Numerical simulation of electric characteristics of deep submicron silicon-on-insulator MOS transistor

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Abstract. Today submicron silicon-on-insulator (SOI) MOSFET structures are widely used in different electronic components and also can be used as sensing elements in some applications. The development of devices based on the structures with specified characteristics is impossible without computer simulation of their electric properties. The latter is not a trivial task since many complicated physical processes and effects must be taken into account. In current study ensemble Monte Carlo simulation of electron and hole transport in deep submicron n-channel SOI MOSFET with 100 nm channel length is performed. The aim of the study is investigation of the influence of interband impact ionization process on the device characteristics and determination of the transistor operation modes when impact ionization process starts to make an appreciable influence on the device functioning. Determination of the modes is very important for adequate and accurate modeling of different devices on the basis of SOI MOSFET structures. Main focus thereby is maid on the comparison of the use of two models of impact ionization process treatment with respect to their influence on the transistor current-voltage characteristics. The first model is based on the frequently used Keldysh approach and the other one utilizes the results obtained via numerical calculations of silicon band structure. It is shown that the use of Keldysh impact ionization model leads to much faster growth of the drain current and provides earlier avalanche breakdown for the SOI MOSFET. It is concluded that the choice between the two considered impact ionization models may be critical for simulation of the device electric characteristics.

Keywords: SOI MOSFET, Monte Carlo simulation, impact ionization.

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Численное моделирование электрических характеристик глубокосубмикронного МОП-транзистора со структурой «кремний на изоляторе»

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На сегодняшний день субмикронные МОП-транзисторные структуры кремний-на-изоляторе (КНИ) широко используются в различных электронных устройствах, а также могут применяться в качестве сенсорных элементов. Разработка приборов с заданными характеристиками на основе этих структур невозможно без компьютерного моделирования их электрических свойств. Для глубокосубмикронных транзисторных структур это весьма трудная задача, поскольку необходимо учитывать многие сложные физические процессы и эффекты, имеющие место в полупроводниковом приборе. В настоящей работе многочастичным методом Монте-Карло проведено моделирование переноса электронов и дырок в глубокосубмикронном n-канальном КНИ МОП-транзисторе с длиной канала 100 нм. Целью настоящей работы явилось исследование влияния процесса межзонной ударной ионизации на характеристики транзистора, а также установление таких режимов его работы, при которых процесс ударной ионизации начинает оказывать существенное влияние на работу прибора. Определение этих режимов является крайне необходимым для адекватного и корректного моделирования различных устройств на основе КНИ-МОП-транзисторных структур. При этом основное внимание обращено на сравнение двух моделей учета процесса ударной ионизации по степени их влияния на вольтамперные характеристики транзистора. Первая, аналитическая модель, основана на широко известном подходе Келдыша, а во второй используются результаты численного расчета зонной структуры кремния. Показано, что применение модели ударной ионизации Келдыша приводит к более быстрому росту тока стока и, как следствие, к скорейшему лавинному пробою КНИ МОП-транзисторной структуры. Сделан вывод о том, что выбор между двумя рассматриваемыми моделями ударной ионизации может быть критиче-

Ключевые слова: КНИ-МОП-транзистор, моделирование методом Монте-Карло, ударная ионизация.
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Introduction

Silicon-on-insulator (SOI) technology in micro- and nanoelectronics has gained a great interest in the last decades. Deep submicron SOI MOSFETs are regarded as promising elements for modern integrated circuits in different electronic applications [1, 2]. Among the advantages of submicron SOI MOSFETs, in comparison with common «bulk» MOSFETs, are the lower power dissipation and increased operation speed, lower leakage currents, and higher radiation hardness. Deep submicron SOI MOSFETs are less vulnerable to short-channel effects in comparison with common MOSFETs [3]. Results of recent investigations show that very promising is the use of submicron SOI MOSFETs as different sensors and detectors. For instance, the possibility to use SOI MOSFETs as electric field sensors was proposed in [4]. Also recently the possibility to use deep submicron SOI MOSFETs as unique single-photon detectors at room temperature was demonstrated in [5, 6].

