

# Impact Ionization Model Using Second- and Fourth-Order Moments of Distribution Function

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## Abstract

This paper describes an impact ionization model suitable for calculation of an impact ionization rate in inhomogeneous electric field. The model is formulated using second- and fourth-order moments of an electron energy distribution function. A set of model equations for carrier transport in semiconductor devices is also presented to perform practical device simulation with the impact ionization model. The calculation result with the new models agrees to Monte Carlo simulation result.

## 1. Introduction

Scaling-down the dimensions of silicon devices without proportional decrease of power supply voltage induces high electric field, which causes hot carrier effects. Device degradation caused by hot carriers has been main concern from the reliability point of view. Because secondary-generated carriers created by impact ionization (I.I.) have great influence on the degradation of gate oxide, accurate modeling of I.I. is necessary.

An ionization coefficient, which is the number of I.I. event per unit length, has been conventionally expressed as a function of electric field[1]. It has also been formulated using average carrier energy[2] to take the effect of non-uniform electric field into account. In the past few years, it has been reported that the average energy is still insufficient to describe nonlocal nature of I.I. in non-uniform electric field[3][4].

We propose an I.I. model which is formulated using second- and fourth-order moments of an electron energy distribution function. A set of model equations to calculate the fourth-order moment is also presented to perform device simulation with the I.I. model.

## 2. Impact Ionization Model

To investigate the I.I. phenomena in inhomogeneous field, we use the Monte Carlo (MC) simulation program with analytical multi-valley band structure, in which phonon

scattering rates [5] and the impact ionization rate [6] are implemented as a function of electron energy.

Calculated average energy,  $\langle \varepsilon \rangle$ , and impact ionization coefficient,  $\alpha$ , in the inhomogeneous electric field (Fig. 1(a)) are shown in Figs. 1(b) and (d), respectively. The symbol,  $\langle A \rangle$ , means  $\int A f d\mathbf{k} / \int f d\mathbf{k}$  hereafter. The ionization coefficient,  $\alpha$ , is obtained from the relation,  $G_{ii} = n \langle \mathbf{u} \rangle \alpha$ , where  $G_{ii}$  is the electron-hole pair generation rate caused by I.I.,  $n$  is the electron density, and  $\mathbf{u}$  is the group velocity of an electron. Note that  $n$ , and  $\langle \mathbf{u} \rangle$  are zeroth-, and first-order moments, respectively. These figures show that in spatially varying electric field, the impact ionization coefficient is no longer determined by the average energy alone, but strongly depends on the high energy tail of distribution function (Fig. 2).

In order to express impact ionization coefficient precisely, we use a fourth-order moment of the distribution function,  $\langle \varepsilon^2 \rangle$ , in addition to second-order moment,  $\langle \varepsilon \rangle$ . The fourth-order moment is parameterized in a normalized form,  $\xi = ((3/5)\langle \varepsilon^2 \rangle)^{1/2} / \langle \varepsilon \rangle$ . The factor  $(3/5)^{1/2}$  is introduced so as to  $\xi = 1$  when the distribution function is Maxwellian. Fig. 1(c) shows the parameter,  $\xi$ , calculated using MC simulation. The figure shows that  $\xi$  starts to increase where the field decreases, which coincides with the fact that the high energy tail of the distribution function remains in spite of the rapid decrease of electric field and average energy.

Fig. 3 shows calculated ionization coefficient for several maximum field ( $E_{\max} = 200, 300, 400, 500 \text{ kV/cm}$ ) in Fig. 1(a) as a function of the inverse of the average energy with several  $\xi$ 's as a parameter. The figure shows that ionization coefficient,  $\alpha$ , is expressed as  $\alpha_0 \exp(-\varepsilon_c / \langle \varepsilon \rangle)$  for a given  $\xi$ , where  $\alpha_0$  is a constant and  $\varepsilon_c$  depends on  $\xi$ . The coefficient,  $\varepsilon_c$ , is plotted as a function of  $\xi$  in Fig. 4 to show the relation,  $\varepsilon_c \propto \exp(-\gamma \xi)$ , where  $\gamma$  is constant. From Figs. 3 and 4, the impact ionization coefficient,  $\alpha$ , is modeled as

$$\alpha = \alpha_0 \exp\left(-\frac{\varepsilon_{c0} \exp(-\gamma \xi)}{\langle \varepsilon \rangle}\right), \quad (1)$$

where  $\alpha_0 = 1.4 \times 10^7 \text{ cm}^{-1}$ ,  $\varepsilon_{c0} = 82.3 \text{ eV}$ , and  $\gamma = 2.56$ . In the homogeneous field case,  $\xi = 0.88$  and  $\varepsilon_c = 8.7 \text{ eV}$  from the MC simulation.

