Modelling of disordering regions in proton-irradiated silicon

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Abstract. A model of disordering regions generation as a result of interstitial atom-vacancy pairs separation in view of neutral and charged pair states was developed. The model allows to define the radius and the mean number of vacancies of a disordering region. Distribution profiles of interstitial silicon, vacancies, divacancies, disordering regions created by low-energy protons in silicon were calculated, as well as the disordering regions parameters dependencies on proton energies. It was shown that the disordering region distribution maximum is spatially separated from interstitial silicon, vacancies and divacancies distribution maximums. This allows to differentially modify superficial and volumetric properties of semiconductor structures.

1. Introduction

Engineering of radiation defects is an actively developing area of semiconductor technology. For the controlled introduction of impurities and changes in the properties of semiconductors, the ion implantation method is used, which has several advantages compared to thermal diffusion from an external source and epitaxy. The interaction of intrinsic defects, impurity atoms, radiation defects, dislocations, and other structural defects causes the appearance of new properties in semiconductor materials.

The formation of radiation defects in silicon during bombardment by protons with an energy of 1–10 MeV was analyzed in [1]. It was shown that, as a result of the separation of Frenkel pairs, point defects are formed: vacancies and interstitial atoms, and nanoscale regions with a high vacancy density (disordering regions) appear in the cascade of displaced Si atoms. During electron bombardment, nanoscale disorder regions are formed if the Si atom receives kinetic energy of more than 7 keV from the incident particle [2], which is consistent with data on neutron irradiation [1]. The disordering regions cause changes in the electrophysical properties of silicon crystals irradiated with protons and high-energy electrons [3]. The existence of nanoscale disorder regions in silicon irradiated with 27 MeV electrons and 1 MeV neutrons was detected by transmission electron microscopy in [4]. The disordering regions in silicon are formed upon irradiation with protons, electrons, and neutrons if an atom knocked out of a lattice site creates a cascade of displacements containing a large number of vacancies.

Irradiation by protons allows controlled changing of material properties in depths ranging from 0.1 μm to 1 mm [5]. The properties and structure of radiation defects depend on the dose of proton irradiation, annealing temperature and a primary impurities concentration [1, 5, 6]. The features of nano- and microelectronics are sensitive to changes in the superficial layer state. Numerical simulation of the process of radiation defect formation is of great interest today, mostly because it gives an opportunity to predict the regularities of variations in semiconductor materials and structures properties [7].
The fact of the existence of disorder regions in silicon irradiated with protons is debatable. The aim of this work is a numerical analysis of disordering regions distribution forming in silicon during irradiation by protons.

2. The model of primary radiation defects generation

An atom of the silicon (Si) lattice receives kinetic energy $T_k$ upon collision with an incident particle. The threshold energy for the formation of a bound Frenkel pair is $T_d$ and of a divided one $T_{dn}$. A Frenkel bound pair which exists at helium temperatures only, is formed if $T_d \leq T_k < T_{dn}$. At higher temperature a vacancy ($V$) and an interstitial silicone atom ($Si_I$) either annihilate, having overcome the energy barrier $E_k$ or split up, having overcome the energy barrier $E_L$. Having received the energy $T_k \geq T_{dn}$, the primary knock-on Si atom creates a Frenkel split pair, then overcomes the energy barrier $E_L$, collides with other lattice atoms, and at the energy $T_k \geq 2T_{dn}$ displaces them from their nodes. This, as a result, leads to the formation of a displacement cascade. The mean quantity of Frenkel split pairs in a displacement cascade may be described by a cascade function $v(T_k)$. In the model introduced by Lindhard, Nielson, Scharff and Thomson [8] this function is as follows:

$$v(T_k) = \begin{cases} 
0, & T_d \leq T_k < T_{dn}, \\
1, & T_{dn} \leq T_k \leq 2T_{dn}/g(T_k), \\
g(T_k)T_k / 2T_{dn}, & 2T_{dn}/g(T_k) \leq T_k. 
\end{cases}$$