Today the development of modern devices of micro- and nanoelectronics, including various sensor devices, can not be done without computer simulation of their characteristics. Thereupon it must be noted that ensemble Monte Carlo method has been widely used as a powerful tool for simulation of carrier transport phenomena in different semiconductor devices. By means of Monte Carlo simulation static, dynamic and noise characteristics of submicron SOI MOSFETs have been calculated [7–10]. One of the advantages of the method is the possibility of incorporation of rather sophisticated models describing different physical processes into the simulation procedure. Ensemble Monte Carlo simulation thus is one of the most promising methods for the simulation of deep submicron SOI MOSFETs, which allows account of all necessary mechanisms of carrier scattering. The simulation procedure also enables inclusion of semiconductor band structure calculations and account of quantum effects as well [10–14].

It is known that inclusion of effects related to impact ionization becomes very important in numerical simulations of short-channel MOSFETs. This is caused by the fact that in such MOSFETs electric field strengths are high enough to make impact ionization rate be comparable or even higher than other dominant scattering mechanisms. The latter may considerably influence the operation of the MOSFET itself as well as the sensor or detector on the basis of the transistor.

The main purpose of this study is to examine the influence of impact ionization process on electric characteristics of a deep submicron n-channel SOI MOSFET with the channel length of 100 nm, compare two different widely used in Monte Carlo simulations models describing impact ionization process in the transistor structure channel, and also to determine the transistor operation modes and conditions when impact ionization process may be neglected.

Outlines of ensemble Monte Carlo transport simulation

The cross-section of the SOI MOSFET structure under consideration is presented in Figure 1. The simulated structure is a fully depleted single gate SOI MOSFET with the conducting silicon channel laying between gate and buried oxides [8, 15, 16]. The device dimensions denoted in the Figure 1 are as follows: the source, gate and drain lengths are \( L_s = L_g = L_d = 100 \) nm, channel thickness \( W_c = 30 \) nm, the thickness of buried oxide layer is \( W_b = 100 \) nm, and the thickness of the silicon substrate layer \( W_{\text{sub}} = 200 \) nm. The gate oxide is 5 nm thick. The doping levels of n+ regions and p-Si are \( 10^{25} \) m\(^{-3} \) and \( 8 \times 10^{23} \) m\(^{-3} \), respectively. Simulation temperature is 300 K. In all our calculations the source and substrate electrode biases (\( V_s \) and \( V_{\text{sub}} \), respectively) are equal to zero and the gate and drain biases (\( V_g \) and \( V_d \), respectively) are applied with respect to the source.

![Figure 1 – Schematic cross-section of the simulated SOI MOSFET](image)

To calculate electrostatic potential and electric field strength within the device as well as other physical parameters of interest our Monte Carlo simulation is coupled self-consistently with the numerical solution of two-dimensional Poisson equation. In brief the procedure can be described as follows. Electron and hole movement within the device is simulated during short time steps \( \Delta t \). After every time step \( \Delta t \) the
Poisson equation with appropriate boundary conditions is solved in order to update the electrostatic potential. The calculation of free carrier charge density within the simulation dimensions is performed using so-called particle technique [17]. The Monte Carlo procedure is two-dimensional in real space and three-dimensional in momentum space. The latter is caused by the fact that state-of-the-art planar technology implies that the device width in the dimension perpendicular to the figure plane (see Figure 1) is much higher than its length \( L = L_g + L_d + L_s \) and depth \( W = W_g + W_d + W_{sub} \). The time step \( \Delta t \) is chosen to be 1 fs. A general description of the Monte Carlo simulation approach may be found elsewhere [18].

It is considered that the contacts of the drain, the source, and the substrate are ideal ohmic contacts. The metallic gate is assumed to be aluminum. Ideal ohmic contact model implies that a contact is in thermal equilibrium though the current is flowing through it. The latter means that the contact injects particles to provide charge neutrality in a small region of semiconductor near the contact edge. We suppose that injected particles have Maxwellian distribution and also we use the injection model which takes into account that particles have Maxwellian distribution and also we use the injection model which takes into account that particles are not injected simultaneously [19]. Particles reaching the contact from inside the simulation domain leave the device freely.

