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Monte Carlo Simulation of Photoresponse in Silicon Photodiodes with *p-n*-Junction and *p-i-n*-Structure

A.V. Borzdov[1], V.M. Borzdov[1], D.N. Buinouski[1], A.N. Petlitsky[2]

[1]*Belarusian State University,*
Nezavisimosty Ave., 4, Minsk 220030, Belarus
[2]*JSC "Integral" – «Integral» Holding Management Company,*
Kazintsa str., 121A, Minsk 220108, Belarus

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Abstract

Numerical modeling of semiconductor photodiodes' electrical characteristics is an important task at the stage of their development and design. In this regard, it should be noted that one of the most promising methods that can be used for this purpose is the ensemble Monte Carlo method, which allows including, along with the dominant mechanisms of charge carriers' scattering in the device structure, also the processes of impact ionization, which is very important for adequate modeling of a wide class of silicon photodiodes operating in the reverse bias mode. The aim of the work was to study the influence of the impact ionization process on the electrical characteristics of silicon photodiodes with a *p-n*-junction and a *p-i-n*-structure operating in the reverse bias mode under the influence of picosecond pulses of visible radiation. Using self-consistent simulation by the ensemble Monte Carlo method, the electron ionization coefficient in bulk silicon at a crystal lattice temperature of 300 K was calculated and compared with known experimental data. Photoresponse in silicon submicron photodiodes with a *p-n*-junction and photodiodes with a *p-i-n*-structure was calculated for different thicknesses of the undoped *i*-region. It was shown that use of simple models similar to the Keldysh model with constant values of the threshold energy and other parameters for calculating the rate of the impact ionization process did not allow obtaining values of the ionization coefficient matched with experimental data in a wide range of electric field strengths. This result raises the question on the adequacy of the device structures' electrical characteristics modeling with a non-uniform electric field when using such simple impact ionization models.

Keywords: Monte Carlo method, photocurrent, silicon photodiode, impact ionization

Адрес для переписки:
Борздов В.М.
Белорусский государственный университет,
пр-т Независимости, 4, г. Минск 220030, Беларусь
e-mail: borzdov@bsu.by

Address for correspondence:
Borzdov V.M.
Belarusian State University,
Nezavisimosty Ave., 4, Minsk 220030, Belarus
e-mail: borzdov@bsu.by

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Моделирование методом Монте-Карло фотоотклика в кремниевых фотодиодах с *p-n*-переходом и *p-i-n*-структурой

А.В. Борздов[1], В.М. Борздов[1], Д.Н. Буйновский[1], А.Н. Петлицкий[2]

[1]*Белорусский государственный университет,*
пр-т Независимости, 4, г. Минск 220030, Беларусь

[2]*ОАО «Интеграл» – управляющая компания холдинга «Интеграл»,*
ул. Казинца, 121А, г. Минск 220108, Беларусь

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Численное моделирование электрических характеристик полупроводниковых фотодиодов является важным этапом на стадии их разработки и проектирования. В этой связи следует отметить, что одним из наиболее перспективных методов, который может быть использован для этой цели, является многочастичный метод Монте-Карло. Данный метод позволяет учитывать и включать наряду с доминирующими механизмами рассеяния носителей заряда в приборной структуре также и процессы ударной ионизации, что является очень важным при адекватном моделировании широкого класса кремниевых фотодиодов, работающих в режиме обратного смещения. Целью работы явилось изучение влияния процесса ударной ионизации на электрические характеристики кремниевых субмикронных фотодиодов с *p-n*-переходом и *p-i-n*-структурой, работающих в режиме обратного смещения при воздействии пикосекундных импульсов излучения видимого диапазона спектра. С помощью самосогласованного моделирования многочастичным методом Монте-Карло проведен расчёт и сравнение с известными экспериментальными данными коэффициента ионизации электронами в объёмном кремнии при температуре кристаллической решётки 300 К. Рассчитан фотоотклик в кремниевых субмикронных фотодиодах с *p-n*-переходом и фотодиодах с *p-i-n*-структурой для различных толщин *i*-области. Показано, что использование для расчёта интенсивности процесса ударной ионизации простых моделей, подобных модели Келдыша, предполагающих постоянные значения пороговой энергии и других параметров, не позволяет согласовать полученные значения коэффициента ионизации с экспериментальными данными в широком диапазоне напряжённости электрического поля. Этот результат ставит вопрос об адекватности моделирования электрических характеристик приборных структур с неоднородным электрическим полем при использовании таких простых моделей ударной ионизации.

