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Improved Monte Carlo algorithm of phonon transport in semiconductor nanodevices

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Abstract. In this work, we present the main features of an algorithm of phonon transport based on the particle Monte Carlo solution of the Boltzmann Transport Equation. In particular, we have developed an injection technique which consists in replacing a costly reservoir of phonons at thermodynamic equilibrium by an equivalent interface injecting in the device the appropriate phonon distribution. Additionally, we have derived a formulation of phonon–phonon scattering rates which includes realistic phonon dispersion of the material giving accurate frequency-dependence. An algorithm is proposed to improve the treatment of phonon interaction.

1. Introduction
Heat dissipation in MOS transistors appears as a severe limit for further increasing the packing density of chips and constitutes a major challenge for the microelectronics industry. It is already one of the main factors contributing to the slowing down of chip frequency enhancement. The appropriate choice of model for describing self-heating and heat conduction is conditional on the characteristic device length compared to the length scales associated with physical mechanisms governing the phonon transport [1]. Heat conduction in quasi-equilibrium regime can be treated by the Fourier law through the concept of thermal conductivity for device lengths larger than the phonon mean free path, i.e. typically 100 nm in usual semiconductors, which is more questionable for smaller structures. The coherence length and wave length of phonons is typically about or smaller than a few nanometers. For larger characteristic length of the structure the wave-like nature of phonons is weakly pronounced at room temperature and phonons can reasonably be treated as particles. In the 10-100 nm range of device length, the Boltzmann Transport Equation (BTE) is an appropriate formalism. Thus the particle Monte Carlo technique is very convenient for solving phonon transport problems in 3D device geometry including phonon-phonon interactions [2]. We develop in the present work (Section 2) an efficient Monte Carlo transport model for the phonon BTE. Phonons are treated as particles in free-flight between interactions with impurities or other phonons. This model is destined to be coupled in the near future with our charge-carrier transport simulator MONACO [3] to study self-heating effects on electrical properties of ultra-small field-effect transistors. It should make possible the accurate description of electro-thermal effects including out-of-equilibrium phonon situation induced by electron transport.

A new efficient technique of particle injection is described in Section 3. An appropriate treatment of boundary conditions at thermal contact and adiabatic interfaces is required. To go beyond the widely used empirical relaxation time associated with phonon scattering suggested
in [4] on the basis of experimental data, we propose in Section 4 a more rigorous formulation of three-body scattering rates that may be integrated within a Monte Carlo algorithm of phonon transport.

2. Transport algorithm

The device is divided in identical spatial cells in which we compute the phonon occupation number \( n(q, j) \) for each polarisation \( j \) (LA, TA, LO and TO) where \( q = |q| \) is the phonon wave vector norm. We consider isotropic quadratic dispersion relations between the phonon pulsation \( \omega \) and \( q \) according to the fitting expression obtained along the (100) crystallographic direction [5]. We quote \( q_{\text{max}} = 2\pi/a_{\text{si}} \) the maximal phonon wave vector norm and \( a_{\text{si}} \) the silicon lattice parameter. The phonon distribution in the device is initialised at thermodynamic equilibrium. For a three-dimensional and isotropic crystal, the number of phonons \( dN(q, j) \) with polarisation \( j \) and wave vector norm between \( q \) and \( q+\text{dq} \) is

\[
dN(q, j) = \langle n(q, j) \rangle \text{DOS}(q, j) g_j \text{dq}
\]