### 3. Moment Conservation Equations

Both second-order moment,  $\langle \varepsilon \rangle$ , and fourth-order one,  $\langle \varepsilon^2 \rangle$ , are required to use the new I.I. model (1) in device simulation. The fourth-order moment is numerically calculated from the conservation equations of the moment incorporated in a hydrodynamic model[7]. The equations are derived from the Boltzmann transport equation (BTE) to be

$$\nabla \cdot (n \langle \mathbf{u} \varepsilon^2 \rangle) = -2q\mathbf{E} \cdot \mathbf{S} - n \frac{\langle \varepsilon^2 \rangle - \langle \varepsilon^2 \rangle_0}{\tau_{\langle \varepsilon^2 \rangle}} - U_{\langle \varepsilon^2 \rangle} \quad (2)$$

$$n \langle \mathbf{u} \varepsilon^2 \rangle = \frac{\tau_{\langle \varepsilon^2 \rangle}}{\tau_{\langle \mathbf{u} \rangle}} \frac{7}{3} \left( \langle \varepsilon^2 \rangle \frac{\mathbf{J}}{-q} - \frac{kT_n}{q} n \mu \nabla \langle \varepsilon^2 \rangle \right), \quad (3)$$

where  $\mathbf{E}$  is the electric field,  $\mathbf{J} \equiv -qn \langle \mathbf{u} \rangle$  is the electron current density,  $\mathbf{S} \equiv n \langle \mathbf{u} \varepsilon \rangle$  is the electron energy flux,  $\langle \varepsilon^2 \rangle_0$  is the fourth-order moment at thermal equilibrium,  $U_{\langle \varepsilon^2 \rangle}$  is the net loss rate of  $\langle \varepsilon^2 \rangle$  due to generation-recombination process,  $\tau_{\langle A \rangle}$  is the relaxation time of  $\langle A \rangle$ ,  $\mu$  is the electron mobility, and  $T_n$  is the electron temperature defined by  $3kT_n/2 \equiv \langle \varepsilon \rangle$ . The parameters,  $\tau_{\langle \varepsilon^2 \rangle} = 0.29 \text{ ps}$ ,  $\tau_{\langle \mathbf{u} \varepsilon^2 \rangle} / \tau_{\langle \mathbf{u} \rangle} = 0.59$  are extracted from MC simulation in homogeneous electric field.

## 4. Results and Discussions

In order to verify the new I.I. model, we calculate I.I. generation rate,  $G_{ii}$ , in an  $n^+nn^+$  structure using moment equations with different I.I. models. They are compared with MC result in Figs. 5(a) and (b). Parameters used in the I.I. models are calibrated to provide the same I.I. coefficient as that obtained from MC simulation in homogeneous electric field. In the MC simulation, the BTE and Poisson equation are solved self-consistently. In the MC simulation, generated carriers by impact ionization are ignored because the number of created carriers has little effect on the total number of carriers in the calculation condition here. Generation terms in the moment equations are also ignored by the same reason.

The calculated results with a local I.I. model,  $\alpha(E)$ , in which the coefficient is determined by the electric field, overestimate maximum I.I. rate nearly one order of magnitude. Moreover, it underestimates the generation rate in the decreasing field region. Although the maximum I.I. rate is improved with  $\alpha(\langle\varepsilon\rangle)$ , in which  $\alpha$  is expressed as a function of average energy only, this model still underestimate  $G_{ii}$  in the region where the electric field decreases. In contrast with the previous two models, the new model ( $\alpha(\langle\varepsilon\rangle, \xi)$ ) provides the generation rate which agrees with the MC result better than that with previous two models, especially in the field decreasing region.

The electric field of the  $n^+nn^+$  structure (Fig. 5(a)), which shows rapid increase and decrease, is similar to the previous field profile (Fig. 1(a)). The large generation rate in the field decreasing region attributes to the fact that the energetic carriers are still exist in spite of the low electric field and the low average energy as shown in Figs. 1 and 2. The parameter,  $\xi$ , incorporated with average energy,  $\langle\varepsilon\rangle$ , is an indicator for the high energy portion of the distribution function which contributes to impact ionization so that the new I.I. model can predict the generation rate better than previous I.I. models.

