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# Physical Model for Deep Submicron Device Simulation

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Impact ionization rate based on rigorous physical model is derived for silicon with anisotropic and nonparabolic band structure. The validity of the model is verified by comparing calculated and experimental results on both impact ionization coefficient and quantum yield. Carrier transport characteristics in the presence of large electric field gradient is investigated using an iterative method based on the Boltzmann transport equation. A phenomenological length constant used in a modified drift-diffusion model is evaluated at room temperature. The length constant increases with applied electric field at low field and flattens out above 30kV/cm, reaching saturation value of 400Å.

## 1 Introduction

The majority of submicron MOSFETs are subject to regions of high electric fields and high carrier gradient which give rise to nonequilibrium transport conditions. Traditional device simulators based on drift-diffusion equations are not capable of modeling accurately future deep submicron MOSFETs. One approach to overcome this difficulty is to use an advanced energy relaxation model [1] which include momentum and energy relaxation effects of carriers. However, numerical calculation of the model under two carrier condition requires excessive amount of computational time and limit the usefulness of the relaxation model from a software engineering point of view. The other practical approach is to use the extended drift-diffusion model proposed by Price [2]. The model parameters, however, are not well investigated so that one has to obtain accurate parameters before applying the extended model to device simulation. The aim of this paper is twofold. We first report the model parameters obtained from Monte Carlo simulation and then we demonstrate carrier transport characteristics in submicron MOSFETs based on the extended drift-diffusion model with accurate model parameters.

## 2 Physical model

### 2.1 Impact ionization model

To properly predict substrate current in submicron MOSFETs by using Monte Carlo simulation, one must use impact ionization model as a function of electron energy instead of electric field. The use of Keldysh model [3] is, however, not adequate for predicting the impact ionization in silicon because the model assumes direct- and isotropic-parabolic band structure. Note that silicon has indirect anisotropic nonparabolic band structure. In order to estimate impact ionization more precisely, we derive a new impact ionization rate based on 'lucky drift' model [4,5] taking account of both anisotropy and nonparabolicity of the conduction band. The calculated impact ionization rate, $P_i(\varepsilon)$ , is found to be well expressed as

$$P_i(\varepsilon) = A\left(\frac{\varepsilon - \varepsilon_{th}}{\varepsilon_{th}}\right)^{2.5} \qquad (1)$$

where $\varepsilon_{th}$ is the threshold energy for impact ionization. Note that the power of the impact ionization rate is 2.5, while that of Keldysh model is only 2.0. This gives higher ionization rate than Keldysh model for higher energy region. The present model also gives soft ionization rate around the threshold energy, which is caused by the indirect and anisotropic band structure of silicon. Comparisons between calculated and experimental results of impact ionization coefficient [6,7,8,9] and quantum yield [10] are shown in Fig. 1(a) and (b) together with physical parameters ($\varepsilon_{th} = 1.7\text{eV}, P = 9.0 \times 10^{12}\text{s}^{-1}$) used in the calculation. The calculated results are in good agreement with the experimental results.

## 2.2 Extended drift diffusion model

It has been recognized that the carrier velocity is not well expressed as a function of the local electric field in the presence of large electric field gradient. In order to include nonlocal effect in the conventional drift-diffusion model, Artaki [11] and Price [2] added a term proportional to the field gradient with a phenomenological length constant $L(F)$ as

$$u = u_0(F)\left(1 + \frac{L(F)}{F}\frac{dF}{dx}\right) - \frac{D(F)}{n}\frac{dn}{dx} \qquad (2)$$

where $u_0(F)$ is the drift velocity corresponding to the homogeneous field $F$. Artaki estimated the length constant by means of Monte Carlo simulation using a simplified band structure: a single spherical and parabolic conduction band. The Monte Carlo simulation showed that $L(F)$ becomes significant only for field above 30kV/cm and flattens out with increasing field at about 400Å. In the field region below 30kV/cm, $L(F)$ is negligible and the data points scattered in a wide range because of stochastic noises due to the Monte Carlo simulation. For that reason, the data at low field are highly qualitative. In the present work, a quite accurate length constant has been estimated by using the iterative method [12] which provide the quite smooth carrier velocity versus space curve without stochastic noise.

