Calculation of Frenkel Pairs Separation, Formed in Silicon as a Result of Ionizing Particles Irradiation

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Abstract
The equations for describing separation probabilities of Frenkel pair were proposed in this paper. These equations take into account neutral and charged states. The dependence of the separation probability on the temperature and the position of the Fermi level in the band gap were calculated. It is shown that the probability of Frenkel pairs separation increases with a decrease in the position of the Fermi level, as well as the temperature increase. These regularities cause the dependence of primary radiation defects concentration on the irradiation temperature and impurity concentration. These results may be there are practical significances for decreasing radiation damage of silicon structures with a surface n-p junction when irradiated with low-energy protons.

1. Introduction
Silicon electronics are used in conditions of increased exposure to ionizing radiation. A radiation defects formation affects parameters of electronic devices. Also, it is one of the reasons of silicon electronics parameters degradation in irradiation conditions [1 – 3].

Radiation defects in silicon have electrical and recombinational activity. An increase in the number of radiation defects changes a concentration and a lifetime of electrons and holes, as a result, electrical characteristics of n-p-junctions change during device operation [4, 5]. Thus, a study of the radiation defects formation is an actual problem of semiconductor physics and technology [6, 7].

The objectives of this paper are to develop and to analyze a model of the Frenkel pairs separation process formed in silicon by irradiation of ionizing particles.

2. The Model of Frenkel Pairs Formation
A radiation defect it is a defect in a material. The defect is formed as a result of exposure to ionizing radiation.

Depending on a mechanism of formation distinguish: simple, primary and secondary radiation defects [8, 9]. The interaction of ionizing radiation with crystalline silicon lattice forms simple defects: separated and bound Frenkel pairs. These defects consist of a vacancy V and a self-interstitial silicon Si.
An incident ionizing particle transfers the kinetic energy to a silicon atom. To get out of a crystal site, a silicon atom must overcome the potential barrier $T_d$ (figure 1).

A type of the Frenkel pair depends on the energy that a silicon atom received from an incident particle. The energy threshold of forming a bound Frenkel pair is $T_d = 12.9$ eV, and separated Frenkel pair is $T_{dm} = 21$ eV [8, 9].

A bound Frenkel pair forms when a silicon atom in the crystal site receives the energy $T_k \in (T_d; T_{dm})$ after collision with an incident particle.

The volume generation rate of Frenkel pair [9]

$$G_{0} = N_0 \Phi \int_{T_d}^{T_{dm}} \frac{d\sigma_d}{dT_k} dT_k$$

(1)

where $N_0$ – the concentration of silicon atoms in the crystal lattice, $\Phi(E)$ – incident particles flux with the energy $E$, $d\sigma_d(E, T_k)$ – differential scattering cross section (characterize the probability of transmission the energy $T_k$ to a site atom from an incident particle with energy $E$).

A bound Frenkel pair exists only at the liquid helium temperature [10]. On temperature growing, an interstitial silicon atom overcomes the energy threshold $E_R$. Then it moves in the crystal site and annihilates or overcomes the energy threshold $E_L$ with separated Frenkel pair formation.

The separation of bound Frenkel pair is described by various models of metastable pairs [9 – 11]. There are neutral and charged bound Frenkel pairs. The probability of the charged state of a bound Frenkel pair is described by the formula:

$$\omega_1 = 1 + g_1 \exp \left( \frac{F - E_f}{kT} \right)^{-1}$$

(2)

where $F$ – the Fermi level, $g_1 = 0.5$, $E_f$ – Frenkel pair energy level in the silicon band gap, $E_c = E_c - 0.07$ eV [10], $k$ – the Boltzmann constant, $T$ – the temperature. The form of the potential barrier of a charged Frenkel pair varies so that it is separated with probability 1.

The probability of a neutral pair separation is described by the formula

$$\omega_n = \left[ 1 + \exp \left( \frac{E_f - E_c}{kT} \right) \right]^{-1}$$

(3)

The probability of a bound Frenkel pair separation with taking into account a charge state of a defect is determined by the quantity $\omega_f$:

$$\omega_f = \omega_n \omega_c + (1 - \omega_n \omega_c) \omega_2$$

(4)

where $\omega_c$ – the additional parameter, it characterizes the probability of the displacement of a silicon atom into spatial position, which permits the charged state, $\omega_f = 0.00887$ [12], $\omega_c = \omega_n \omega_c$ – the charged state probability of a silicon atom in an interstitial position (a charged Frenkel pair is divided), $\omega_2 = (1 - \omega_n \omega_c) \omega_1$ – the separation probability of bound Frenkel pair in the neutral state.

