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Monte Carlo Simulation of Carrier-Carrier Interaction for Silicon Devices

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Abstract

This paper presents a Monte Carlo approach to electron-electron $(e-e)$ scattering in silicon which is suitable for applications to device analysis. A generalization of the theoretical approach of Bohm and Pines [1] to the case of an arbitrary isotropic multiband model is used. Results for the effect of the Coulomb interaction on the electron distribution function and on the energy-loss properties of the electron gas are presented.

1. Introduction

Hot-carrier effects still represent the major threat for MOSFET reliability. In order to effectively design modern submicron technologies such effects must be correctly simulated since the knowledge of the carrier distribution function is necessary to quantitatively describe physical phenomena, such as carrier injection and trapping into the SiO_2, responsible for device degradation. In this frame, the Monte Carlo method can be considered the most settled, but particular care must be taken to the microscopic transport physics in order to have quantitative confidence on the modeling of the distribution function. Inter-carrier Coulomb interaction is generally neglected in Monte Carlo simulations since it is considered sufficiently low inside most of the channel region to make the interaction irrelevant. However, since in a MOSFET the point of maximum carrier heating falls just inside the drain junction, where the concentration of cold carriers is high, the Coulomb scattering can be very significant. In addition, due to the high carrier concentrations in the channel of modern MOSFETs, it is also questionable whether this interaction can be neglected in this region. E-e interaction has been considered by several researchers so far, with as few approximations as possible [2, 3, 4], but usually the amount of CPU time needed imposes very severe limitations to its practical applicability.

2. Theoretical approach and the Monte Carlo simulator

In the present paper, following the approach of Bohm and Pines [1], the inter-carrier Coulomb interaction has been analyzed in terms of short and long-range components. The short-range contribution can be described by two-particle collisions through the introduction of a screened Coulomb potential. The long-range contribution can be formally transformed into the coupling of a single carrier with the *sea* of the other electrons, whose coherent behavior gives rise to plasma oscillations. We have studied, in particular, the generalization of this approach to the case of an arbitrary isotropic multiband model [5, 6, 7], which allowed us to consistently include the Coulomb interaction in the Monte Carlo simulator for MOSFET devices described in [8, 9].

The scattering probability for the short-range two-particle interaction is given by

$$P_{e-e}(\mathbf{k}_{1b}) = \frac{2\pi}{\hbar}\left(\frac{e^2}{V\epsilon}\right)^2 \sum_{\mathbf{k}_{2b},n_{2b}} \sum_{\mathbf{k}_{1a},n_{1a}} \sum_{\mathbf{k}_{2a},n_{2a}} f(\mathbf{k}_{2b}) \frac{1}{||\mathbf{k}_{2a}-\mathbf{k}_{2b}|^2+q_D^2|^2} \delta(\mathbf{k}_{1b}+\mathbf{k}_{2b};\mathbf{k}_{1a}+\mathbf{k}_{2a}) \delta(\varepsilon_{k_{1a}}-\varepsilon_{k_{1b}}+\varepsilon_{k_{2a}}-\varepsilon_{k_{2b}}) \quad (1)$$

where q_D is the inverse of the Debye screening length, 1 and 2 are labels for the two particles involved in the scattering process (supposed to be distinguishable), b and a refer to states "before" and "after scattering", respectively, and n are the band indices.

Since the distribution function $f(\mathbf{k})$ of the counterparts in any given two-carrier scattering is not known a priori, an overestimation-rejection of the short-range scattering probability has been used in order to compute the carrier free-flight [10], thus allowing to treat the short-range term without any analytical assumption on the shape of $f(\mathbf{k})$. This numerical procedure, that will be described in details in a longer paper, has the effect of reasonably contain the CPU time necessary for the Monte Carlo simulation (about 2-3 CPU hours on an IBM RISC/6000).

The carrier-plasmon interaction has been explicitly included among the considered scattering mechanisms by using the following scattering probability:

$$P_{el-pl}(\mathbf{k}) = \frac{2\pi}{\hbar}\frac{e^2\hbar^3}{8m^{*2}V\epsilon\omega_p} \sum_{q<q_c} \frac{1}{q^2}(2\mathbf{qk}+q^2)^2(1-n_{k+q})n_k \{n_q\delta[\varepsilon(k+q)-\varepsilon(k)-\hbar\omega_p] + (n_{-q}+1)\delta[\varepsilon(k+q)-\varepsilon(k)+\hbar\omega_p]\} \quad (2)$$

where ω_p is the plasma frequency.

The long-range Coulomb interaction has been accounted for as an explicit scattering mechanism because, as described in [8, 9], Poisson equation is solved for carrier densities averaged during intervals much longer than the plasma frequency. This avoids the double estimation of the long-range coupling. The plasma frequency must be evaluated, in this case, for each space cell in the simulator, provided that the cell dimensions are much larger than the carrier screening length.

3. Numerical results

Numerical results have been obtained from Monte Carlo simulations of electrons in homogeneous silicon. Fig.1 reports the electron distribution function for homogeneous silicon at low temperature. The results obtained including the short range $e-e$ interaction are compared with those obtained by considering only optical phonon interaction: the $e-e$ mechanism clearly washes out the oscillations introduced by the periodicity of the optical phonons [11]. For this example a simple parabolic band was used.