(1)

where \( g_j \) is the degeneracy factor (1 for longitudinal modes, 2 for transverse ones), DOS is the density of states for wave vector \( q \) and polarization \( j \), \( \langle n(q, j) \rangle \) is the mean occupation number. At thermodynamic equilibrium, \( \langle n(q, j) \rangle \) is the Bose-Einstein distribution. The algorithm starts with the estimation of the initial number \( N(j) \) of phonon of polarisation \( j \). The expression (1) of \( dN(q, j) \) is used as a probability law for the random selection of each phonon wave vector norm. As we assume the crystal to be isotropic, the direction of the wave vector is uniformly distributed. According to the isotropic quadratic expressions of phonon dispersion \( \omega(q, j) \), the phonon group velocity \( v_g(q) \) is collinear to \( q \). During a time step \( \Delta t \), the appropriate number of phonons are injected from thermal contacts into the device according to the method described below in Section 3. Each phonon trajectory is broken down in free flight of duration \( \tau_f \) randomly selected. After each free flight the phonon experiences either a phonon-phonon scattering or a phonon–impurity scattering (see Section 4), which modifies its wave vector. At any device boundary, the possibility of transmission or reflection may be treated according to the acoustic mismatch model [6]. At the end of the iteration, we calculate a pseudo-temperature and occupation number for each cell. At thermodynamic equilibrium:

\[
E = \sum_j \int_q \left( f_{\text{BE}}(\omega) + \frac{1}{2} \right) h\omega(q, j)\text{DOS}(q, j) g_j \text{dq}
\]

(2)

By equalling expression (2) with the total phonon energy in each cell, we obtain temperature by inverting the Bose-Einstein distribution. Note that the concept of temperature is relevant only near thermodynamic equilibrium. The output data for charge carrier transport algorithm is the occupation number in each spatial cell.

3. Phonon injection

In contrast to other Monte Carlo algorithms of phonon transport, we do not use adiabatic walls. Indeed, this kind of boundary condition is not appropriate for a real transistor MOSFET, which is not really thermally isolated even with a Silicon-On-Insulator (SOI) technology. In our code, phonon are injected through each face considering that they come from an equilibrium cell at a given temperature. If \( u_z \) is the unit vector normal to the surface contact, the phonon number per surface unit and per time unit with polarisation \( j \) and component \( q_z \) belonging to interval \([q_z; q_z + dq_z]\) is given by

\[
dN_{nij}(q_z, j) = q_z dq_z \int_{q_z}^{q_z + dq_z} \langle n(q, j) \rangle \text{DOS}(q, j) g_j dq_z dq_y
\]

(3)
Variables $q_x$, $q_y$ and $q_z$ cannot be separated in the integral. Accordingly, the probability law for selecting $q_z$ and $q_y$ is conditional on $q_x$ value. Figure 1 shows phonon distribution for a 100 nm edge cube with boron impurity. The phonon number is plotted as a function of $q_z$. Initially, the structure contains a thermodynamic equilibrium phonon population at 500 K. The faces are not adiabatic, so the phonons can leave the device if the transmission probability condition is satisfied. Such phonons are called exiting phonons. We also plot the imposed injected phonon distribution. These phonons are randomly selected from probability law (3) by considering the transmission probability condition. Figure 1 points out that both distributions are similar, except for the particle noise. Consequently, the equilibrium distribution of $q_z$ in the cell is conserved. This can be verified for any property of phonon population in the cell, as $\omega$ or any $q$ component distribution for each polarization. This injection algorithm is thus able to well reproduce the phonon flux which leaves the device.

4. Phonon scattering

The phonon transport simulator we have developed can include two types of interaction mechanisms: phonon-phonon and phonon-impurity scattering. These events are independent, so we obtain the total scattering rate $\Gamma(q)$ by summing $\Gamma_{ph-ph}$ and $\Gamma_{ph-i}$, the scattering rates associated with phonon-phonon and phonon-impurity interaction, respectively. The time of free flight $\tau_f$ between two scatterings is selected according to :

$$\tau_f = -\frac{\ln(R)}{\Gamma(q)}$$ (4)

where $R$ is a random number between 0 and 1. After this free flight, the phonon should experience a scattering event whose type is randomly selected. The phonon-impurity scattering rate is calculated using the Vincenti and Kruger model [7]. It is an elastic process which only changes the direction of $q$ isotropically. For phonon-phonon scattering, we use the perturbed Hamiltonian for three phonons to define scattering rate $\Gamma_{ph-ph}$ [8]. The simulator should include four phonon-phonon interactions :

