Moment Expansion Approach to Calculate Impact Ionization Rate in Submicron Silicon Devices

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Abstract

A method to calculate the impact ionization rate in submicron silicon devices is developed using both an average energy and an average square energy of electrons. The method consists of an impact ionization model formulated with the average energy and conservation equations for the average square energy in the framework of an energy transport model. Parameters for the transport equations are extracted in such a way that calculated moments based on these equations match Monte Carlo simulation results. The impact ionization generation rate in an n^+nn^+ structure calculated with this method agrees well with the results obtained from Monte Carlo simulation. The new method is also applied to a submicron n-MOSFET. The calculated distribution of the generation rate is found to be quite different from the results based on a conventional method.

1. Introduction

Much effort has been devoted to device miniaturization into a deep submicron region to accomplish higher density of integration and better circuit performance. Device degradation caused by hot carrier effects has been a primary concern in recent years because the power supply voltage has not been scaled down along with the physical dimensions of MOSFETs. A device simulator is a powerful tool to optimize device structure by satisfying both current drive capability and suppression of device degradation. Although it is mandatory to utilize accurate physical models to obtain precise simulation results, the presence of a large field gradient and the multi-dimensional nature of the physical phenomena make it difficult to simulate the hot carrier effects in deep submicron MOSFETs.

The most popular approach for the calculation of impact ionization (I.I.) is a local field (LF) model in the framework of a drift-diffusion model. In the LF model, an I.I. coefficient, α, which is the number of ionization events per unit length along a current path, is determined[1]

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*on leave from ULSI Laboratory, Mitsubishi Electric Corporation, Mizuhara, Itami, Hyogo, 664 Japan by the local electric field, E, with the characteristic field strength, E_c, as $\alpha \propto \exp(-E_c/E)$. Strictly speaking, the LF model holds only in a homogeneous electric field because the energy distribution function of carriers is not described using a local electric field in the case where the field varies within the energy relaxation length, which is the product of the saturation velocity and the energy relaxation time for electrons, $v_{sat}\tau_{\langle\varepsilon\rangle}(\sim 0.05\mu\mathrm{m})$. The value, $\tau_{\langle A\rangle}$, is the relaxation time of $\langle A\rangle \equiv \int fA\,d\boldsymbol{k}/\int f\,d\boldsymbol{k}$, which are used hereafter. The LF model tends to overestimate the I.I. rate in an increasing-field region; a simulated substrate current is normally much larger than its experimental counterpart.

In order to overcome these shortcomings, a non-local field (NLF) model[2–4] was proposed. In this model, carrier trajectories are traced back along an electric field path to a point where the electrostatic potential difference is equal to the effective threshold energy for impact ionization, V_I. The ionization coefficient is expressed[4] with the path length d as $\alpha \propto \exp(-d/\lambda_p)$, where λ_p is the effective mean free path without being scattered by the optical phonons. In a homogeneous field, the model reduces to the local field model with the relation of $\lambda_p = V_I/E_c$. In the non-local field model, the impact ionization phenomenon is treated as a one-dimensional problem. In reality, high energy electrons move around in three-dimensional space so that it is questionable whether this method can be adapted to multi-dimensional device structure.

The exact calculation of the impact ionization coefficient demands the use of an energy distribution function, because impact ionization events are caused by energetic carriers. The average energy of the distribution function is a basic physical parameter to characterize the energy distribution. It is more appropriate to use the average energy rather than the electric field to express the impact ionization coefficient. In a homogeneous high electric field,the average energy, $\langle\varepsilon\rangle$, is given by the electric field, E, as $\langle\varepsilon\rangle = qEv_{sat}\tau_{\langle\varepsilon\rangle}$. This relation is combined with the local field model to give

$$\alpha \propto \exp\left(-\frac{\varepsilon_c}{\langle\varepsilon\rangle}\right). \tag{1}$$

This model is called a local energy (LE) model because the ionization coefficient is expressed as a function of the local average energy. The characteristic energy, ε_c, is obtained from $\varepsilon_c = qE_c v_{sat}\tau_{\langle\varepsilon\rangle}$. This model is often used in energy transport models[5–7]. Other expressions for the impact ionization generation rate have been proposed[8–10] using the average energy of carriers.

