Monte Carlo Simulation of Impact ionization processes in silicon

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Abstract

The energy-dependent impact ionization rate in silicon is derived by a first-order perturbation theory. The scattering rate is close to that obtained experimentally with a soft x-ray photo-emission spectroscopy. The reasonableness of the calculated results is also supported by the close agreement of simulation results to available experimental data. Key features of the derived impact ionization rate are (1) impact ionization rate for initial electrons with energy below 3 eV shows strong anisotropy, and (2) energy-dependent impact ionization rate has a large power exponent. For practical device simulation, we also derived a simple analytical expression of impact ionization rate under exponentially varying electric field conditions.

I. Introduction

The down-scaling of MOSFETs induces higher electric fields in the channel because the power supply voltage has been scaled less aggressively than device geometries. In deep submicron MOSFETs, the number of hot carriers is expected to increase quite rapidly, leading to the degradation of device characteristics. In order to ensure long term operation of MOSFETs, it is essential to model the behaviors of high energy electrons.
Device simulators developed in the last decade now make it possible to reproduce device characteristics but none of these can accurately estimate the distribution of high energy carriers. Note that high energy carriers directly affect long term reliability of devices as well as electron injection efficiency in FLASH memory. For more predictable T-CAD, high energy carriers have to be simulated more accurately. This requires the use of precise physical models instead of a traditional parameter fitting approach. Among several physical models, an impact ionization rate model is far more important in order to estimate the distribution of high energy carriers. The aims of this paper are twofold: (1) to derive impact ionization rate theoretically and a simple impact ionization model applicable for practical device simulation and (2) to verify the reasonableness of the derived impact ionization rate through the comparison with available experimental data.

II. Theory of impact ionization

Impact ionization process is a kind of electron-electron interaction taking place at the presence of high electric field. When a high energy electron collides with a valence electron, it gives up its kinetic energy to the valence electron which is ionized over the band gap. Thus two conduction electrons and a hole are left.

Theory of impact ionization process in silicon has been well established[1]. The impact ionization rate is obtained from the Fermi's golden rule.

$$S_{I.I.}(1,2 \rightarrow 1',2') = \frac{2\pi}{\hbar}\left[|M_a|^2 + |M_b|^2 + |M_a - M_b|^2\right] \times \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_{1'} - \varepsilon_{2'})$$

Where 1 and 2 denote the conduction and valence electron states before scattering, while 1' and 2' the conduction electron states after scattering. We used the Coulomb potential as an interaction Hamiltonian. The direct matrix element M_a is given in the forms as

$$M_a = \left\langle \phi_1'(r_1)\phi_2'(r_2) \left| \frac{e^2}{4\pi\epsilon(q,\omega)|r_1 - r_2|} \right| \phi_1(r_1)\phi_2(r_2) \right\rangle$$

To calculate the matrix elements, we need (1) wave functions of electrons involving impact ionization process and (2) a frequency- and wave vector-dependent dielectric function. After expanding the Coulomb potential into Fourier series, the direct matrix element is given by

$$\begin{aligned} M_a = & \sum_{G_1,G_2,G_{1'},G_{2'}} \frac{e^2}{q^2 V \epsilon(q,\omega)} A_{1'}^*(G_{1'},k_{1'}) A_{2'}^*(G_{2'},k_{2'}) A_1(G_1,k_1) \\ & \times A_2(G_2,k_2)\delta(-k_{1'} + k_1 - k_{2'} + k_2 + G) \end{aligned}$$

In the calculation, both momentum and energy among the particles are conserved through the delta functions. Also, both the normal and umklapp processes were took into account. Final wave vector-dependent impact ionization rate was derived from the integration over an eight-dimensional k space numerically. In our calculations, we used 113 plane waves and 15 reciprocal lattice vectors.

III. Calculated impact ionization rate

Figure 1 shows the calculated impact-ionization rate as a function of initial electron energy. The calculated results scatter in a rather wide range for initial electrons with kinetic energy below 3 eV because of its strong anisotropic nature. The anisotropy diminishes with increasing the electron energy. In Fig. 1, several reported analytical impact ionization rates[2-5] are also plotted. Although they differ in three orders of magnitudes, they all reported that the calculated impact ionization coefficients agree with experimental data. This means that none of these impact ionization rates have not been well verified. In other words, simulated results could be fitted to any experimental data by simply adjusting phonon scattering rates.
Recently Cartier et al. reported a new combined experimental and theoretical effort to find the electron-hole pair production rate[6]. This was achieved by using soft X-ray photoemission spectroscopy and by performing Monte Carlo simulations. The thin solid curves shown in Fig. 1 is the results of their experiment. Although there exist some undulations in the curves due to an artificial fitting to three sets of Keldysh formula[7], our calculated data are essentially the same as theirs.