Ключевые слова: метод Монте-Карло, фототок, кремниевый фотодиод, ударная ионизация

Адрес для переписки:
Борздов В.М.
Белорусский государственный университет,
пр-т Независимости, 4, г. Минск 220030, Беларусь
e-mail: borzdov@bsu.by

Address for correspondence:
Borzdov V.M.
Belarusian State University,
Nezavisimosty Ave., 4, Minsk 220030, Belarus
e-mail: borzdov@bsu.by

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Introduction

It is well known that silicon photodiode structures are widely used in optoelectronics as converters of optical radiation into electrical signals. Semiconductor photodiodes, in particular silicon ones, are the main elements for creating detectors of visible and infrared spectral range radiation. Such photodiodes can operate both in the usual current mode and in the mode of counting single photons [1–4]. The relevance of the study and modeling of the operation of silicon photodiodes of various constructions is due, in particular, to the significant development of silicon technology and the widespread use of silicon in modern microelectronics. Due to this, it is possible to integrate silicon photodiode structures into various microelectronic systems within the framework of existing and promising technological processes used in the production of integrated circuits.

During the process of development and design of modern semiconductor photodiodes and other integrated microelectronics devices, an important task, without which any production cannot do, is numerical computer modeling. The purpose of such modeling is to predict the electrical characteristics of devices in various operating modes. On the other hand, computer modeling allows us to give recommendations on optimizing the design and topological parameters of devices based on numerical calculations of their electrical characteristics. For computer modeling of integrated submicron photodiodes and phototransistors, one of the most promising methods is numerical self-consistent simulation based on the ensemble Monte Carlo method [5–9]. The ensemble Monte Carlo method, as a method of kinetic simulation, allows us to simulate the processes of charge carrier transport in semiconductor device structures. The simulation is able to take into account the main, most significant, processes of charge carrier scattering, as well as the processes of their generation-recombination. In the case of diodes with a *p-n*-junction and *p-i-n*-structure operating in reverse bias mode, it is especially important to take into account the processes of avalanche multiplication of charge carriers due to interband impact ionization [10–12].

The aim of this work was to numerically simulate, using the ensemble Monte Carlo method, the dependence of current density on time in submicron silicon photodiodes with a *p-n*-junction and a *p-i-n*-structure operating in the reverse bias mode under the influence of picosecond pulses of visible spectrum radiation, and taking into account the processes of impact ionization of charge carriers.

Photodiode model

The two-dimensional simulation regions of silicon photodiodes with a *p-i-n*-structure considered in this work are schematically shown in Figure 1. For diodes with a *p-n*-junction, the difference from the structure shown in Figure 1 is the absence of an intrinsic undoped *i*-Si layer. It is assumed that the radiation is directed perpendicular to the interface between the silicon and the external environment, and penetrates only into the region located between the electrodes of the photodiode. The length of the region is $L_C = 0.25$ μm. Thickness of the photodiode into substrate is $W_S = 0.5$ μm. For the doped *n*- and *p*-layers of Si the doping levels are supposed equal. Concentrations of the donor and acceptor impurities in the layers are 10^{24} m^{-3}, respectively. The diodes with different thicknesses of the doped Si layers are regarded as follows: $W_{d1} = W_{d2} = 250$ nm (diode with a *p-n*-junction), 225 nm, 200 nm and 150 nm (diodes with a *p-i-n*-structure and the thickness of the *i*-layer equal to 50 nm, 100 nm and 200 nm, respectively). The lattice temperature for the simulation is supposed to be 300 K.