(1)

The factor $g(T_k)$ in $v(T_k)$ (1) describes the primary displaced atom energy share spent on elastic collisions. Vacancies and interstitial Si atoms, created in result of the Frenkel pairs separation are called Basic Radiation Defects [9]. Basic Radiation Defects interact at the stage of the cascade propagation. Multivacancy complexes act as a nucleus of amorphous phase or disordering regions (DR). Interstitial atoms $Si_I$ and vacancies $V$ that didn’t recombine, as well as divacancies $W$, multi-vacancy defects and disordering regions created in displacement cascades are referred to as primary radiation defects (PRD) [9].

The influence of the temperature and charge state on the probability $w_f$ of the Frenkel pair separation and the generation of PRD in silicon with different donor and acceptor concentrations has been analyzed in [10]. The probability of the Frenkel pair separation increases with temperature, as well as with lowering of the Fermi level from the bottom of the conduction band to the mid of the forbidden energy bandgap.

The phenomenological model of the primary radiation defects generation in silicon has been built in [11]. We will match two experimentally defined threshold energy intervals [12] with creation of a bound $T_d = 12.9$ eV and a divided $T_{dn} = 21$ eV Frenkel pairs, and the threshold energy for the formation of DR will choose $T_{do} = 20$ keV [9].

For randomly placed $k$ vacancies in the volume of the instability zone $v_w$ (or reaction sphere) the probability of their merging $w_f$ is defined from the Poisson distribution (2):

$$\omega_k = \frac{(N_{v_p}v_w)^k}{k!} \exp\{-N_{v_p}v_w\},$$

(2)

where $N_{v_p}$ is the mean vacancy concentration in the cascade region.

Assume $T_m$ being the maximum energy, transferred to an interstitial atom by an incident particle. Then the mean number of interstitial silicon atoms and vacancies created by a single ionizing particle at a projected path length unit, with $T_{dn} \leq T_k \leq T_m < 2T_{dn}$ is described by the following equation (3):
\[
G_{Si} = G_{\nu} = N_0 \left\{ \omega_f \int_{T_d}^{T_{dm}} d\sigma_d \frac{dT_k}{dT} + \omega_d \int_{T_{dm}}^{T_p} v(T_k) \frac{d\sigma_d}{dT} dT_k \right\}, \tag{3}
\]

where \( N_0 \) – is the Si atoms concentration in the crystal lattice, \( d\sigma_d(E, T_k) \) – is the differential scattering cross section, representing the probability of \( T_k \) energy transfer from an incident particle (having energy \( E \)) to a node atom, \( \omega_d \) – is the probability for the separated \( V \) and \( Si_i \), placed at a distance of \( r \leq r_{vi} = 2.8 \) \( a \) (\( r_{vi} \) – mean reaction radius, \( a \) – lattice period) to avoid annihilation.

The region of the cascade appearing in case the recoil atom energy is \( \frac{dE}{dt} \geq 10^4 \) eV has previously been developed in [15]. At \( \frac{dE}{dt} < 10^4 \) eV there were used extrapolated \( R_p \) values.

Consider two cases corresponding to inequalities \( K_{vi} \geq K_{we} \) and \( K_{vi} < K_{we} \). In the first one \( K_{we} \) number of \( V \) and \( Si_i \) pairs annihilate while the rest of the \( Si_i \) atoms are at \( r > r_{vi} \) distance away from vacancies and contribute to the primary defects concentration. In the second case, \( K_{ie} \) number of \( V \) and \( Si_i \) pairs annihilate, the core volume \( v_c \) increases due to the inner part of the shell occupied by unannihilated vacancies (ratio (5)):

\[
\Delta v_c = \begin{cases} 
0, & K_{ie} \geq K_{we} \\
(K_{we} - K_{ie}) / N_{we}, & K_{ie} < K_{we}.
\end{cases}
\tag{5}
\]

