An Impact Ionization Model Including Non-Maxwellian and Non-Parabolicity Effects

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Abstract

Accurate modeling of impact-ionization is a critical issue for submicron devices. It is well known that models based on the electric field or on the average carrier energy give a rather poor description of the problem. We show that by accounting for the average square energy an accurate analytical description of the distribution function can be given which can then be used to evaluate microscopic models in a macroscopic device simulator. The new model is accurate for both bulk and submicron devices and involves only local quantities.

1 Introduction

For fast and accurate evaluation of CMOS reliability issues in sub-100 nm technology very precise high field transport models are needed. In particular, hot-carrier effects like impact ionization are poorly described by models using the local average carrier energy as parameter. To obtain a more accurate description, equation sets based on six moments of Boltzmann's equation have been considered where in addition to the carrier concentration and temperature the next higher even moment, the average square energy of the distribution function is taken into account. First promising results were obtained by Sonoda *et al.* [1] who proposed an analytical expression for the impact ionization rate as a function of the average energy and the average square energy by fitting Monte Carlo (MC) results. Being a fit-formula, the model lacks theoretical background and we obtained poor accuracy for other channel lengths and biases than those used in [1]. Therefore we developed an analytical model for the symmetric part of the distribution function which goes beyond the Maxwellian approximation. This model is then used to derive a macroscopic impact ionization model based on microscopic descriptions used in MC simulators. Impact ionization models based on six moments of the distribution function (DF) nicely fit into the concept of conventional device simulators and do not require e.g., integration along current paths, as only local quantities are involved.

2 The new model

It has been frequently shown that the shape of the DF depends on whether the gradient of the field is positive or negative with respect to the current density. Several cases have been considered and evaluated and we found that

$$f(\mathcal{E}) = A \exp\left[-\left(\frac{\mathcal{E}}{a}\right)^b\right] \tag{1}$$

which is a generalization of [2] and [3], neatly captures the main features of the distribution function throughout the whole device. The parameters $a = a(T_n, \beta_n)$ and $b = b(T_n, \beta_n)$ are functions of the local temperature and kurtosis. Instead of using the average square energy directly, we define the kurtosis of the distribution function as $\beta_n = (3/5)\langle\mathcal{E}^2\rangle/\langle\mathcal{E}\rangle^2$. We now take the moments of order l of the analytical energy distribution function (1)

$$m_l = \int \mathcal{E}^l g(\mathcal{E}) f(\mathcal{E})\, \mathrm{d}\mathcal{E} \tag{2}$$

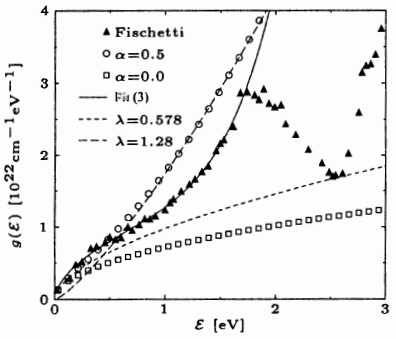

Fig. 1: Comparison of different expressions for the density of states

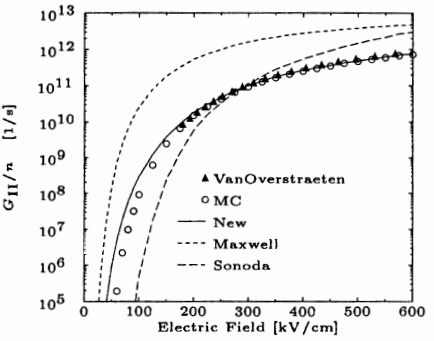

Fig. 2: Comparison of the new expressions with other models for the bulk case

To evaluate (2) an expression $g(\mathcal{E})$ for the density of states is needed. Results based Kane's first-order non-parabolicity correction [4] cannot be handled analytically. As can be shown, a power-law approximation $g(\mathcal{E}) = g_0\,\mathcal{E}_C(\mathcal{E}/\mathcal{E}_C)^\lambda$ similar to the one given by Cassi and Riccò [2] cannot capture the non-parabolic nature of the bands, because only the low- or the high-energy part can be fit accurately, but not both simultaneously as shown in Fig. 1. Instead, we use the expression

$$g(\mathcal{E}) = g_0\sqrt{\mathcal{E}}\Big(1 + (\eta\mathcal{E})^\zeta\Big) \tag{3}$$

with $\eta = 1.4\ \mathrm{eV}^{-1}$ and $\zeta = 1.08$ which were obtained by a fit to Kane's expression. In addition (3) can be nicely fit to the pseudo-potential data obtained by Fischetti and Laux [5] using the parameter values $\eta = 0.9\ \mathrm{eV}^{-1}$ and $\zeta = 1.4$ (cf. Fig. 1).