The figure 2 shows us the dependence of the separation probabilities of a neutral $\omega_n$ and a charged $\omega_c$ Frenkel pair on the temperature in the range [250 K; 607 K]. Curves 1, 2 and 3 characterize the separation probability of a charged Frenkel pair for various Fermi levels in the band gap. The curve 4 shows the separation probability of a neutral Frenkel pair $\omega_{dn}$. Note that $\omega_{dn}$ practically doesn’t depend on Fermi level position. The main contribution to the separation probability of bound Frenkel defects is made by charged pairs. The contribution of neutral pairs is negligibly small.

A separated Frenkel pair forms when a silicon atom in a crystal site receives the energy $T_k \geq T_{dm}$. The form of the potential barrier changes after formation of the separated Frenkel pair. The formation of the separated Frenkel pair leads to a decrease in the energy barrier of the reverse transition (figure 3). An interstitial silicon atom $\text{Si}_i$ is within the sphere of reaction with radius $r_0$. $\text{Si}_i$ can either migrate from or annihilate with a corresponding vacancy.

An interstitial silicon atom needs to overcome the reverse
transition barrier $E_{iv}$ for annihilation of a separated Frenkel pair. The barrier height depends on a state of an annihilating pair. According to the theory of impurity reactions, a reaction is called activation-controlled when the diffusion activation energy $E_{im}$ less than the reverse transition barrier ($E_{iv}$ on the figure 3). If the energy $E_{im}$ more than the reverse transition barrier, then reaction is called diffusion-controlled ($E_{iv}$ on the figure 3) [9, 11].

Taking into account a shape of the potential barrier (Figure 3), the probability of avoiding annihilation for a neutral separated Frenkel pair is described by the following equation [11, 13]:

$$\omega_d = \left[1 + \exp\left(-\frac{E_{iv} - E_{im}}{kT}\right)\right]^{-1}, \quad (5)$$

where $E_{iv}$ – the energy of the reverse transition barrier, $E_{im}$ – the activation energy of an interstitial silicon migration ($E_{iv} = 0$, $E_{im} = 0.13$ eV according to [14]).

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**Figure 3. The form of the potential barrier of a separated Frenkel pair.**

1 – the potential energy for activation-controlled reactions,
2 – the potential energy for diffusion-controlled reactions.

The variable $\omega_d$ characterizes the probability to avoid annihilation of Si$_I$ with corresponding V. The probability is defined as follows. Let’s pretend that the charged state of a metastable pair V and Si$_I$ is formed in one of the six symmetrical directions with respect to a vacancy. Then

$$\omega_d = 6\omega_{dc} + (1 - 6\omega_{dc})\omega_{dn}, \quad (6)$$

where $\omega_{dc} = 6\omega_{e1}\omega_{e2}$ – the probability to avoid annihilation of charged Si$_I$ – V pair, $\omega_{dn} = (1 - 6\omega_{e1}\omega_{e2})\omega_{dn}$ – the probability to avoid annihilation of neutral Si$_I$ – V pair.

Figure 4 and figure 5 show temperature dependencies of $\omega_d$ for separated Frenkel pairs. These dependencies allowance neutral and charged states of pairs for different Fermi level positions in the temperature range [250 K; 607 K].

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**Figure 4. The temperature dependencies of the probability $\omega_d$ (on a logarithmic scale).**

1 – $F = E_c - 0.28$ eV, 2 – $F = E_c - 0.07$ eV,
3 – $F = E_c - 0.02$ eV, 4 – $F = E_c$.

**Figure 5. The temperature dependencies of probabilities $\omega_{dc}$ and $\omega_{dn}$ (on a logarithmic scale).**

1 – $\omega_{dc}$, $F = E_c - 0.28$ eV, 2 – $\omega_{dc}$, $F = E_c - 0.07$ eV,
3 – $\omega_{dc}$, $F = E_c - 0.02$ eV, 4 – $\omega_{dc}$, $F = E_c$, 5 – $\omega_{dn}$.