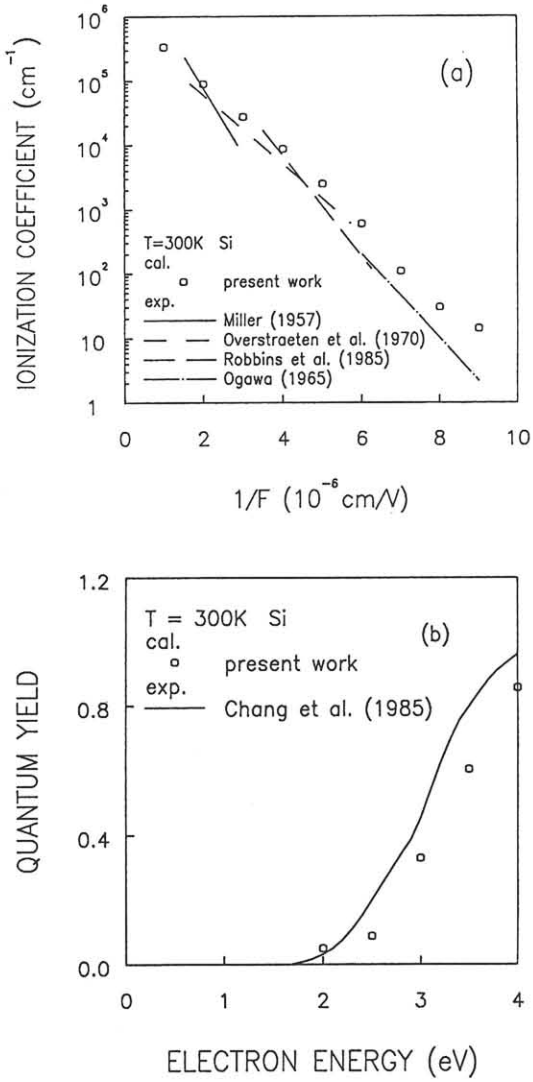


**Fig. 1** (a) Impact ionization coefficient versus inverse electric field for electrons at T=300K in Si. (b) Quantum yield versus electron energies at T=300K in Si.

## 3 Results and discussion

Figure 2 shows the calculated carrier velocity versus space curve at room temperature, using the iterative method. This simulation was carried out in a periodic field configuration with a strong field discontinuity at $x = 0.5\mu$m. The figure exhibits a velocity overshoot in the high field region near the interface. Figure 2 demonstrates that the requirement of carrier continuity forces electrons to be accelerated by diffusion in the low field region before experiencing

the high field. One further worth mentioning is that the carrier velocity undershoot is also observed at the high-low field interface. The calculation in Fig. 2 requires approximately 2 hours on a SX-2 supercomputer.

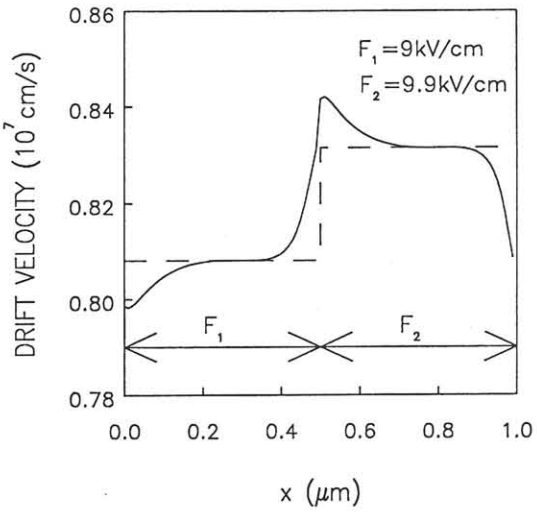


**Fig. 2** Electron velocity versus distance in a periodic field.

Figure 3 shows the length coefficient, $L(F)$, evaluated using the iterative method [12] and the formula proposed by Price [2]. In the low electric field region, the calculated $L(F)$ linearly increases with field, while it saturates to the value of 400 Å at 30kV/cm. The discrepancy between our results and the data obtained from the Monte Carlo simulation by Artaki [11] attributes to the stochastic noise at low field in the Monte Carlo simulation. In order to verify the hypothesis, the length coefficient is estimated by a different approach using analytical formula. Although this would be a rough estimation, the qualitative feature of the length coefficient is obtained. By using a generalized Einstein relation and the Caughey-Thomas expression [13] for field dependent mobility, the electron temperature can be directly related to the applied field in stedy-state conditions as follows

$$T_e = T_0 \sqrt{1 + \left(\frac{\mu_{n0} F}{v_s}\right)^2}. \qquad (3)$$

Using the above equation, the length constant is given by

$$L(F) = \frac{1}{e}\frac{d\langle\epsilon\rangle}{dF} = \frac{3k_B}{2e}\frac{dT_e}{dF}. \qquad (4)$$

Using equations (3) and (4), the length coefficient can be obtained by simply differentiating the average electron temperature with respect to the electric field. The analytical result agrees well with our simulation.