Next the model of the Coulomb interaction has been applied to homogeneous silicon simulations using the multiband model described in [5]. Fig.2 reports, for the first conduction band, the short range $e-e$ scattering rate as obtained *a posteriori* from the simulations in the two cases of electron density $n = 10^{17} cm^{-3}$ and $n = 10^{20} cm^{-3}$. The data show similar behavior for the scattering rates, but the actual effect of the mechanism on the distribution function is markedly different for the two densities. To show this point, Fig.3 reports the number of $e-e$ interactions as a function of the energy exchanged in the interaction between the colliding carriers. While in the case of $n = 10^{17}$ the number of the events with high energy exchange is very limited, the opposite happens for the high density case. As a consequence, the effect of the $e-e$ interaction is noticeable in the shape of the distribution function only in the case of $n = 10^{20} cm^{-3}$, as shown in Fig.4 for different electric field strengths.

Fig.5 shows the effect of the interaction on the average quantities of the electron gas, namely mean energy and drift velocity, for the high density case. The mean energy is marginally affected by the interaction while a noticeable reduction is observed for the drift velocity, probably due to the enhanced symmetrical shape of the k distribution function.

Finally, the model has been applied to the inhomogeneous case of the silicon $n-i-n$ diode. Fig.6 shows the effect on the distribution function of the introduction of electron-plasmon interaction together with the short-range $e-e$ scattering. The distribution function refers to the space point located $10nm$ inside the heavily doped ($10^{20} cm^{-3}$) drain junction: the hot electron gas interacts with the "sea" of cold electrons in the drain region and the long-range mechanism dominates the electron cooling effect.

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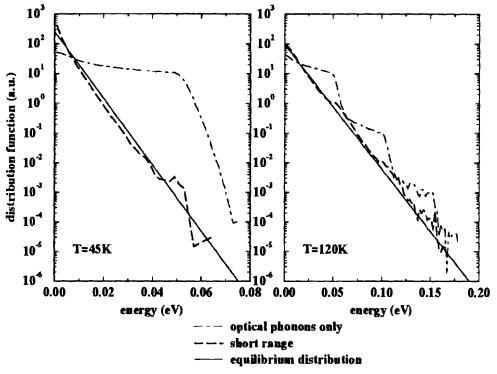

Fig.1: electron distribution function in bulk silicon at low temperature.

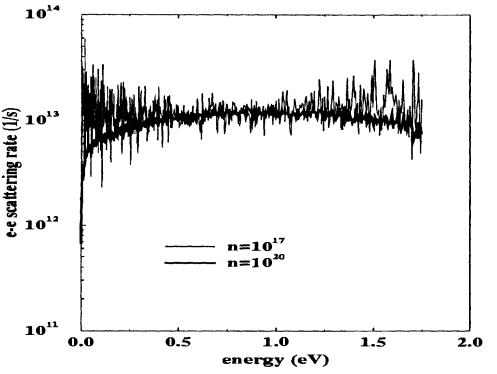

Fig.2: short range $e-e$ scattering rate for the first conduction band of the model [5].

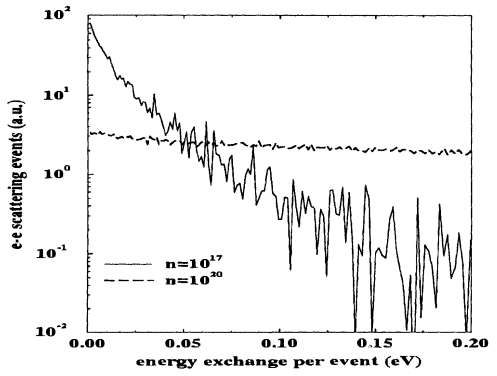

Fig.3: number of short range $e-e$ interactions as a function of the energy exchanged between the colliding carriers.

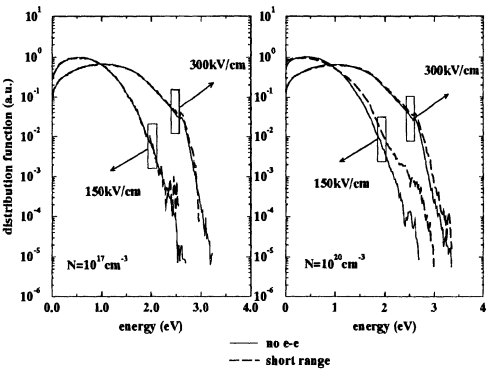

Fig.4: electron distribution function at different electric fields and different electron densities.

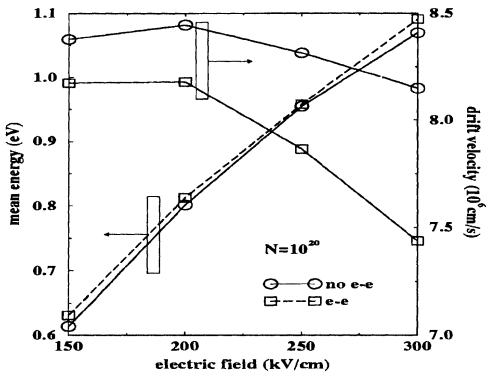

Fig.5: Mean energy and drift velocity at different electric field strengths.

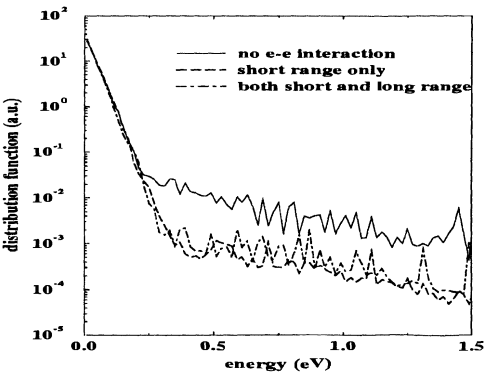

Fig.6: electron distribution function $10nm$ inside the heavily doped drain junction of an $n-i-n$ diode.