of ultra-small DG-MOSFET

T.T. Trang Nghiêm, J. Saint-Martin, P. Dollfus

Institute of Fundametal Electronics, University of Paris Sud, F91405 Orsay cedex, France e-mail: jerome.saint-martin@u-psud.fr

Abstract

To study the self-heating effects, we have developed a new efficient tool that solves selfconsistently the Boltzmann transport equation (BTE) for both electrons and phonons. A Monte Carlo solver for electrons is coupled with a direct solver for the phonon transport (pBTE). In this work, this simulator is used to investigate the selfheating in a 20 nm-long double gate MOSFET.

For electrons, the Monte Carlo model used is a semi-classical ensemble simulator self-consistently coupled with a 2-D Poisson solver. All details of the analytic band structure and the scattering parameters may be found in [1,2]. This approach evaluates very accurately the phonon emission and absorption spectra in both real and energy space.

In the relaxation time approximation, for each phonon polarization s (i.e. LA, TA, LO, TO), the BTE for phonons can be expressed as

$$\vec{v}_{g,s} \cdot \nabla_{\vec{r}} N_s(\vec{r}, \vec{q}) = -\frac{N_s(\vec{r}, \vec{q}) - N_{s, T_{Fourier}}(\vec{r}, \vec{q})}{\tau_s(T_{Fourier}(\vec{r}), \vec{q})}$$
(1)
+ $G(\vec{r}, \vec{q})$

where $v_{g,s}$ is the group velocity, $N_s(\vec{r}, \vec{q})$ is the particle number, \vec{r} is the position and $G(\vec{r}, \vec{q})$ is the phonon generation term provided by the electron transport solution. $N_{s,TFourier}$ is the equilibrium phonon number at temperature $T_{Fourier}$, where $T_{Fourier}$ is the temperature obtained by solving the heat equation. τ_s is the total relaxation time computed via the Mathiessen's rule including three-phonon, phonon-impurity [3] and phononboundary scattering [4] mechanisms. The optical decay into acoustic phonon modes is considered too [5]. An analytical parabolic dispersion was used for phonons [6]. An out-of-equilibrium effective temperature T_{eff} is derived from the local phonon energy density, and is reinjected in the electron MC simulator via the update of electron-phonon scattering rates. The loop is repeated until a convergence is reached.

Fig. 1 shows the simulated Silicon-based DG-MOSFET with film thickness of 20 nm. In Fig. 2 the potential profiles along the device reveal the presence of high electric field at the drain-end of the channel, where, under high drain bias, hot electrons can emit many high-energy phonons, as shown in Fig. 3. In Fig. 4 the profile of effective temperature is plotted for different numbers of loops. We observe that the temperature evolves significantly between the 1^{st} loop and the 2^{nd} loop. However, after the 3rd loop the convergence is reached. Finally, the temperature in the channel reaches 430 K, which has an impact on the electron transport in the channel. For instance, Fig. 6 shows that the fraction B_{int} of electrons that cross the channel ballistically [1] is reduced when taking the self-heating effect into account. This leads to a significant reduction of current, as shown in Fig. 7. In this device, the reduction reaches 16% for $V_{DS} = 1.5$ V.

Our new self-consistent electron-phonon Finally, BTE solver provides very detailed insight into electro-thermal effect at the nano-scale.

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Fig. 1. Simulated Double-Gate MOSFET.



Fig. 2. Potential profile (bottom of conduction band) for various V_{DS} at $V_G = 0.5$ V (isotherrmal simulations).



Fig. 3. Energy spectrum of generated phonons along the device at $V_G = 0.5$ V and $V_{DS} = 1.5$ V.



Fig. 4. Profile of effective temperature T_{eff} along the device obtained at a given bias point after different loop numbers.



Fig. 5. Intrinsic ballisticity as a function of V_{DS} for V_G =0.5V. Isothermal–open loop (dashed line) and self-consistent simulation (continuous line).



Fig. 6. I_D - V_{DS} characteristics for $V_G = 0.5 \text{ V}$ for different numbers of loops of electron and phonon transport simulation.