The mean number of interstitial atoms avoided annihilation:

\[
v_i = \begin{cases} 
v(T_k) \left( 1 - \frac{2r_{vi}}{R_p} \right)^3, & K_{ie} \geq K_{we} \\
v(T_k) \omega_d, & K_{ie} < K_{we}.
\end{cases}
\tag{6}
\]

In the formation of a divacancy the closest vacancy to a given one within the volume \( v_w \) takes part. The probability \( \omega_{vw} \) of detecting the closest vacancy in the volume \( v_w \) can be found from the formula (2): \( \omega_{vw} = 1 - \exp\{-N_{vw} v_w\} \). The parameter \( v_w = 4 \pi a^3 / 3 \). In a cascade induced by an atom with the energy \( T_k < 2T_{dm} \), \( N_{vw} v_w \ll 1 \), therefore, the multi-vacancy cluster formation can be neglected in this case. Using \( \omega_{vw} \), one can find the mean number of divacancies \( v_{wu} \) and vacancies \( v_v \) left in the middle cluster:
\[ \nu_w = 0.5N_vv_c(1 - \exp\{-N_vv_w\}), \nu_v = N_vv_c \exp\{-N_vv_w\}. \quad (7) \]

These ratios (7) are also valid in DR under the \( \nu_v > \nu_w \) condition as long as it’s accurate for all of the calculation parameters. The mean number of the primary radiation defects created by a single ionizing particle at its projected path length unit, at the recoil atom energy \( 2T_{dn} \leq T_k \leq T_m \leq T_{do} \) can be obtained by using the ratios (6)-(7):

\[
\begin{align*}
\left\{ \begin{array}{l}
G_{Si} \\
G_v \\
G_W
\end{array} \right\} &= N_0 \int_{T_{dn}}^{T_m} \begin{pmatrix}
\nu_i \\
\nu_v \\
\nu_w
\end{pmatrix} \frac{d\sigma_d}{dT_k} dT_k.
\end{align*}
\quad (8)
\]

At the \( T_k > T_{do} \) neither vacancies nor divacancies contribute to \( G_v, G_W \), as they stay within the disordering region core. The \( G_{Si} \) value is calculated the same way as in (8), where \( 2T_{dn} \) is replaced with \( T_{do} \).

For DR the following values can be determined:

\[
\begin{align*}
R_{do} &= \int_{T_{do}}^{T_m} \left( \frac{3\nu_v}{4\pi} \right)^{1/3} \frac{d\sigma_d}{dT_k} dT_k, \quad N_{vdo} = \int_{T_{do}}^{T_m} N_v \nu_v \frac{d\sigma_d}{dT_k} dT_k, \quad G_{do} = \int_{T_{do}}^{T_m} \frac{d\sigma_d}{dT_k} dT_k.
\end{align*}
\quad (9)
\]

In (9) \( R_{do} \) – is the radius, \( N_{vdo} \) – is the number of unannihilated in DR vacancies, \( G_{do} \) – is the number of DR, created by one ionizing particle at a projected path length unit.

The differential cross section \( d\sigma_d(E, T_k) \) of a classic proton was calculated according to the Lindhard-Nielson-Scharff formula [16] with consideration to energy dependencies of ionization loss, electronic and nuclear stopping power in a range of low and high energy.

3. Calculation of the formation of disordered regions

The depth distribution of the mean number of primary radiation defects produced in silicon by a proton with energy \( E_p = 180 \text{ keV} \) at a temperature of 300 K was calculated using the ratios (3), (8) and (9) (figure 1).

Protons with the energy \( E_p = 180 \text{ keV} \) produce disordering regions in silicon with their distribution maximum being on the surface, and the interstitial atoms and vacancies distribution maximums are located in volume at \( x = 1490 \text{ nm} \) (figure 1). Changing DR parameters \( R_{do}(x), N_{vdo}(x) \) at the distance of \( x \leq 272 \text{ nm} \) from the surface is shown in figure 2. Disordering regions are nanoscale objects with the average radius \( R_{do} \leq 15 \text{ nm} \) and mean vacancies number \( N_{vdo} \leq 111.8 \) (figure 2).

