Formation of primary radiation defects in a non-equilibrium silicon structure by electron irradiation

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Abstract. Based on numerical simulation, the influence of the position in the band gap of the Fermi quasilevel of electrons on the dependence of the linear generation rate of interstitial silicon, vacancies, divacancies, and disordering regions in silicon irradiated with electrons is analyzed. From the obtained results it follows that, if the quasi-Fermi level of electrons is located in the upper quarter of the band gap and approaches the bottom of the conduction band, then the linear rate of generation of primary radiation defects created by electrons decreases. Consequently, under nonequilibrium conditions caused by a high level of illumination or the passage of an electric current through the n+-p junction in the forward electric bias mode, as well as in the n'-region of silicon, it is possible to differentially vary the concentration of radiation defects when exposed to electrons. The results obtained can find application in the development of new methods for modifying the properties of semiconductor structures.

1. Introduction
Radiation defects change physical properties of semiconductor structures [1 – 4]. Apart from controlled processes of defect-impurity engineering, there are uncontrolled processes of formation of radiation defects under operating conditions, which are one of the reasons for the degradation of semiconductor devices [4]. Therefore, the study of the processes of radiation defects formation is of interest [5 – 7]. The influence of nonequilibrium conditions such as temperature, the quasi-Fermi level position, energy of ionizing particles, on radiation defect formation in semiconductors was discussed in [2, 8].

Theoretical and experimental studies [7, 9] have shown that the number of radiation defects created in the Bragg peak by low-energy protons in the n⁺ layer of the n⁺-p junction is significantly less at the temperature of the irradiated samples \(T_p = 83\) K than at \(T_p = 300\) K and also much less than in the p-region. The listed regularities are due to the dependence of the separation of charged Frenkel pairs on the position of the quasi Fermi level in n and p type silicon.

The purpose of this work is modelling the formation of primary radiation defects (PRD) caused by electrons in silicon under nonequilibrium conditions of stationary charge carriers transport.

2. The model of primary radiation defects generation
The concentration of nonequilibrium electrons \(n\) and holes \(p\) in semiconductors in the local equilibrium approximation is expressed by the formulas (1):

\[
\begin{align*}
n &= N_e e^{\frac{E_n - E_F - q\Phi}{kT}}, \\
p &= N_h e^{\frac{-E_p + E_F - q\Phi}{kT}}.
\end{align*}
\]
Here \( N_e \) is the effective density of electronic states in the extent of the conduction band bottom, \( F_n \) – electron quasi-Fermi level, \( E_c \) – the conduction band bottom level, \( q \) is elementary charge, \( \varphi \) – internal electric field potential, \( k \) – Boltzmann constant, \( T \) – absolute temperature, \( N_e \) – effective density of electronic states in the extent of the top of the valence band, \( E_v \) – the top of the valence band level.

The system of equations for the charge carriers transport in inhomogeneous semiconductors has the following form (2):

\[
\begin{align*}
\frac{\partial n}{\partial t} & = -\mu_n n \left( -\nabla \varphi + \frac{1}{q} \nabla E_c \right) - D_n \nabla n + D_n n \nabla \ln N_e, \\
\frac{\partial p}{\partial t} & = \mu_p p \left( -\nabla \varphi + \frac{1}{q} \nabla E_v \right) - D_p \nabla p + D_p p \nabla \ln N_v, \\
\frac{\partial \varphi}{\partial t} & = G - R,
\end{align*}
\]

(2)

In (2) \( \nabla n \) – electron flow, \( \mu_n \) – electron mobility, \( D_n \) – electron diffusion coefficient, \( \nabla p \) – hole flow, \( \mu_p \) – hole mobility, \( D_p \) – hole diffusion coefficient, \( G \) – volumetric generation rate, \( R \) – rate of volumetric recombination of electron-hole pairs, \( N_p^+ \) – ionized donor concentration, \( N_A^- \) – ionized acceptors concentration.

Under stationary conditions, the system of equations (2) is transformed to the system of equations (3) for unknown variables \( F_n, F_p, \varphi \):

\[
\begin{align*}
\frac{\Delta F_n}{q} + \left( \frac{\nabla (F_n - E_c + q \varphi(x))}{kT} + \nabla \ln N_e + \nabla \ln \mu_n \right) \frac{\nabla F_n}{q} &= -\frac{G - R}{\mu_n n(x)}, \\
\frac{\Delta F_p}{q} + \left( \frac{\nabla (-F_p + E_v - q \varphi(x))}{kT} + \nabla \ln N_v + \nabla \ln \mu_p \right) \frac{\nabla F_p}{q} &= -\frac{G - R}{\mu_p p(x)}, \\
\Delta \varphi &= -\frac{q}{\varepsilon \varepsilon_0} \left( N_e e^{\frac{F_n - E_c}{kT}} - N_ie^{\frac{F_n - E_c - \varphi(x)}{kT}} + N_D^{+} - N_A^{-} \right).
\end{align*}
\]

(3)

In equilibrium, \( F_n = F_p = F \), where \( F \) is the Fermi level, taking a constant value in the volume of the semiconductor.