The probability $\omega_d$ increases when the Fermi level position decreases or the temperature increases (figure 4). The contribution to the separation probability of the considered neutral and charged Frenkel pairs is shown in figure 5. The separation probability of a neutral Frenkel pair $\omega_{dn}$ practically doesn’t depend on the Fermi level position (the curve 5 on the figure 5). Points $T_1 = 533.7$ K, $T_2 = 462$ K, $T_3 = 364.1$ K, $T_4 = 296.1$ K on the figure 5 correspond to the intersections of curves 1, 2, 3 and 4 with the curve 5. A decay of a neutral Frenkel pairs prevails at $T > T_i$ (i=1, 2, 3, 4) for corresponding Fermi levels, and at $T < T_i$ – for charged.

As it follows from the figure 5, the location of points $T_i$ depends on the Fermi level position. The dependence is shown in the figure 6. It shows that the lower Fermi level position relative to the bottom of the conduction band, the higher the temperature $T_i$ is. At this temperature the decay probabilities of neutral and charged Frenkel pair are equal.
3. Discussion

The paper proposes equations that describe the separation probabilities of Frenkel pair. These equations take into account neutral and charged states. Neutral pairs give a negligible contribution to the separation probability of bound Frenkel pairs, in comparison with charged pairs.

The dependence of the separation probability on the temperature and the position of the Fermi level F in the band gap were calculated. It is shown that the probability of Frenkel pairs separation increases with a decrease in the position of the Fermi level, as well as the temperature increase.

The probability of the neutral Frenkel pair separation does not depend on the position of the Fermi level. Denote the temperature $T_c$ at which the probabilities to avoid annihilation of separated Frenkel pair in neutral and charged states are equal. $T_c$ depends on the Fermi level position in the band gap. The probability to avoid annihilation of separated Frenkel pair in the neutral state prevails at $T > T_c$. At $T < T_c$ it prevails for the pair in charged state. The function $T_c(E_F - F)$ increases from $T_c = 296.1$ K at $F = 0$ to $T_c = 533.7$ K at $F = 0.15$ eV. At $F > 0.15$ eV the function has constant value $T_c = 533.7$ K.

The considered regularities cause the dependence of primary radiation defects (PRD) concentration on the irradiation temperature and impurity concentration. In figure 7 and 8 show calculated the depth distribution of the mean number of PRD: $G_{Si}$ – interstitial silicon atoms, $G_V$ – vacancies created by one proton (with the energy $E_p = 40$ keV) per unit length of projected range in silicon at temperature 300 K (figure 7) and at temperature 83 K (figure 8).

At $T = 300$ K (figure 7), there is a sharp maximum of the distribution of interstitial silicon atoms and vacancies at $x \approx 390$ nm. The values of $G_{Si}$, $G_V$ at the maximum practically don’t change with increasing phosphorus concentration up to $N_D = 10^{17}$ cm$^{-3}$ and decrease at $N_D > 10^{17}$ cm$^{-3}$.

At $T = 83$ K (figure 8) the absolute maximum at $x \approx 390$ nm exists only for $N_D \leq 10^{15}$ cm$^{-3}$. With increasing $N_D$, values of $G_{Si}$, $G_V$ decrease and at $N_D > 10^{17}$ cm$^{-3}$ the maximum at $x \approx 390$ nm disappears. Consequently, the region of the greatest material damage disappears.

4. Conclusion

The calculated dependence of the separation probability on the temperature and the position of the Fermi level in the band gap is a consequence of the existence of Frenkel pairs in the charged and neutral states. The separation probability increases with a decrease in the position of the Fermi level, so the concentration of primary radiation defects decreases with increasing donor concentrations.

In n-type silicon, the separation probability decreases if the irradiation temperature decreases. These results may be there are practical significances for decreasing radiation damage of silicon structures with a surface n-p junction when irradiated with low-energy protons.

The obtained results allow to draw a conclusion about higher radiation stability of silicon structures with a surface n-p junction in comparison with p-n junction structures when irradiated with low-energy protons.

References