It must be mentioned that in present work we neglect size quantization effects and consider electron and hole gases as purely three-dimensional. Such approximation must be reasonable for considered channel width [8, 15]. Another problem, which arises while simulating charge carrier transport in SOI MOSFETs, is the treatment of carrier scattering by Si-SiO₂ interfaces. For three-dimensional electron and hole gases the scattering of charge carriers by the interfaces is usually regarded as the combination of diffusive and specular reflections of particles from the interface. The amount of diffusive scattering must depend on the quality of the interface and is not a priori known. The variation of the amount of diffusive scattering makes an influence, for example, on drift velocity and particle distribution functions in the transistor channel. As a result it also makes an influence on current-voltage characteristics of the device and may be used as additional fitting parameter in Monte Carlo simulations. Since it is not the aim of present work to examine the role of interface scattering on the transport properties, electron and hole scattering by Si-SiO₂ interfaces is regarded as purely specular.

Electron transport in the conduction band of silicon is simulated in valleys \( X \) and \( L \), with account of the nonparabolicity effect. The intravalley and inter-valley electron scattering by phonons, scattering by the ionized impurity, plasmons, and impact ionization process are taken into account [18, 20].

It is known that the band structure of silicon in valley \( X \) can be represented by three pairs of equivalent valleys, the isoenergetic surfaces of which in \( k \) space are ellipsoids of a revolution with the axes of symmetry oriented along crystallographic directions of the type \((100)\). In present simulation it is assumed that the axes of real space coordinates coincide with these directions. Then, taking into account nonparabolicity, the dispersion relation for electrons can be written as:

\[
E(1 + \alpha E) = \frac{\hbar^2}{2} \sum_{i=1}^{3} \frac{k_i^2}{m_i}.
\]

In the equality (1) \( E \) is the electron energy, \( \alpha \) is the nonparabolicity coefficient, which equals 0.5 eV⁻¹; \( \hbar \) is the reduced Planck constant, and \( k_i \) and \( m_i \) are the components of the wave vector and the tensor of the effective mass along the \( i \)-th direction. To simulate the electron transport in valley \( L \), we use a relatively simplified model, in which the isotropic effective mass of conductivity is used when solving the equations of motion. When simulating n-channel MOSFETs, holes are often considered in the quasi-equilibrium approximation. However, in the presence of strong electric fields in the channel and high impact ionization rate, this approximation can be inadequate. In this study, the hole transport is simulated similarly to the electron transport in the effective mass approximation allowing for the nonparabolicity and anisotropy of the dispersion relation in the valence band. To do that we follow the work by Rodriguez-Bolivar et al. [21]. The transport is taken into account in the band of heavy and light holes, and in the split-off band. The scattering of holes by acoustic and optical phonons and by ionized impurity are involved in the model [22, 23]. Dispersion relations for holes can be written in the form:

\[
E_g(k) = \frac{\hbar^2 k^2}{2m_h} \left[ 1 - g(0, \varphi) \right] \chi_{hh}(E), \ E \geq 0;
\]

\[
E_e(k) = \frac{\hbar^2 k^2}{2m_h} \left[ 1 + g(0, \varphi) \right] \chi_{ee}(E), \ E \geq 0;
\]

\[
E_m(k) = \frac{\hbar^2 k^2}{2m_h} \chi_{mm}(E) + \Delta_m, \ E \geq \Delta_m;
\]

\[
g(0, \varphi) = \sqrt{\frac{B^2}{A^2} + \frac{C^2}{A^2} (\sin^4 \theta \sin^2 \varphi \cos^2 \varphi + \cos^2 \theta \sin^2 \varphi)}.
\]
In equalities (2)–(5), indices «H», «L», and «so» denote the band of heavy holes, the band of light holes, and the split-off band, respectively; \( k \) is the wave vector of holes; constants \( A = -4.22; B = -0.78; C = 4.80; \theta \) and \( j \) are the angles in a spherical coordinate system in the space of wave vectors; \( m_e \) is the free electron mass; \( m_{so} \) is the hole effective mass in the split-off band; \( \Delta_{so} = 0.044 \) eV; and \( \chi \) are the functions that describe the nonparabolicity of the dispersion relation in the valence band, the form and approximation of which are presented in [21].