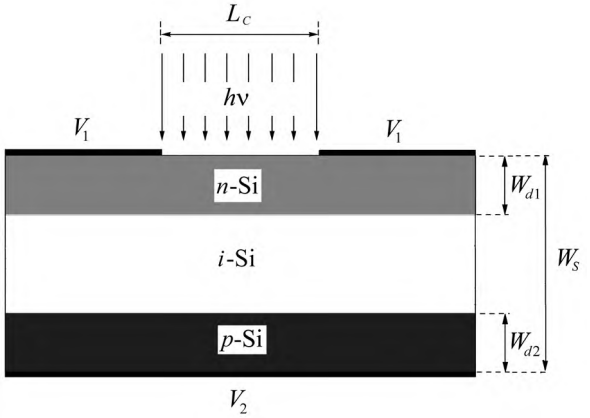

Figure 1 – Schematic cross-section of a photodiode with *p-i-n*-structure

The calculation of the electrical characteristics of considered diode structures is carried out by the ensemble Monte Carlo method within the framework of self-consistent two-dimensional simulation based on the particle method. The description and basics of this method can be found, for example, in the monographs [5, 6]. When carrying out the calculations, we consider the effect of radiation in the visible range of the spectrum with the following characteristics: the radiation wavelength is equal to 650 nm, the intensity of the radiation is $5 \cdot 10^{10}$ W/m^2, the radiation pulse duration is 1 ps. As a model approximation,

we also assume that the intensity of the radiation pulses is constant during the exposure time and is uniformly distributed over the surface area of the diode structure.

The processes of electron and hole transport in the considered photodiodes are generally simulated in the same way as in silicon MOS transistors [13, 14]. When simulating the processes of electron transport in the conduction band of silicon, the population of the X and L valleys of the semiconductor is taken into account. The analytical dispersion law for electrons in both valleys assumes a nonparabolicity coefficient of $0.5\ \text{eV}^{-1}$. To simulate the processes of hole transport in the valence band of silicon, an analytical dispersion law is also used, which takes into account nonparabolicity and anisotropy, and is considered in the band of heavy and light holes, as well as in the split-off band due to spin-orbit interaction. The Monte Carlo simulation procedure includes the processes of electron scattering on acoustic and optical phonons, on plasmons, on ionized impurity, as well as the process of interband impact ionization initiated by electrons. For holes, the simulation includes processes of scattering on phonons and ionized impurity, as well as the process of interband impact ionization initiated by holes. The simulation procedure also includes processes of optical generation of electron-hole pairs during intrinsic absorption of the radiation. The numerical model takes into account reflection processes of optical radiation from the interfaces of materials.

The process of impact ionization by electrons and holes in the Monte Carlo simulation procedure is considered as an additional scattering mechanism, in which electron-hole pairs are generated. When simulating the processes of charge carrier transport in semiconductor device structures by the Monte Carlo method, the Keldysh model and similar models are often used to describe the impact ionization scattering rate for both electrons and holes. In the case of the Keldysh model, the expression for the rate of the impact ionization process in general can be presented in the following form [10, 13]:

$$W_{\text{II}}(E) = A_{\text{II}}\left(\frac{E - E_{th}}{E_{th}}\right)^{b}, \tag{1}$$

where A_{II} and b are some constants; E is the electron kinetic energy; E_{th} is the so called threshold energy of impact ionization. Along with formula (1), in some works devoted to the numerical calculation of the scattering rate of the impact ionization process by electrons and holes taking into account the full band structure of silicon, an interpolation formula of the form [11, 14, 15] is used for its calculation:

$$W_{\text{II}}(E) = C_{\text{II}}\left(E - E_{th}\right)^{b}, \tag{2}$$

where the parameters C_{II} and b, as in formula (1), are constants. Formula (2) in principle corresponds to formula (1), reduced to the appropriate form.