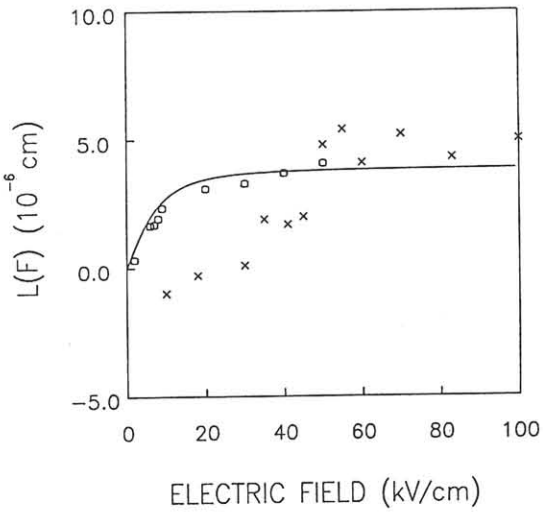


**Fig. 3** Length coefficient as a function of electric field calculated from iterative method ( o ) , Monte Carlo (Artaki 1988) ( × ) and Eq. (4) (solid line).

Finally, carrier transport characteristics of submicron devices are investigated from the practical point of view. In Fig. 4 we show the velocity profile in submicron MOSFET along the channel. Equation (2) indicates that in a field increasing along current flow, the carrier velocity exceeds $u_0$, meaning the velocity overshoot, while in a field decreasing along current flow, Eq. (2) leads to the velocity undershoot as shown in Fig. 3. This fact means that the advantage of nonequilibrium carrier transport cannot be easily taken of the velocity overshoot because both accelerating and decelerating field coexist in the actual devices. Note that the benefit of velocity overshoot in the channel of a MOSFET cannot be realized until the carriers are overshooting very near their injection point from the source into the channel. For that reason, the nonequilibrium transport effect should be taken into account for deep submicron device simu-

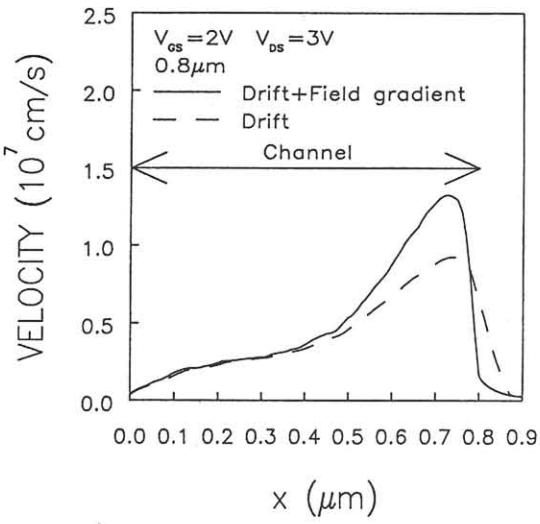


**Fig. 4** Electron drift velocity parallel to the interface at 300K in Si MOSFET.

lation by adopting the extended drift-diffusion model with accurate model parameter.

## 4 Conclusions

We derived a new impact ionization model applicable for a wide range of electron energy based on the non-parabolic and anisotropic band structure. The energy dependence of the impact ionization rate shows a 2.5 power law. The model well explains the reported experimental data; (1) the field dependence of impact ionization coefficient and (2) the quantum yield as a function of electron energy. By using the iterative method, we evaluate the phenomenological length parameter, $L(F)$ . In the low electric field regime, the calculated $L(F)$ linearly increases with field, while it saturates to the value of 400 Å at 30kV/cm. In order to check the usefulness of the extended drift-diffusion model with the obtained length parameter, we simulate the carrier transport characteristics with strong discontinuity of electric field. Both carrier velocity overshoot and undershoot are clearly demonstrated. These results proves that the extended drift-diffusion model will be suitable for a next generation device simulator without requiring any excessive amount of computational time.

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