For more practical use, we derived analytical form of impact ionization rate averaged over all initial electron states with a given energy.

$$S_{I.I.}(\varepsilon) = 1.0 \times 10^{11}(\varepsilon - 1.1eV)^{4.6}$$

Compared with the Keldysh form with power exponent of two, the new isotropic impact ionization rate has much larger power exponent of 4.6, indicating soft impact ionization threshold.

Figure 2 shows the impact ionization rates based on other first principle calculations[8-11]. The overall trend of the calculated results shows similar characteristics since the impact

ionization rate simply reflects the energy band structure of silicon. However, one point to note is that there still exists about one order of magnitude discrepancy among the reported values. The reasons for the discrepancy are not clarified yet. There may be several reasons: choices of the integration method, pseudopotential form factors used, dielectric function, energy allowance used in the numerical calculation.

IV. Comparison with experimental results

(1) *Transient impact ionization using anisotropic and isotropic I.I. rates*

In order to study the reasonableness of the derived isotropic impact ionization rate, we simulated the number of impact ionization events under non-steady state conditions by using isotropic and anisotropic scattering rates. No appreciable differences between the two cases indicate that it is reasonable to use isotropic impact ionization rate instead of more elaborate anisotropic ones without losing any physical meaning. In addition, the use of the isotropic impact ionization rate greatly improves the efficiency of Monte Carlo simulation in terms of memory capacity as well as computational time.

(2) *Impact ionization coefficient*

The number of impact ionization events produced by one carrier per unit length is defined as impact ionization coefficient, which varyies with the electric field as Aexp(-B/E). The open circles shown Fig. 3 are the simulated impact ionization coefficient under constant electric field. Good agreement with the experimental data demonstrates the validity of the impact ionization rate derived.

(3) *Non-local impact ionization coefficient in exponentially varying electric field*

In MOSFETs electric field in the velocity saturation region changes so rapidly that the channel electrons are no more equilibrium. According to simulation studies, the electric field in MOSFETs was found to vary exponentially with distance from the pinch-off point toward the drain. The data points in Fig. 4 show calculated impact ionization coefficients under exponentially varying electric field conditions. All the points below the solid line are the data calculated under increasing electric field condition, while the solid points above the solid line are the data for decreasing electric field conditions. Simulated characteristics length, λ, of the velocity saturation region is simply expressed with the gate oxide thickness and junction depth.

Figure 4 shows two interesting features: (1)under the increasing electric field, non-local impact ionization coefficient is significantly smaller than that in equilibrium state and (2)at lower electric field, the decrease of the impact ionization rate becomes more pronounced.

(4) *Simulation of substrate current*

Figure 5 shows the substrate currents calculated using two different impact ionization models. The solid line shows the experimental data.

A conventional drift-diffusion simulation using the local impact ionization coefficient overestimates substrate current. However, the use of the non-local impact ionization coefficient shown in Fig. 4 results in a reasonable agreement with experimental data. Note that even quite simple device simulator based on the drift-diffusion model can predict impact ionization current correctly once the non-local impact ionization coefficient is implemented in a device simulator.

(5) *Quantum yield*

We simulated quantum yield to further verify the derived impact ionization rate. By using p-ch MOSFET, electrons are injected from the gate electrode to the silicon substrate through the gate oxide. If the injected electrons has enough energy to make impact ionization, some of them create electron-hole pairs in the silicon substrate. The generated holes are collected into the inversion layer while electrons flow to the substrate electrode. By measuring the electrode currents, the average number of generated electron-hole pairs per injected electron is calculated. This is the definition of quantum yield.

Figure 6 shows the calculated quantum yields using the MC simulation together with experimental data[13-15]. The calculated data agree quite well with the data reported by Takagi and Toriumi. The discrepancy among the reported quantum yields may originate from the calibration error of the injected electron energy.

(6) *Transient impact ionization*

We investigated the anisotropic impact ionization in Si MOSFETs reported by Takagi[16]. The devices used for their experiment were n-ch Si MOSFETs with single drain structures on the (100) surface. The measured data shows the gate voltage dependence of the substrate current with different channel directions. They found that the substrate current along the 45° off the ⟨011⟩ direction, meaning ⟨001⟩ direction, becomes larger than that along 0 or 90°. The anisotropy decreases with increasing substrate current. We simulated impact ionization process with similar device structures.

The calculated impact ionization agrees well with the experimental data; the anisotropy diminishes with increasing ionization rate.