Formulas (1) and (2) have become widespread due to their relative simplicity. The rate of the impact ionization process, specified by these formulas, is a function of only the energy of the charge carrier E, which makes it very convenient for use in simulating transport processes by the Monte Carlo method. The parameters A_{II}, C_{II}, b and E_{th} are considered as some constant values. For both formula (1) and formula (2), different values of the specified parameters are found in the literature. So, for the Keldysh model (1) in [13] it was proposed to define the parameters as follows: $A_{\text{II}} = PW_{ph}(E_{th})$, where P is the constant; $W_{ph}(E_{th})$ is the total electron scattering rate on phonons for the electron energy equal to E_{th}. According to the theoretical estimate given in [13], the threshold energy E_{th} and constant P take the following values: $E_{th} = 1.2$ eV and $P = 0.38$ for the so called "soft" threshold, and $E_{th} = 1.8$ eV and $P = 100$ for so called "hard" threshold. Constant b is equal to 2 in both cases. For formula (2), taking into account the effects associated with the real band structure of silicon gives values of the coefficient b greater than 2. So, for example, according to [11], the value of C_{II} is equal numerically to $9.5\cdot10^{10}\ \text{s}^{-1}\text{eV}^{-4.79}$, $b = 4.79$, and the value of E_{th}, given in electron-volts, is equal to 1.1 eV. Somewhat different values of these parameters are present in [14]. It can be assumed that these values depend on the approximate description of the semiconductor band structure used and are determined by matching the simulation results with the experimental data, taking into account the values of any parameters or characteristics of the structure under study, for example, the avalanche multiplication factor, the current-voltage characteristics of the p-n-junction, etc. As was shown in [16], the results of simulation of the current-voltage characteristics of silicon submicron MOS transistors taking into account the impact ionization process in accordance with different models and parameters from [13, 14] have significant differences. Thus, in the general case, the parameters A_{II}, C_{II}, b and E_{th} can be considered as fitting parameters.

In this paper, we study the effect of the electron impact ionization process on the photocurrent response in the photodiode structure shown in Figure 1. In this case, formula (2) is used to calculate the scattering rate of electron impact ionization. For definiteness, we will assume the constant values of the exponent $b = 4.79$ and the threshold energy $E_{th} = 1.1$ eV, taken from [11]. The constant C_{II} is considered to be a fitting parameter, and its value can be determined from the results of simulating the electron ionization coefficient α using the ensemble Monte Carlo method in such a way that the value of α, calculated using the Monte Carlo method with a given accuracy, agrees with the known experimental results. Taking into account the fact that the available literature data on the experimental determination of the dependence of the electron ionization coefficient on electric field strength differ somewhat [17–20], for definiteness, we use the interpolation of the experimental data from [17] as a basis.

For the calculation of the hole impact ionization scattering rate in all cases we will use the formula (2) with the following parameter values from [15]: $C_{II} = 1.4 \cdot 10^{12}$ s^{-1}eV$^{-3.4}$, $b = 3.4$, and $E_{th} = 1.49$ eV.

The results of calculations

Figure 2 shows the experimental dependence of the electron impact ionization coefficient in bulk silicon α on the electric field strength F for a crystal lattice temperature of 300 K, taken from [17] (solid curve). The range of electric field strength variation is from $1.25 \cdot 10^7$ to 10^8 V/m. The presented experimental dependence of the electron ionization coefficient corresponds to bulk silicon. The electric field strength vector is directed along the main crystallographic direction <100>. It should be noted that the dependences of the electron ionization coefficient on the electric field strength are somewhat different for the conditions under consideration when the field strength vector is directed along the <100> and <111> axes. However, this difference can be considered insignificant [17]. Figure 2 also shows the corresponding dependence of the C_{II} coefficient calculated by us when using the formula (2) for the impact ionization process scattering rate. The results are obtained by numerically calculating the α coefficient by the Monte Carlo method and matching its values with the corresponding experimental data. The calculated C_{II} values (dashed curve) ensure the accuracy of ionization coefficient simulation by the Monte Carlo method with respect to the interpolation of the experimental values from [17] within 1 % in the 98 % confidence interval within the framework of the used analytical model of the silicon band structure.