(1) : $LA_{(q)} \rightarrow LA_{(q')} + TA_{(q'')} 
(2) : LA_{(q)} \rightarrow TA_{(q')} + TA_{(q'')}$

(3) : $LA_{(q')} + TA_{(q'')} \rightarrow LA_{(q)} 
(4) : TA_{(q')} + TA_{(q'')} \rightarrow LA_{(q)}$

The scattering rate $\Gamma_{ph-ph}$ for a phonon $q$ is given by summing over all possible final states compatible with total energy and momentum conservation.

$$\Gamma_{ph-ph}(q) = \frac{\hbar}{16\pi^2}\rho^3\omega(q,j) \int_0^{2\pi} d\theta \sin(\theta) \int_0^{q_{\text{max}}} |q'| d|q'| \frac{M(q,q',q \pm q',j,j,j'' \pm j')^2}{\omega(q',j') \omega(q \pm q',j'')} \delta(\Omega)$$ (5)

Where $\delta(\Omega)$ ensure energy conservation, $j, j'$ and $j''$ stand for the phonon branch index involved in the considered process, $\rho$ is the silicon density and $M$ is the matrix element defined in [8] which depends on the angle $\theta$ between $q$ and $q'$. Prior to the simulation, we calculate and tabulate the whole possible phonon-phonon scattering rates. For each $q$ we calculate phonon-phonon scattering rates for the possible $q'$ in the four interactions, and associated conditional probabilities needed for $q'$ selection. First, in expression (5) the integral is performed over $\theta$ and then over $|q'|$. The resulting values are ranged in a look-up table used for the selection of $|q'|$, i.e. the wave vector norm of one of the created/destroyed phonons. Then for this $|q'|$ value, the integral (5) is performed over $\theta$ and ranged in another look-up table for the selection of the angle $\theta$. In phonon–phonon interactions (1) and (2), one of the resulting wave vector $q'$ is obtained through expression (5). Then, the second will be $q - q'$. Even if $q$ and $q'$ belong to the
first Brillouin zone (here a sphere of radius $q_{\text{max}}$), $\mathbf{q} - \mathbf{q}'$ can leave it. In this case of Umklapp process, a reciprocal wave vector is subtracted in order to bring $\mathbf{q} - \mathbf{q}'$ back to the first Brillouin zone. In phonon–phonon interactions (3) and (4), the resulting wave vector $\mathbf{q}' + \mathbf{q}''$ may also have a norm higher than $q_{\text{max}}$. The resulting Umklapp process is treated as the previous one.

5. Conclusion
We have presented a Monte Carlo algorithm for phonon transport which ensures conservation of both energy and momentum for each phonon–phonon process. Moreover, appropriate phonon injection from boundaries avoids using adiabatic walls. At the moment, phonon injection algorithm and transport algorithm including phonon–impurity scattering are fully validated. Introduction of phonon–phonon scattering is currently underway and this work will be continued by coupling this algorithm with the existing Monte Carlo simulator of charge carrier transport MONACO. This two algorithms will be connected through the electron–phonon scattering, which requires the knowledge of the phonon occupation number in each cell. This simulator would allow an accurate description of the self-heating effect in the MOSFET channel.

Figure 1. Phonon distribution of a 100 nm edge cube for a boron density of $5 \times 10^{18} \text{cm}^{-3}$. On the left-hand side, initialisation from equilibrium state at $t = 0$ (line) and after 1 ns (dots). Equilibrium distribution is conserved during these 1000 time steps. On the right-hand side, exiting phonon (line) and injected phonon distribution (dots) cumulated on a time step $\Delta t$.

Figure 2. Total phonon–phonon scattering rates for the four interactions considered here. Curves (1) and (2) refer to a LA phonon to be destroyed before creation of TA+LA and TA+TA phonons, respectively. Curves (3) and (4) refer to a LA phonon to be destroyed together with either a LA or a TA phonon, respectively, to create a LA phonon.

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