Recent studies[11–14] have shown that the average energy is not a good measure to predict impact ionization generation rate in an inhomogeneous field. The authors have proposed[14] the impact ionization model using the average square energy of electrons $\langle\varepsilon^2\rangle$ in addition to the average energy $\langle\varepsilon\rangle$. The pair creation rate by impact ionization in an inhomogeneous field is expressed as

$$G_{ii} = n g_{ii\,0} \exp\left(-\frac{\varepsilon_c}{\langle\varepsilon\rangle_{eff}}\right), \tag{2}$$

$$\langle\varepsilon\rangle_{eff} = \langle\varepsilon\rangle \exp(\gamma(\xi - \xi_h)), \tag{3}$$

$$\xi \equiv \frac{\sqrt{(3/5)\langle\varepsilon^2\rangle}}{\langle\varepsilon\rangle} \tag{4}$$

which gives higher accuracy compared with previous models. The values of the parameters that appear in the above expressions are shown in Table II.

In this paper, we propose a new method to calculate impact ionization generation rate in deep submicron MOSFETs. It is based on the moment expansion of distribution functions. The transport equations for the average square energy as well as the carrier concentration and the average energy are derived from the Boltzmann transport equation (BTE) in Section 2. Simulation results for an n^+nn^+ structure and an n-MOSFET are shown in Section 3.

2. Moment Expansion Method

There are two ways to derive the energy transport model from the BTE: the energy balance (EB) model[15] and the hydro-dynamic (HD) model[16]. Both of them are derived by multiplying the BTE by a group velocity $\boldsymbol{u}$ and/or an energy ε and integrating them over $\boldsymbol{k}$-space. A major difference between these models lies in the treatment of the collision term in the BTE. In the HD model, the relaxation times for each moment (average velocity, average energy, etc.) are introduced to express the collision terms after the integration over $\boldsymbol{k}$-space. In the EB model, on the other hand, the collision term in the BTE is expressed as $-(f-f_0)/\tau$, in which only a microscopic relaxation time, τ, is included. The resulting equations of these models take different forms. From the practical point of view, however, they are regarded as similar, except for the definition of the parameters used in the equations[17,6].

Several attempts have been made to clarify which model is more suitable for semiconductor device simulation[6,18], and it has been concluded that neither the EB nor the HD model correctly describes the moments in an inhomogeneous field. We treat the parameters in the equations only as fitting variables to reproduce the moments which are close to those obtained from Monte Carlo simulation.

The energy transport model used in this study consists of the following equations[18]:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\langle \boldsymbol{u} \rangle) = \left(\frac{\partial n}{\partial t}\right)_{\mathrm{GR}}, \tag{5}$$

$$\frac{\partial n\langle\varepsilon\rangle}{\partial t} + q\boldsymbol{E}\cdot(n\langle\boldsymbol{u}\rangle) + \nabla\cdot(n\langle\varepsilon\boldsymbol{u}\rangle) = -n\frac{\langle\varepsilon\rangle - \langle\varepsilon\rangle_0}{\tau_{\langle\varepsilon\rangle}} + \left(\frac{\partial n\langle\varepsilon\rangle}{\partial t}\right)_{\mathrm{GR}}, \tag{6}$$

with the consecutive equations

$$n\langle\boldsymbol{u}\rangle = -n\mu\boldsymbol{E} - \mu\frac{kT_n}{q}\nabla n - \mu\frac{k}{q}(1+\nu_0)n\nabla T_n, \tag{7}$$

$$n\langle\varepsilon\boldsymbol{u}\rangle = \frac{\tau_{\langle\varepsilon\boldsymbol{u}\rangle}}{\tau_{\langle\boldsymbol{u}\rangle}}\frac{5}{3}\left(kT_n(n\langle\boldsymbol{u}\rangle) - qn\mu\left(\frac{k}{q}\right)^2(1+\nu_1)T_n\nabla T_n\right). \tag{8}$$

The electron temperature, T_n, is defined by $\langle\varepsilon\rangle = (3/2)kT_n$. The terms $(\partial n/\partial t)_{\mathrm{GR}}$ and $(\partial n\langle\varepsilon\rangle/\partial t)_{\mathrm{GR}}$ mean the relaxation rates for the electron density and the average energy due to the generation-recombination (GR) process, respectively. In the consecutive equations (7) and (8), $n\langle\boldsymbol{u}\rangle$ and $n\langle\varepsilon\boldsymbol{u}\rangle$ are particle- and energy-fluxes, respectively.