## 5. Conclusion

We proposed the I.I. model including second- and fourth-order moments of the distribution function, which is applicable for spatially varying electric field. The validity of the new model was verified through the comparison between the numerical calculation based on the generalized moment conservation equations and MC simulation in the  $n^+nn^+$  structure.

## References

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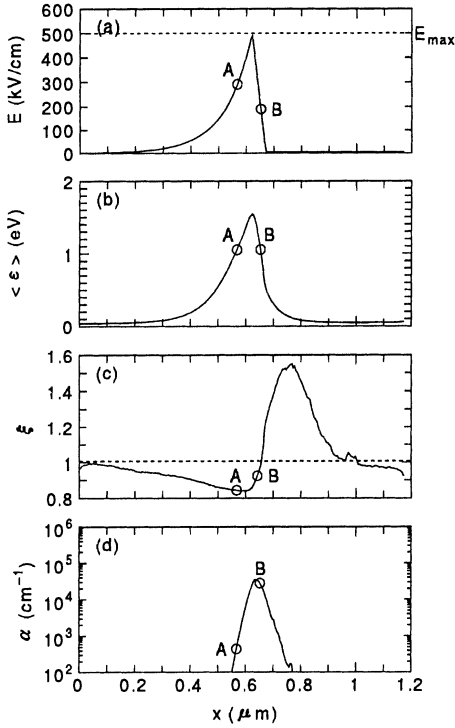


Figure 1: Results of Monte Carlo simulation at a given electric field profile. (a) Electric field,  $E$  (increases exponentially and decreases linearly), (b) Average energy,  $\langle \epsilon \rangle$ , (c)  $\xi \equiv \sqrt{(3/5)\langle \epsilon^2 \rangle / \langle \epsilon \rangle}$ , (d) Impact ionization coefficient,  $\alpha$ .

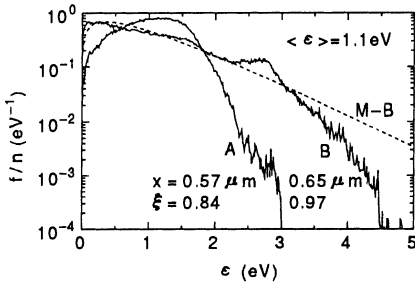


Figure 2: Electron energy distribution functions at points A and B in Fig. 1 where the average energy  $\langle \epsilon \rangle = 1.1 \text{ eV}$ . The dotted curve means Maxwell-Boltzmann distribution function for the same average energy.

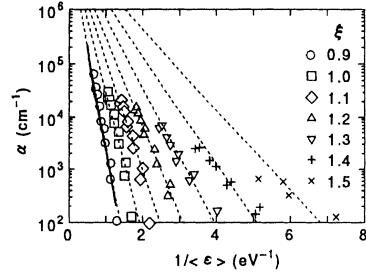


Figure 3: Impact ionization coefficient as a function of inverse average energy for different  $\xi$  values. Dashed lines are obtained from a least square fit to the data. Solid line indicates the value in homogeneous electric field.

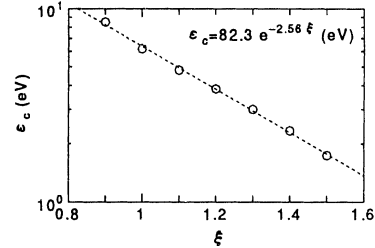


Figure 4: The slope of the data in Fig. 3,  $\epsilon_c$ , as a function of the parameter,  $\xi$ . Dashed line indicates the least square fit to the data.

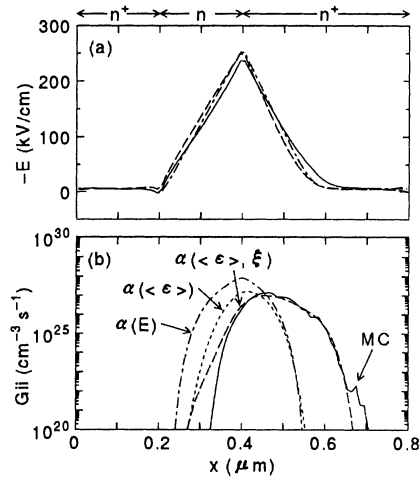


Figure 5: Calculated electric field and impact ionization rate in an  $n^+nn^+$  structure ( $n^+ = 2 \times 10^{17} \text{ cm}^{-3}$ ,  $n = 5 \times 10^{15} \text{ cm}^{-3}$ ). Applied voltage is 5V. (a) Electric field, (b) Impact ionization generation rate.