With this approximation for $g(\mathcal{E})$ expressions for $T_n(a,b)$ and $\beta_n(a,b)$ can be found

$$T_n = \frac{2}{3}\frac{a}{k_B}\frac{m_1}{m_0} \qquad \beta_n = \frac{3}{5}\frac{m_0\,m_2}{m_1^2} \tag{4}$$

$$m_l = Ag_0\frac{a^{l+3/2}}{b}\left[\Gamma\Big(\frac{2l+3}{2b}\Big) + (\eta a)^\zeta\Gamma\Big(\frac{2l+2\zeta+3}{2b}\Big)\right] = Ag_0\frac{a^{l+3/2}}{b}F_l(a,b) \tag{5}$$

As there is no analytical inversion of (4) with respect to a and b, the solution has been obtained by a two-dimensional Newton procedure. A comparison of DFs obtained by Monte Carlo (MC) simulation and their analytical counterparts is given in Fig. 3 and Fig. 4 for the bulk case and the short channel device, respectively. Also shown are the results based on a parabolic band approximation ($\eta = 0$). The analytical expression slightly overestimates the high-energy tail when the curvature of the DF is too strong. However, with a more realistic MC model employing a fullband structure and including electron-electron scattering, the temperature of the high-energy tail is increased and the curvature of the DF diminished which in turn improves the quality of the analytical expression.

With this analytical description for the distribution function, microscopic scattering rates can be evaluated to yield models suitable for macroscopic transport models. We considered the anisotropic model of Quade *et al.* [6], the isotropic expressions given by Keldysh [7], and the extension used by Fischetti *et al.* [8]. In the following we

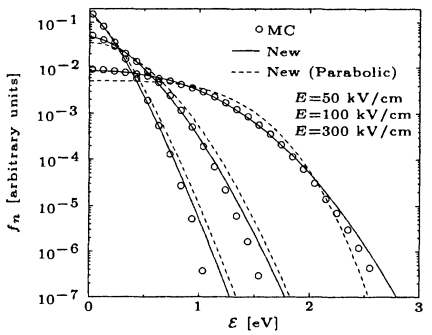

Fig. 3: Comparison of analytical expressions for the DF with MC results for the bulk case

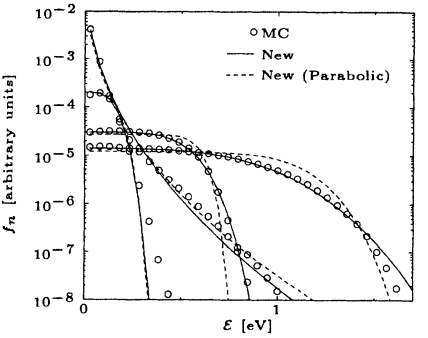

Fig. 4: Comparison of analytical expressions with MC results for the short channel device

restrict ourselves to the Keldysh formula $P_{\mathrm{II}}(\mathcal{E}) = P_0(\mathcal{E}-\mathcal{E}_{\mathrm{th}})^2/{\mathcal{E}_{\mathrm{th}}}^2$, because it gives rather compact results and can be easily extended to Fischetti's expression. For the six moments model [9] the additional terms to the right hand side of the balance equations are required which can be obtained via

$$G_{\mathrm{II},l} = \int_{\mathcal{E}_{\mathrm{th}}}^{\infty} \mathcal{E}^l \, P_{\mathrm{II}}(\mathcal{E}) \, f(\mathcal{E}) \, g(\mathcal{E}) \, \mathrm{d}\mathcal{E} \tag{6}$$