**Impact ionization process simulation**

Impact ionization is a threshold process [24–26]. In a simple case, threshold energy \( E_{th} \) can be determined using the energy and momentum conservation laws and minimization of the energy of final particles. For accurate impact ionization process simulation in bulk silicon or in silicon devices one must take into account the fact that silicon has a complex energy band structure. Subject to this it can be assumed that several values of threshold energies are possible and it may be concluded that the effective (or average) threshold energy of charge carriers depend on electric field strength. The effective threshold energy can be defined as the energy corresponding to maximum value of the product of impact ionization cross section and electron distribution function [25]. When simulating the electric properties of bulk silicon and silicon MOSFETs by the Monte Carlo method, in order to calculate the dependence of impact ionization scattering rate \( W_{\phi}(E) \) with specified threshold energy \( E_{th} \) on energy \( E \), many authors currently use Keldysh formula [24, 27]:

\[
W_{\phi}(E) = PW_{\phi}(E_{th}) \left( \frac{E - E_{th}}{E_{th}} \right)^2,
\]

where \( P \) is a parameter and \( W_{\phi}(E_{th}) \) is the total scattering rate of electrons by phonons for energy equal to \( E_{th} \). The model has two fitting parameters \( P \) and \( E_{th} \). The most common values for these parameters for silicon are \( E_{th} = 1.2 \) eV and \( P = 0.38 \) for so-called «soft» threshold model and \( E_{th} = 1.8 \) eV and \( P = 100 \) for so-called «hard» threshold model [27]. Briefly the difference between these two kinds of Keldysh models can be described as follows. In the hard threshold model it is assumed that during the impact ionization event the rules of energy and momentum conservation must be fulfilled. In the soft threshold model participation of, particularly, phonons may be expected. Due to this fact restriction associated with the momentum conservation may be neglected. Previously, the comparison of soft and hard threshold models was done while simulating electrical characteristics and effective threshold energy in deep submicron MOSFET in [28]. Also in the framework of Keldysh model some aspects of impact ionization effective threshold energy in deep submicron silicon MOSFETs were investigated in [16, 29]. In this study we will use the parameters of the soft threshold model as by now it is supposed that impact ionization process is more likely to occur within the soft threshold model and estimations based on full-band calculations indicate this.

The main advantage of Keldysh model is its relative simplicity and easiness of inclusion into Monte Carlo simulation. At the same time the problem is that the model does not take into account the complexity of real semiconductor band structure and thus it has the lack of universality. As a result the model has two fitting parameters mentioned above: threshold energy \( E_{th} \) and \( P \). The values of these parameters are usually obtained in order to match theoretical results with known experimental data.

Another important problem that must be discussed is the definition of electron and hole states after the impact ionization event. The most common situation for Keldysh model is the definition of particle final states after scattering via the assumption that near threshold the group velocities of the final particles are equal and for spherical parabolic bands all wave vectors are collinear [27].

By now more sophisticated models of impact ionization process based on full-band calculations have been developed [25, 30–32]. These types of models usually have no fitting parameters, but their implementation is restricted by the complexity of scattering rate calculation and definition of the particle final states which result in too much computational effort. Basing on the full-band approach in [32] the expression for impact ionization scattering rate for silicon was derived in a rather simple fitted form:

\[
W_{\phi}(E) = 10^{11} (E - 1.1)^{2.6},
\]