V. Conclusions

We theoretically derived impact ionization rate. The energy dependence of the rate was found to be the same as the pair generation rate obtained from the soft x-ray photo-emission spectroscopy. The reasonableness of the models is also supported by the close agreement of the simulation results to available experimental data. Key features of the derived impact ionization rate are (1) impact ionization rate for initial electrons with the energy below 3 eV shows strong anisotropy which directly reflects energy band structure of silicon, (2) energy dependent impact ionization rate shows large power exponent, indicating the soft threshold of impact ionization, (3) we demonstrated that both isotropic and anisotropic impact ionization rates lead to the same results. This means that for more practical Monte Carlo simulation we can use the energy dependent impact ionization rate instead of more complicated wave-vector dependent impact ionization.

Using the Monte Carlo simulation, we derived a simple analytical expression of non-local impact ionization coefficient under exponentially varying electric field conditions. We demonstrated that the newly derived impact ionization coefficient well reproduces substrate current of MOSFETs even in a drift-diffusion device simulation.

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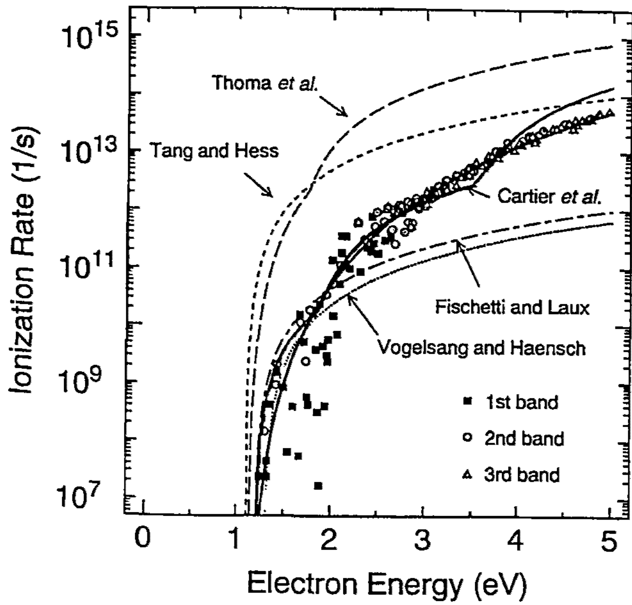

Figure 1. Calculated impact ionization rates. Bold solid line represents a best fitted curve to the calculated impact ionization rates. The other four lines except the solid lines represent impact ionization rate expressed by Keldysh formula. The thin solid curves show the impact ionization rate fitted to a set of three Keldysh formula.

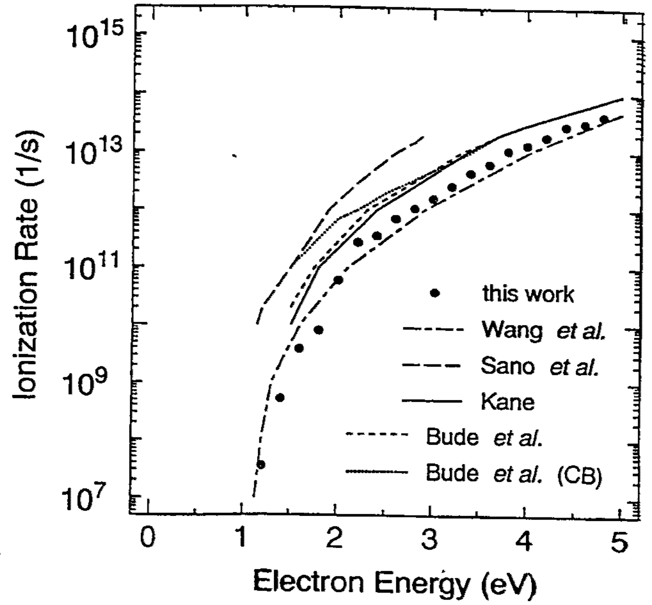

Figure 2. Comparison of reported impact ionization rates averaged over all initial electron states as a function of energy measured from the bottom of the conduction band.

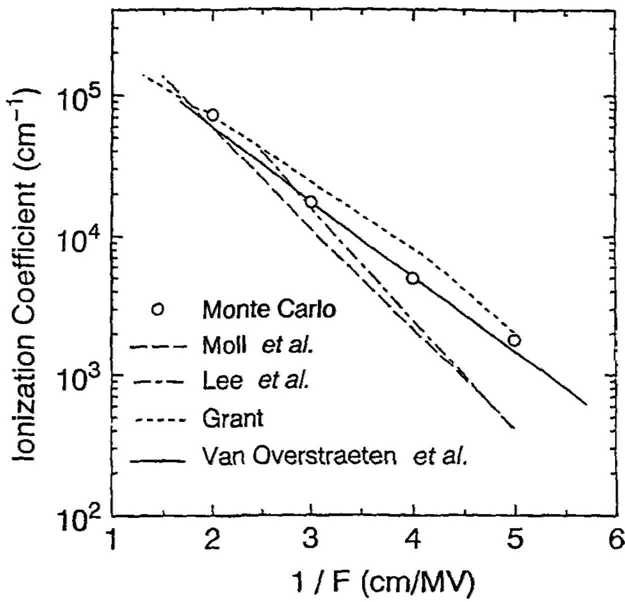

Figure 3. Calculated impact-ionization coefficient as a function of reciprocal electric field with reported experimental data.