The DR parameters dependence on proton energies is shown in figure 3. Protons with the energy \( E_p < 150 \text{ keV} \) do not produce disordering regions. The dependence of \( G_{do} \) on the proton energy has its maximum at \( E_p = 300 \text{ keV} \), the maximal value \( G_{do_{max}} = 1.9 \text{ cm}^{-1} \). The value \( G_{do} \) decreases from \( G_{do_{max}} \) to 0.011 \text{ cm}^{-1} at \( E_p = 100 \text{ MeV} \). The average radius \( R_{do} \) as well as the vacancies number \( N_{vdo} \) in DR evenly increase with the proton energy increasing from 150 keV up to 100 MeV.
Figure 1. The number of PRD, produced at a projected path length unit by a proton having energy $E_p = 180$ keV: 1 – interstitial silicon $G_{Si}$; 2 – vacancies $G_V$; 3 – divacancies $G_W$; 4 – disordering regions $G_{do}$.

Figure 2. Coordinate dependence of the parameters DR created by a proton with an energy $E_p = 180$ keV: 1 – $R_{do}$; 2 – $N_{vdo}$.
Figure 3. The dependence of the parameters of disordering regions on the proton energy:
1 – $v_{doN}$; 2 – $doG$; 3 – $doR$.

4. Conclusion
PRD interact with each other, with atoms of the crystal lattice, impurities and other defects, forming secondary radiation defects (SRD) [9]. The SRD distribution can be calculated by numerically solving the system of equations of quasi-chemical reactions [9, 11]. The result depends on the concentration of donors, acceptors, uncontrolled impurities of oxygen, carbon, etc., as well as the temperature of the samples. The structure of the SRD is different in silicon grown by various methods [9, 11, 17].

Hydrogen-containing centers are formed in silicon upon irradiation with protons. The structure and depth distribution of hydrogen-containing centers depends on the energy of protons, the time of irradiation and samples temperature [18], the time and temperature of annealing following irradiation [19]. In this article, the distribution of the PRD was calculated for the proton energy of 180 keV and the temperature of the samples 300 K. In this case, the hydrogen-containing centers are located at a depth of the projective range of protons $s = 1510$ nm and do not affect the disordering regions located at a distance from the surface of less than $sd = 272$ nm. Modeling of the SRD and hydrogen-containing centers is beyond the scope of this article.

The proton energy of 180 keV was chosen in the calculations in such a way that the PRD is created in the entire space charge region of the silicon structure with an n+-p junction depth of 450 nm. Protons with energy of 180 keV create the DR in the emitter and the PRD with a maximum located near the boundary of the space charge region and the base. This statement was experimentally substantiated in [7].

DR formation is a random process. The probability of creating a DR by one proton is small. The proton flux with a dose $F_p$ creates DR with an average surface density $S_{do} = F_p \int_0^{s_p} G_{do}(x)dx$. The calculated dependence $G_{do}(x)$ gives the value $S_{do} = 3.3 \cdot 10^9$ cm$^{-2}$ for $F_p = 10^{15}$ cm$^{-2}$. The disordering
regions have average radius $R_{do} \leq 15 \text{ nm}$, then the conditions $E_p = 180 \text{ keV}$ and $F_p > 4 \cdot 10^{16} \text{ cm}^{-2}$ can correspond to a uniform surface distribution of DR.

The calculated dependence $G_{do}(x)$ means that the maximum of the DR distribution is always spatially separated from the maximum of the PRD distribution (the Bragg peak), which is located closer to the end of the projective path of protons. The maximum of the DR distribution shifts from the silicon surface to the volume if the energy of the incident protons increases $E_p > 300 \text{ keV}$. A flux of protons with energy $E_p \geq 1 \text{ MeV}$ can create DR in the layer between the irradiated surface and the region of the Bragg peak. Thus, it is possible to differentially modify the various regions properties of the semiconductor structure.

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