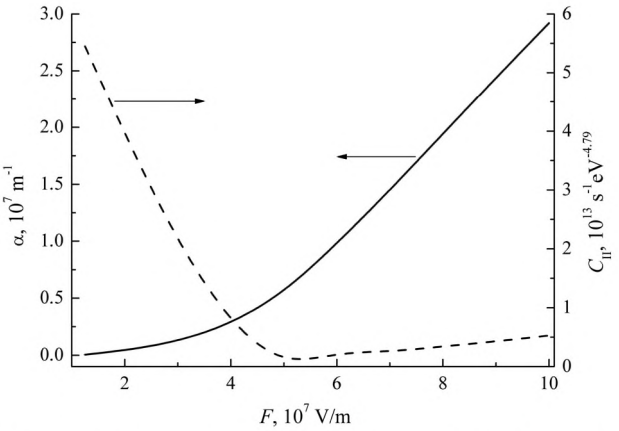

Figure 2 – Dependences of the electron ionization coefficient (solid curve) and the constant C_{II} (dashed curve) versus electric field strength in bulk silicon

As it can be seen from the Figure 2, the dependence of the coefficient C_{II} on the electric field strength F is not monotonic. The minimum of the dependence is observed for the value of the electric field strength $F \approx 5 \cdot 10^7$ V/m. With a decrease in the electric field strength from $5 \cdot 10^7$ to $1.25 \cdot 10^7$ V/m, a sharp increase in the coefficient C_{II} is observed from $1.61 \cdot 10^{12}$ to $5.45 \cdot 10^{13}$ s^{-1}eV$^{-4.79}$. For the electric field strength F equal to 10^7 V/m, the calculated value of C_{II} is already $4.3 \cdot 10^{14}$ s^{-1}eV$^{-4.79}$ (not shown in the figure). Thus, using a simple approximation with a constant value of the parameter C_{II}, it is not possible to reconcile the calculated using the ensemble Monte Carlo method and the experimental values of the ionization coefficient α. The non-monotonic dependence of the C_{II} coefficient can be explained by the fact that, first of all, the threshold energy of impact ionization E_{th} is not constant and depends on the electric field strength [21].

To assess the influence of different values of the C_{II} parameter on the electrical characteristics of photodiodes Figure 3 shows simulated dependences of the current density on time under the influence of picosecond radiation pulses in a diode with a *p-n*-junction (*a*) and in diodes with a *p-i-n*-structure (*b*), (*c*) and (*d*) with a reverse bias between the electrodes $V_1 - V_2 = 5$ V, assuming different constant values of the C_{II} coefficient. The thickness of the undoped *i*-layer for the structure in Figure 3*b*) is 50 nm, for the structure in Figure 3*c*) is 100 nm, and for the structure in Figure 3*d*) is 200 nm. Solid

curves correspond to the calculated C_{II} values for the constant electric field strength in bulk silicon $F = 10^7$ V/m, dashed curves – $F = 5 \cdot 10^7$ V/m, dotted curves – $F = 7 \cdot 10^7$ V/m, and dash-dotted curves – $F = 10^8$ V/m. The radiation begins to affect the diode structures at the time $t = 1$ ps.