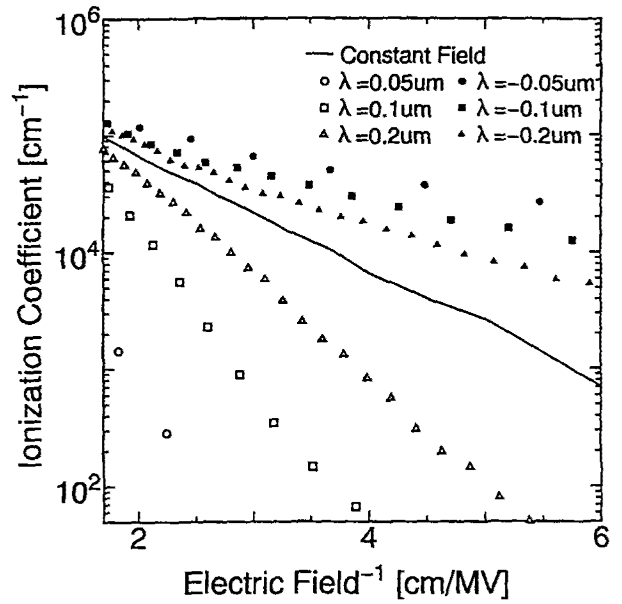

Figure 4. Calculated impact ionization coefficients under exponontially varying electric field conditions.

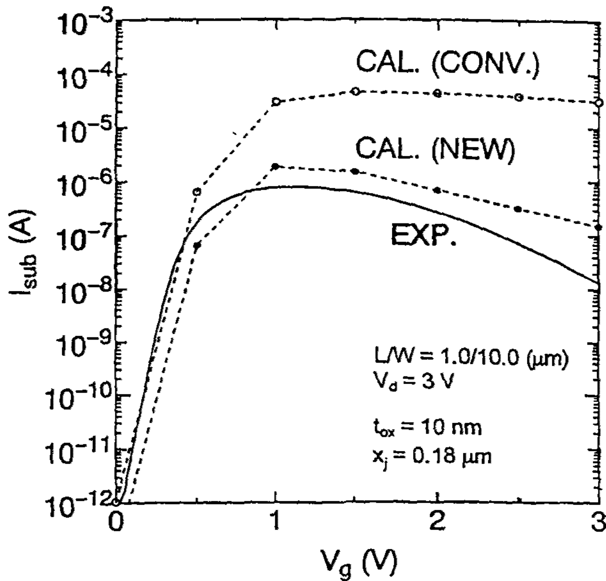

Figure 5. Simulated substrate current together with experimental result at V_D=3.0V for an n-ch MOSFET with the channel length of 1.0 μm. Gate oxide thickness of 10 nm and channel doping concentration of $1.2\text{x}10^{17}/\text{cm}^2$.

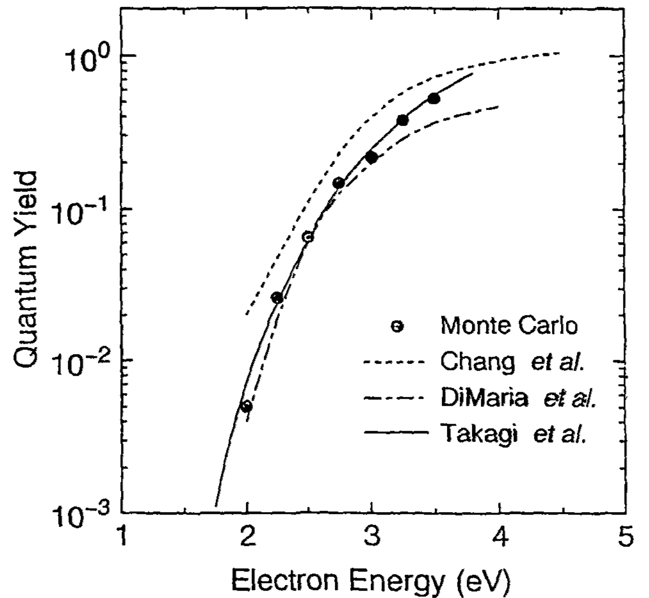

Figure 6. Quantum yield at room temperature as a function of electron energy. Open circles show the calculated results. Curves are the experimental results.