For the relaxation rate caused by the GR process, only the I.I. is taken into account in this study, i.e. $(\partial n/\partial t)_{\mathrm{GR}} = G_{\mathrm{ii}}$. The relaxation rate of the average energy due to I.I. is formulated as $(\partial n\langle\varepsilon\rangle/\partial t)_{\rm GR} = \varepsilon_{\rm loss}G_{\rm ii}$, where $\varepsilon_{\rm loss}$ is the net average energy loss by impact ionization.

The physical parameters, μ, $\tau_{\langle\varepsilon\rangle}$, $\tau_{\langle\boldsymbol{u}\varepsilon\rangle}/\tau_{\langle\boldsymbol{u}\rangle}$ and $\varepsilon_{\rm loss}$ are determined to fit the E-$\langle u\rangle$, E-$\langle\varepsilon\rangle$ and E-$\langle\varepsilon u\rangle$ curves obtained from MC simulations[14] in homogeneous fields as shown in Fig. 1. The values of these parameters are summarized in Table I. For the mobility, μ, the empirical expression

$$\mu = \frac{\mu_0}{\left(1+\left(\dfrac{\mu_0 E(\langle\varepsilon\rangle)}{v_{\rm sat}}\right)^{\beta}\right)^{1/\beta}} \tag{9}$$

is used, where $E(\langle\varepsilon\rangle)$ is the electric field as a function of the average energy in a homogeneous field.

The remaining parameters ν_0 and ν_1, which relate to the non-local transport effect, cannot be determined uniquely because they depend on the field profile[19]. In order to derive these parameters, we employ the one-dimensional test structure as shown in Fig. 2 which has a similar field profile along the channel of the deep submicron MOSFETs. The parameters ν_0 and ν_1 are calibrated to fit the average velocity and the average energy to MC results.

The average square energy, $\langle\varepsilon^2\rangle$, is calculated using the particle concentration and the average energy, which are obtained from the energy transport model. The conservation equations for $\langle\varepsilon^2\rangle$ are derived from the BTE as follows:

$$\frac{\partial n\langle\varepsilon^2\rangle}{\partial t} + 2q\boldsymbol{E}\cdot(n\langle\varepsilon\boldsymbol{u}\rangle) + \nabla\cdot(n\langle\varepsilon^2\boldsymbol{u}\rangle) = -n\frac{\langle\varepsilon^2\rangle - \langle\varepsilon^2\rangle_0}{\tau_{\langle\varepsilon^2\rangle}} + \left(\frac{\partial n\langle\varepsilon^2\rangle}{\partial t}\right)_{\rm GR}, \tag{10}$$

$$n\langle\varepsilon^2\boldsymbol{u}\rangle = \frac{\tau_{\langle\varepsilon^2\boldsymbol{u}\rangle}}{\tau_{\langle\boldsymbol{u}\rangle}}\frac{7}{3}\left(\langle\varepsilon^2\rangle(n\langle\boldsymbol{u}\rangle) - n\mu\frac{kT_n}{q}(1+\nu_2)\nabla\langle\varepsilon^2\rangle\right). \tag{11}$$

Equations (10), (11) together with the energy transport model (5)–(8) are solved using the box integration method[20] to give the average square energy of the electrons. The relaxation rate of the average square energy due to I.I. is formulated as $(\partial n\langle\varepsilon^2\rangle/\partial t)_{\rm GR} = {\varepsilon^2}_{\rm loss}G_{\rm ii}$, where ${\varepsilon^2}_{\rm loss}$ is the net loss of the average square energy by impact ionization.