The probability of separation of interstitial silicon \( Si_i \) and vacancy \( V \) depends on the pair charge state. The energy level of the Frenkel pair in the bandgap of silicon is located close to the bottom of the conduction band \( E_f = E_c - 0.07 \text{ eV} \), therefore, electron transitions between the energy levels of the pair and the conduction band are occurred. In the case of the charge carriers transport, for the formula of the probability of the charged state of a bound Frenkel pair \( F_n \) will replace \( F \) (4):

\[
\omega_i = \left[ 1 + g_i \exp \left\{ \frac{F_n - E_f}{kT} \right\} \right]^{-1}.
\]

(4)
In (6) $F_{m}$ is the equation system (3) solution, $g_{t} = 0.5$. The probability of a neutral pair separation is described by the expression (5):

$$
\omega_{z} = \left[1 + \exp\left(-\frac{T_{d} - T_{dm}}{kT}\right)^{-1}\right].
$$

(5)

In (5) $T_{d} = 12.9$ eV is the threshold energy for the formation of a bound Frenkel pair, $T_{dm} = 21$ eV is the threshold energy for the formation of a separated Frenkel pair in silicon. The nodal silicon atom that received energy from the incident particle $2T_{dm} \leq T_{l} < T_{do}$ ($T_{do}$ is the threshold energy for the formation of disordering regions; for silicon $T_{do} = 20$ keV), leaves its position and travels within the crystal volume. The displaced atom transfers energy to neighboring atoms due to elastic collisions, which leads to their displacement from their site positions and in the end, to the formation of a displacement cascade.

The probability of a bound Frenkel pair separation with respect to the charge state of the defect, is determined by the value $\omega_{f}$. For the separated $Si_{l}$ and $V$ located within a reaction sphere with the radius $r_{ci} = 2.8\alpha$ ($\alpha$ is the lattice period), the probability to avoid annihilation is defined by the $\omega_{f}$ value (6):

$$
\omega_{f} = \omega_{c}\omega_{t} + (1 - \omega_{c}\omega_{t})\omega_{z}, \quad \omega_{d} = 6\omega_{c}\omega_{t} + (1 - 6\omega_{c}\omega_{t})\omega_{z}.
$$

(6)

In (6) $\omega_{c}$ is used as an additional parameter, that describes the probability of a silicon atom displacement into spatial position allowing a charged state, $\omega_{c} = 0.00887$, $\omega_{t}$ is the probability of avoiding annihilation for a neutral separated Frenkel pair (7):

$$
\omega_{3} = \left[1 + \exp\left(-\frac{E_{r}^{\prime} - E_{m}^{\prime}}{kT}\right)^{-1}\right].
$$

(7)

In (7) $E_{r}^{\prime}$ – the reverse transition barrier energy, $E_{m}^{\prime}$ is the activation energy of interstitial silicon migration ($E_{r} = 0$, $E_{m} = 0.13$ eV).

Probabilities $\omega_{f}$ and $\omega_{d}$ (6) depend on the electron quasi-Fermi level $F_{e}$ via $\omega_{t}$ (4). Linear primary radiation defects generation rates that are the average quantity of interstitial silicon atoms $G_{Si}$, vacancies $G_{v}$, divacancies $G_{w}$ disordering regions $G_{do}$, created by one ionizing particle per unit of the projective path length were calculated according to the formulas [10], containing $\omega_{f}$ and $\omega_{c}$. The differential scattering cross section of a relativistic electron was calculated using the McKinley - Feshbach formula.

3. Calculation of the linear primary radiation defects generation rates

Figure 1 shows the calculated dependence of the linear generation rate of interstitial silicon $G_{Si}(E_{c}, T)$ on the electron energy $E_{c}$ in the range [0.1; 100] MeV and irradiation temperature $T$ in the range [20; 600] K. In the considered ranges of $E_{c}$ and $T$ values, the dependence $G_{Si}(E_{c}, T)$ increases and does not have extreme values both in the section $T = \text{const}$ and in the section $E_{c} = \text{const}$. $G_{Si}(E_{c}, T)$ has a maximum value at the point corresponding to $G_{Si}(100$ MeV; 600 K) = 1.6 cm$^{-1}$.

The dependence $G_{Si}(E_{c} = \text{const}, T)$ shows two regions of the function growth. The first one is the region of rapid growth in the temperature range (76; 136) K. The second region is the region of smooth growth in the range (136; 600) K. This feature is determined by the nature of the dependence $\omega_{d}(T)$.