Here $l = 0, 1, 2$ denote the entries for the continuity, energy balance, and kurtosis balance equations, respectively. As we are only interested in the high energy part of the density of states, Cassi's expression can be savely used to give the final expression

$$G_{\mathrm{II},l} = n \, P_0 \, {\mathcal{E}_{\mathrm{C}}}^{1-\lambda} \, \frac{a^{l+\lambda-1/2}}{F_l(a,b)} \left(\Gamma_{1,l} - 2{z_{\mathrm{th}}}^{-1/b}\Gamma_{2,l} + {z_{\mathrm{th}}}^{-2/b}\Gamma_{3,l} \right) \tag{7}$$

with $\lambda = 1.32$, $\mathcal{E}_{\mathrm{C}} = 0.07$ eV, $\Gamma_{j,l} = \Gamma[(j+l+\lambda)/b, z_{\mathrm{th}}]$ where $\Gamma[a,x]$ is the incomplete Gamma function and $z_{\mathrm{th}} = (\mathcal{E}_{\mathrm{th}}/a)^b$. We used $P_0 = 4.18 \cdot 10^{12}$ s^{-1} and $\mathcal{E}_{\mathrm{th}} = 1.12$ eV consistently with the MC simulation, values which fit available experimental data as shown in Fig. 2.

A comparison of $G_{\mathrm{II}} = G_{\mathrm{II},0}$ from (7) with the MC results and the model proposed by Sonoda *et al.* is given in Fig. 5 and Fig. 6 for n^+-n-n^+ test-structures with channel lengths of 1.5 μm and 0.2 μm, respectively. The short channel device was taken from [1] and the channel length was increased to give the long channel version. The maximum electric fields where 120 kV/cm and 320 kV/cm for the long and short channel devices, respectively. Note that the models were evaluated using T_n and β_n from the MC simulation. To fit the short channel device the parameters of Sonoda's model had to be adjusted whereas the new model uses the same parameters as in the MC simulation. For the long channel device, the new model slightly overestimates the ionization rates because the high energy tail in the DF is overestimated by the analytical model. For the short channel device, the new model predicts the tail in the drain region. Unfortunately, the high energy tail is overestimated because the analytical DF cannot capture the turning point.

(7) can also be used to demonstrate the inaccuracies introduced by assuming a heated Maxwellian distribution when deriving macroscopic impact-ionization rates as done

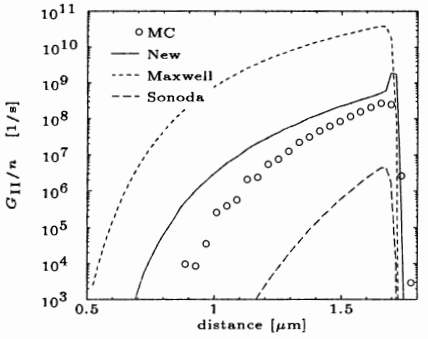

Fig. 5: Comparison of the new expressions with other models for a long channel device

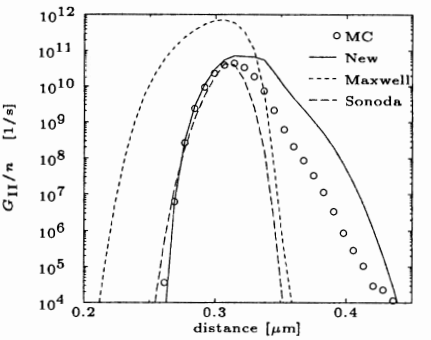

Fig. 6: Comparison of the new expressions with other models for a short channel device

e.g. in [6]. For a heated Maxwellian distribution function which is characterized by $a = k_B T_n$ and $b = 1$, (7) delivers results similar to local energy models [10] which considerably overestimate the ionization rates as also shown in Fig. 2, Fig. 5, and Fig. 6. This overestimation leads to non-physical calibrations of the model parameters which are only valid for a very narrow range of devices. Furthermore, impact ionization caused by hot electrons in the drain cannot be captured because the cold carriers dominate the average energy which is close to the lattice temperature in the drain region.

3 Conclusion

We have demonstrated that the average square energy provides the necessary information to develop an analyical expression for the distribution function which goes beyong the heated Maxwellian assumption. Replacing the heated Maxwellian DF with the new expression allows for accurate evaluation of microscopic impact ionization rates for bulk and submicron devices. The new model nicely fits into the concept of macroscopic device simulators as it only employs local quantities.

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