The parameters in the equations, $\tau_{\langle\varepsilon^2\rangle}$, $\tau_{\langle\varepsilon^2\boldsymbol{u}\rangle}/\tau_{\langle\boldsymbol{u}\rangle}$ and ${\varepsilon^2}_{\rm loss}$, are determined using Monte Carlo simulation in a homogeneous electric field, whereas the nonlocal transport parameter, ν_2, is determined in such a way that the numerically calculated average square energy fits those obtained from MC simulations in the structure shown in Fig. 2. The set of physical parameters is summarized in Table I.

3. Results and Discussion

Impact ionization generation rates in the n^+nn^+ structure calculated with several impact ionization models described in Section 1 are shown in Fig. 3. The calculated results using the MC simulation are also shown. Parameters used in these models, which are shown in Table II, are adjusted so as to give the same generation rate in a homogeneous electric field.

Note that the LF model overestimates the generation rate by more than one order of magnitude. The NLF model yields a smaller generation rate in the up-field region and better accuracy in the down-field region than the LF model. This model, however, still shows an excessive generation rate in the up-field region. Unlike previous two models, the LE model, which is often used in device simulation with an energy transport model, gives a reasonable maximum generation rate which is closer to the MC result. In the down-field region, this model gives poor agreement with the generation rate derived from MC simulation because the average energy in the region is lowered due to the existence of cold electrons diffused from the high concentration region.

In contrast to the models described above, the new impact ionization model Eq. (2), formulated with $\langle\varepsilon\rangle$ and $\langle\varepsilon^2\rangle$, well describes the impact ionization rate in both up- and down-field regions. In this model, the distribution functions at a given average energy in up- and down-field regions is differentiated by the use of the average square energy.

We also calculate the I.I. generation rate in an n-MOSFET with gate length of 0.55 μm, to study the applicability of the new method to a two-dimensional problem. Figure 4 shows the calculated average energy of electrons near the drain junction. The calculated I.I. generation rates using the LE model and the new model are compared in Fig. 5. Although the calculated substrate currents are the same order of magnitude, the new model demonstrates that most of the I.I. events occur in regions farther away from the Si/SiO_2 interface. In order to clarify the relation between the location of the I.I. events and device degradation caused by carrier injection into gate oxide, further investigation will be necessary.

Comparisons with previous works are mentioned below. Concerning the numerical aspect to solve the BTE, it is not new to expand the distribution function with appropriate functions (Legendre polynomial, etc.) in order to translate the BTE into a more tractable form. The series expansion of the Legendre polynomial[21] has been extensively used to calculate impact ionization in high electric field[22–25]. This method, however, requires the discretization in an energy- or momentum-space as well as in a real-space which results in computational burden. On the other hand, the moment approach or a Taylor series expansion, which is used in this study, is the extension of the conventional drift-diffusion or energy transport device simulation technologies, and the discretization in the energy space is not necessary.

Several attempts have been made to improve the accuracy of high-energy population of the distribution function by solving conservation equations for the high energy tail[12,13]. In these works, however, some ambiguity remains in defining the boundary conditions between the low- and high-energy regions. In our method, on the other hand, there is no need to draw the line between the low- and high-energy range of distribution functions.

We also mention the average energy of carriers obtained from energy transport equations. In the calculation of the energy transport equations reported by several authors[26,7], the peak of the average energy shifts along the current direction because the cold electrons diffused from the high density region are ignored. The resulting generation rate coincides with that from MC simulation. However, the "average energy" in this case has a different physical meaning from the conventional one.

4. Conclusions

A method to calculate impact ionization in submicron silicon devices has been developed, in which the impact ionization is formulated using the average energy and the average square energy. A set of transport equations to obtain the average square energy has been proposed in the framework of an energy transport model. Parameters used in the equations were extracted in such a way that the calculated results based on these equations agree well with Monte Carlo simulation results in both homogeneous and inhomogeneous fields. The new method was applied to investigate the impact ionization generation rate in a submicron n-MOSFET. The calculated results show that impact ionization events occur in deeper channel regions than the LE model's prediction.

Acknowledgment

K. Sonoda wishes to thank Dr. N. Kotani of ULSI Laboratory, Mitsubishi Electric Corporation for his encouragement and constant support.

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TABLES

Table I. Values of parameters used in the energy balance model.