The threshold values of the electron energies $E_{c1} = 2.22 \cdot 10^{-1}$ MeV, $E_{c2} = 3.91 \cdot 10^{-1}$ MeV, and $E_{c3} = 15.7$ MeV correspond to the maximum energies of the recoil atom $T_{dm}$, $2T_{dm}$, and $T_{do}$, respectively. The threshold value of the electron energy $E_{c3} = 2.83$ MeV corresponds to the maximum energy of the recoil atom, at which the average projective range of the displaced silicon atom is $R_{p} = 2r_{ci}$. For $E_{c} > E_{c3}$, there is a core of the displacement cascade with a volume $V_{c} > 0$.

Regularities similar to $G_{Si}(E_{c}, T)$ are observed in the dependence of the generation rate of vacancies $G_{v}(E_{c}, T)$. This is explained by the fact that the values of $G_{Si}$ and $G_{v}$ are similar to each other and exceed the generation rate of divacancies $G_{w}$ by an order of magnitude.
Figure 2 shows the calculated dependence of the linear generation rate of interstitial silicon $G_{Si}$ on the electron energy $E_e$ and the position of the quasi-Fermi level of electrons below the bottom of the conduction band $F_{cn} = E_c - F_n$ in the ranges $E_e \in [0.01; 100]$ MeV, $F_{cn} \in [0.017; 0.56]$ eV at the temperature of 300 K.

In the considered ranges of values of $E_e$ and $F_{cn}$, the $G_{Si}(E_e, F_{cn})$ function increases and does not have extreme values both in the section $F_{cn} = \text{const}$ and in the section $E_e = \text{const}$. The maximum values of the function $G_{Si}(E_e, F_{cn})$ for all cross sections $F_{cn} = \text{const}$ are observed at $E_e = 100$ MeV.

In the dependence shown in figure 2 there is a region of a sharp increase of $G_{Si}(E_e = \text{const}, F_{cn})$ and the region of stable values where the $G_{Si}$ almost does not change. Intense growth of the $G_{Si}(E_e = \text{const}, F_{cn})$ at the energies of 100 MeV, 10.8 MeV and 0.32 MeV can be seen in the range of $F_{cn} \in [0.017; 0.17]$ eV, $F_{cn} \in [0.017; 0.16]$ eV and $F_{cn} \in [0.017; 0.15]$ eV, respectively. Calculations of the dependence of the linear generation rate of vacancies $G_{V}(E_e; F_{cn})$ under electron irradiation show regularities similar
These regularities are due to the probability of the charged state of the $Si$, $V$ pair. The $G_{Si}$ and $G_{V}$ values are close and are approximately 20 times higher than the rate of generation of divacancies $G_{W}$.

The disordering regions under electron irradiation are formed in a displacement cascade if $E_{e} > 15.7$ MeV. The area of the displacement cascade is characterized by the concept of the "middle cluster", which approximately has the shape of an ellipsoid. Without taking into account the channeling effect, the middle cluster looks like a sphere with a diameter $R_p$ equal to the average projective range of the initially displaced $Si$ atom [11]. In the emerging cascade of displacements, interstitial $Si$ atoms move to the boundary of the cascade region, while the $V$ are located inside the region, in a core with a radius $r_c$.

Some of the $Si$ atoms return to the core, annihilating with the $V$ in the region characterized by the reaction radius $r_{vi}$, while the other part diffuses in the crystal volume. As a result of this interaction, the nucleus remains, which is a region of disordering. In the considering model, the linear generation rate of disordering regions does not depend on the temperature and position of the quasi-Fermi level (figure 3).

![Figure 3. Dependence of the disordered regions rate of generation on the electron energy.](image)

4. Conclusion
Under nonequilibrium conditions caused by a high level of illumination or by the flow of electric current through the $n^-p^+$ junction in the forward electric displacement mode, the concentration of electrons and holes increases. If the concentration of excess electrons exceeds the concentration of the equilibrium ones ($\Delta n > n_0$), the electron quasi-Fermi level position approaches the conductivity band bottom $E_c$.

As follows from the results obtained, the linear generation rate $G_{Si}$, $G_{V}$, $G_{W}$ in that part of the silicon structure where the following criteria is met: $E_c – F_n < 0.2$ eV turns out to be less than in the rest of the volume upon electron irradiation. The $G_{Si}$, $G_{V}$, $G_{W}$ values evenly increase as with increasing $E_c$ and $T$.

Part of the energy of the electron flow is spent on heating the irradiated semiconductor and for the internal photoelectric effect, what leads to creation of electron-hole pairs with their volumetric generation rate $G$ included into the equation system (3). Thus, the processes of PRD formation, heat release, generation and transport of charge carriers in semiconductor structures are interrelated, which requires generalization of the radiation defect formation model.

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