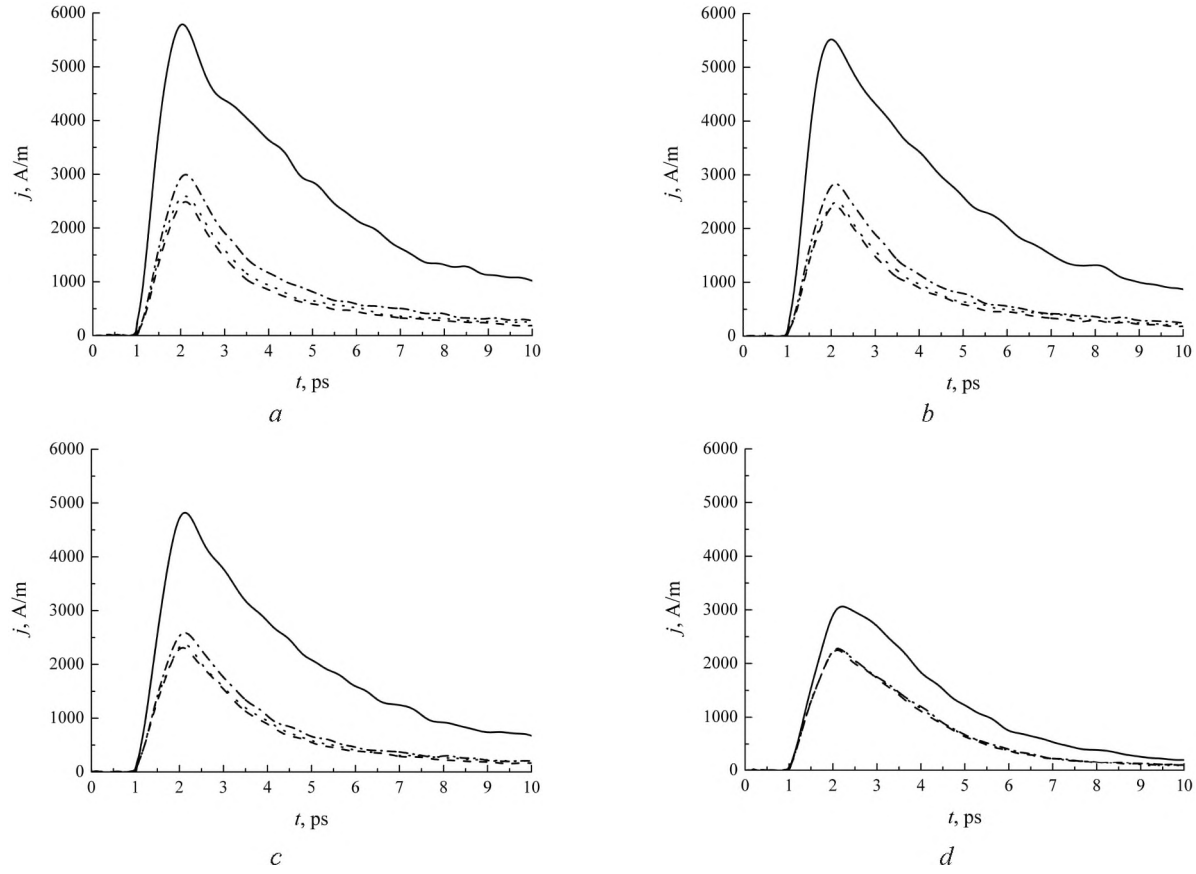

Figure 3 – Dependence of electric current density j versus time in a diode with p-n-junction (*a*) and p-i-n-structure (*b*), (*c*), and (*d*) under the reverse bias of 5 V

Thus, as can be seen from the current density versus time dependences shown in Figure 3, for all photodiode structures there is a significant difference in the calculated current density when using different values of the C_{II} coefficient corresponding to different values of the constant electric field strength in bulk silicon. Thus, the use of formula (2) with constant values of the C_{II}, b and E_{th} parameters for calculating the rate of the impact ionization process by electrons in semiconductor device structures with a significantly non-uniform electric field raises certain questions. Within the framework of the proposed model, it is apparently possible to use a variable value of the C_{II} coefficient, depending on the electric field strength. In this case, for self-consistent simulation of charge carrier transport processes by the ensemble Monte Carlo method, the impact ionization process rate becomes dependent not only on the charge carrier energy, but also on the local value of the electric field strength, and, consequently, on the spatial coordinates and time. Thus, it can be concluded that such an approach will require constant recalculation of the impact ionization rate at each time step, which complicates the algorithm and should lead to an increase in computational costs when modeling the electrical characteristics of semiconductor device structures in which the electric fields are significantly non-uniform.

Conclusion

Dependence of the current density on time in submicron silicon photodiodes with a p-n-junction and a p-i-n-structure under the effect of picosecond radiation pulses with a wavelength of 650 nm and an intensity of $5 \cdot 10^{10}$ W/m^2 is calculated by means of numerical self-consistent simulation based on the ensemble Monte Carlo method. It was shown that taking into account the impact ionization process significantly affects the results of simulating

the photocurrent response. At the same time, simple models most often used in Monte Carlo simulation for calculating the rate of the impact ionization process, such as the Keldysh model, do not allow adequately reproducing dependence of the ionization coefficient on the electric field strength for a wide range of field strength values. Accordingly these models cannot properly take into account processes of avalanche multiplication of charge carriers during their optical generation in silicon photodiodes. Taking into account the obtained results, in order to improve the simulation's adequacy, it is proposed to use in the Keldysh formula the proportionality coefficient which depend on the local value of the electric field strength.

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