Parameters	Values
μ_0	1350 $\mathrm{cm}^2/\mathrm{Vs}$
v_{sat}	9.0×10^6 cm/s
β	2.0
$\tau_{\langle\varepsilon\rangle}$	0.55 ps
$\tau_{\langle\varepsilon^2\rangle}$	0.30 ps
$\tau_{\langle\varepsilon\boldsymbol{u}\rangle}/\tau_{\langle\boldsymbol{u}\rangle}$	0.90
$\tau_{\langle\varepsilon^2\boldsymbol{u}\rangle}/\tau_{\langle\boldsymbol{u}\rangle}$	0.65
$\varepsilon_{\mathrm{loss}}$	1.5 eV
${\varepsilon^2}_{\mathrm{loss}}$	8.0 eV^2
ν_0	-0.2
ν_1	-2.0
ν_2	-1.5

Table II. The impact ionization models investigated and their physical parameters.

Models	Formulas and Parameters
Local Field (LF) model	$\alpha = \alpha_0 \exp\left(-\frac{E_c}{E}\right)$, $\alpha_0 = 1.40 \times 10^6\ \mathrm{cm}^{-1}$, $E_c = 1.32 \times 10^6\ \mathrm{V/cm}$
Non-Local Field (NLF) model	$\alpha = \alpha_0 \exp\left(-\frac{d}{\lambda_p}\right)$, $V_I = \int_{x-d}^{x} \boldsymbol{E} \cdot d\boldsymbol{l}$, $\lambda_p = V_I/E_c$, $V_I = 1.1\ \mathrm{eV}$
Local Energy (LE) model	$G_{ii} = n g_{ii\,0} \exp\left(-\frac{\varepsilon_c}{\langle\varepsilon\rangle}\right)$, $g_{ii\,0} = 1.39 \times 10^{14}\ \mathrm{s}^{-1}$, $\varepsilon_c = 8.78\ \mathrm{eV}$
New model	$G_{ii} = n g_{ii\,0} \exp\left(-\frac{\varepsilon_c}{\langle\varepsilon\rangle_{\mathrm{eff}}}\right)$, $\langle\varepsilon\rangle_{\mathrm{eff}} = \langle\varepsilon\rangle \exp(\gamma(\xi - \xi_h))$, $\gamma = \begin{cases} 4.2 & (\xi < \xi_h) \\ 1.6 & (\xi > \xi_h) \end{cases}$, $\xi_h = 0.88$

FIGURES

Fig. 1. Moments in a homogeneous electric field calculated using Monte Carlo (solid symbols) and energy balance equations (lines): (a) the average velocity, $\langle u \rangle$, (b) the average energy, $\langle \varepsilon \rangle$, and the energy flux, $\langle \varepsilon u \rangle$, and (c) the average square energy, $\langle \varepsilon^2 \rangle$, and the flux of square energy, $\langle \varepsilon^2 u \rangle$.

Fig. 2. (a) An n^+nn^+ structure used to determine the nonlocal transport parameters, ν_0, ν_1 and ν_2. Calculated results from MC and energy balance model: (b) the electric field, (c) the average velocity, and (d) the average energy and average square energy. Solid and dashed lines indicate the calculated results of MC and energy balance model, respectively.

Fig. 3. Calculated impact ionization generation rates in the n^+nn^+ structure shown in Fig. 2. The parameters in the impact ionization models are set so as to give the same generation rate in a homogeneous electric field.

Fig. 4. The average energy of electrons at the drain junction of an n-channel MOSFET at $V_{\mathrm{d}} = 2$V and $V_{\mathrm{g}} = 1$V. The gate length is 0.55 μm ($-0.275 \le x \le 0.275\mu$m). The Si/SiO$_2$ interface lies at $y = 0$. The solid line indicates the metallurgical p-n junction.

Fig. 5. Calculated electron-hole pair generation rates due to impact ionization (I.I.) near the drain junction of the n-channel MOSFET shown in Fig. 4: (a) with the local energy (LE) I.I. model, and (b) with the new I.I. model (the average energy and the average square energy dependent). The solid lines indicate the metallurgical p-n junction.