where electron energy \( E \) is in eV. Moreover, the calculation revealed that the average energy of secondary generated particles depends linearly on the primary electron energy after the scattering event. The latter provided an ability to develop a procedure based on normal distribution simulation which makes it pos-
sible to define carrier states after the impact ionization event. In our opinion the procedure is the most suitable for application in Monte Carlo simulations among other approaches based on full-band calculations. The aim of current study was to compare the influence of the choice between soft threshold Keldysh [27] and full-band [25] electron impact ionization models on the calculation of the SOI MOSFET characteristics and determine the device operation modes when impact ionization starts to make sufficient influence on the channel current. In current study we regard only impact ionization by electrons since they are the main charge carriers in the SOI MOSFET. Also the threshold energy for holes is high enough (1.49 eV) [33].

**Results and discussion**

The current–voltage ($I–V$) characteristics of the simulated SOI MOSFET both with and without account of the impact ionization process are presented in Figure 2.

*Figure 2 –* Current-voltage characteristics of the SOI MOSFET: solid curves – impact ionization process is not taken into account, dashed curves – full-band [25] and dotted curves – Keldysh [27] model of impact ionization

Analysis of Figure 2 shows that the linear region of the $I–V$ characteristics for the transistor corresponds to the drain voltage range $0 \leq V_D \leq 0.5$ V. The saturation region occurs at voltages $V_D > 0.5$ V, up to approximately 1.5 V. While calculating $I–V$ characteristics we restricted the drain bias by the value of 3.5 V, since in current work we concern only impact ionization as breakdown mechanism. As can be seen from the figure, Keldysh model sufficiently overestimates the influence of impact ionization by electrons on current-voltage characteristics. For a given transistor structure Keldysh model gives a rapid rise of current density in the channel for $V_D > 1.5$ V. While the full-band model [25] gives a rather moderate avalanche multiplication in the channel under considered simulation conditions. The latter proves that the use of more rigorous models based on the calculation of realistic silicon band structure may be crucial for calculation of submicron SOI MOSFET characteristics.

*Figure 3 –* Electron drift velocity ($a$) and average kinetic energy ($b$) along the transistor channel at $V_D = 2.5$ V and $V_G = 1.5$ V: solid curves correspond to the case when impact ionization process is neglected, dashed curves – full-band model [25], and dotted curves – Keldysh model [27]

In the Figures 3 and 4 the results of calculated electron drift velocities and average energy versus the distance along the transistor channel with the use of both Keldysh and full band models are presented. Figure 3 stands for $V_D = 2.5$ V while Figure 4 is for $V_D = 3.5$ V. The gate voltages in both cases is 1.5 V. As can be seen from the figures, the effect of impact ionization on electron drift velocity and kinetic energy is not pronounced at $V_D = 2.5$ V. At the same time the difference in current densities (see Figure 2) for given models is already significant. The latter may be
referred to much higher electron-hole pair generation rate provided by Keldysh model. For $V_D = 3.5 \text{ V}$ the effect of impact ionization on the drift velocity and kinetic energy is sufficient. In this case higher Keldysh generation rate leads to much more intensive energy loss of electrons near the drain end of the channel then for full-band model. At the same time the procedure of definition of electron and hole states after ionization event also makes an influence on particle energy distribution in the channel.

**Conclusion**

In this study electric characteristics of a deep submicron SOI MOSFET with 100 nm channel length have been simulated by means of ensemble Monte Carlo method. Both electron and hole transport was included into the simulation with account of all dominant scattering mechanisms for considered transistor structure. The influence of two different models of impact ionization process (Keldysh model with soft threshold and full-band model) on the transistor current-voltage characteristics has been ascertained. It is shown that the use of accurate model based on the full-band approach is crucial while simulating electrical characteristics of deep submicron SOI MOSFET since the use of Keldysh model leads to sufficient overestimation of the current density in the transistor channel and earlier breakdown. Results of our calculations also indicate that at $T = 300 \text{ K}$ and drain voltages $V_D \leq 1.5 \text{ V}$ impact ionization does not make sufficient influence on the transistor current-voltage characteristics for both models. Thus in these modes impact ionization may be neglected.

**References**

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