TEMPERATURE DEPENDENCE OF THE EFFICIENCY OF VACANCY GENERATION IN *n*-Si AT THE 1-MeV ELECTRON IRRADIATION

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UDC 621.315.592

Temperature dependence of the efficiency of the generation of free vacancies, i.e. the vacancies formed as a result of the dissociation of Frenkel pairs (FPs) into independent components – vacancies and interstitial atoms, has been obtained experimentally in *n*-Si at the 1-MeV electron irradiation in the temperature range 100–633 K. It is established that this dependence is an increasing function in the range of temperatures 100–300 K, which tends to saturate at T>300 K. It is shown that the change in the efficiency of free vacancy generation is governed by the function of the FP distribution in distances between FP components, the steepness of which rises with the increase in the temperature of the samples at irradiation. It is found that the change in the steepness of the FP distribution function is caused by an additional scattering of the "hot" interstitial atoms, formed in the process of irradiation, by the phonon oscillations of lattice atoms.

It is known that the efficiency of the creation of secondary radiation defects in silicon is determined in the first place by the ratio between the processes of annihilation and dissociation of FPs formed at irradiation [1]. At the 1-MeV electron irradiation, silicon atoms obtain different energies – from a threshold value (12–13 eV [2]) to 150 eV, where the latter is the maximal energy that a silicon atom knocked out of a lattice site can obtain. As a result, the knocked atoms are thermalized at different distances from a vacancy V. A portion of FPs, for which the distance between the components V and I is less than a critical one, will annihilate. All other FPs dissociate into independent V and I and subsequently form the secondary radiation defects which are detected afterwards in experiment. The critical distance, the so-called capture radius r_c, is determined from the condition of equality between the energy of electrostatic interaction of the oppositely charged V and I and the thermal energy.

The aim of this work is to specify the dependence of the efficiency of free vacancy generation on the specimen temperature at the 1-MeV electron irradiation of *n*-Si in a wide temperature range from 100 to 633 K.

The objects of investigation were silicon specimens doped with phosphorus. The concentration of phosphorus was 10^{15} cm^{-3}, the concentrations of oxygen and carbon were $N_{\rm O} = 7\times10^{17}$ cm^{-3} and $N_{\rm C} \le 5\times10^{16}$ cm^{-3}, respectively. The specimens were subjected to the 1-MeV electron irradiation with the electron beam intensity 0.5 μA/cm^{-2}. The irradiation dose was $\Phi = (0.5 \div 2)\times10^{16}$ cm^{-2}. For the temperature range T<300 K, the irradiation was carried out in a helium cryostat. At higher temperatures, T>300 K, the specimens were heated in a quartz tube. The temperature was measured with the chromel-alumel thermocouple. After irradiation, the temperature dependence of the Hall effect was studied, from which the concentration of the secondary irradiation defects, VO-complexes, as well as its dose dependence were studied. Under the conditions of the experiment, the influence of other irradiation defects can be neglected, since their concentration is at least by one order of magnitude less than the concentration of VO-complexes ($N_{VO} \gg N_{VP,V_2,C_iC_s}$).

For the temperatures lower than that of the annealing of VO-complexes, a linear (as a function of irradiation time t) accumulation of defects is observed ($N_{\rm VO} \ll N_{\rm O}$)

$$N_{VO} = \lambda_V t, \tag{1}$$

where $\lambda_{\rm V}$ is the efficiency of the generation of free vacancies, i.e. those vacancies which were formed as a result of the dissociation of FPs into independent components. At T>300 °C, the VO-complexes become movable and are trapped by oxygen atoms, forming VO_2 defects [3–5]. Then

$$N_{VO} = \frac{\lambda_V}{\chi_{VO_2} N_{\rm O}}\left[1 - \exp\left(-\chi_{VO_2} N_{\rm O} t\right)\right], \tag{2}$$

where χ_{VO_2} is the constant of the formation of VO_2 defects .

From Eqs. (1), (2), and the experimentally obtained dose dependence of N_{VO}, the value of λ_V can be determined.

Figure 1 shows the experimentally obtained (solid circles) dependence of the efficiency of vacancy

generation λ_V on the specimen temperature at irradiation. It is seen that λ_V rises with temperature in the range 100–300 K and saturates upon the further increase in temperature.

The features of the λ_V change in the range 100–300 K were studied in work [6] in detail. There, the analytical form for the FP distribution function was found, and it was shown that

$$\lambda_V = \lambda_{\rm FP}\left[e^{-(r_c/\rho)} - e^{-(r_{\max}/\rho)}\right] / \left(1 - e^{-(r_{\max}/\rho)}\right), \quad (3)$$

if the condition that the FP components can be found in opposite charge states is fulfilled. Here, $\lambda_{\rm FP}$ is the efficiency of the FP creation, i.e. the concentration of FPs produced by one electron, $r_{\max}$ is the maximally possible distance between V and I, and ρ is the parameter of the distribution function. Curve *1* in Fig. 1 represents the temperature dependence of λ_V calculated according to expression (3). It is evident that there is a lack of coincidence between the calculated and experimental data, especially for T>300 K.

To make the calculated curve describe the experimental data more precisely, it is necessary to assume that either $r_{\max}$ or ρ changes with temperature. As follows from the results of work [2], the value of $r_{\max}$ keeps constant over a wide temperature range from 100 to 1200 K. Thus, we have to conclude that it is ρ that changes with T. The parameter ρ of the FP distribution function is determined by the processes of deceleration of "hot" interstitial atoms created at irradiation. It was shown in [7] that the energy lost by a "hot" atom depends on its interaction with lattice atoms and is proportional to its kinetic energy. The efficiency of such a deceleration doesn't depend on temperature ($\rho = \rho_0$ =const). Thus, we are forced to look for such deceleration process, whose efficiency would increase with temperature. The mechanisms of deceleration of "hot" atoms were well studied for the processes occurring at the ionic doping of crystals (see, e.g., [8]). It was shown that, in such a case, only the process of ion channeling is dependent on temperature. In our case, however, the channeling of interstitial atoms is unlikely.

To move further, we assume that, at high temperatures, an additional deceleration of "hot" atoms is possible owing to their interaction with the phonon oscillations of lattice atoms and, thus, the efficiency of this process is proportional to the number of phonons.

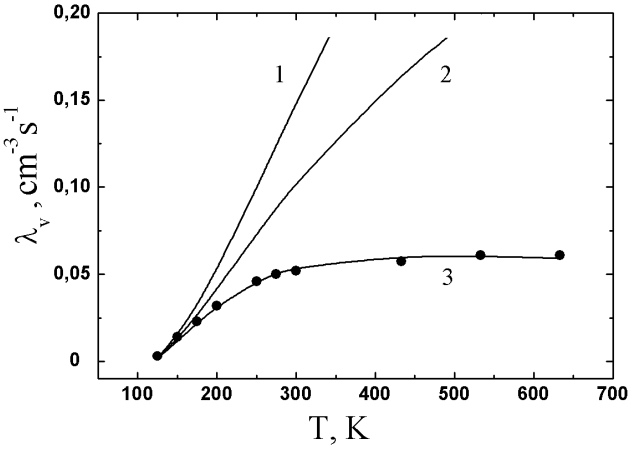

Fig. 1. Dependences of the vacancy generation efficiency λ_V on the specimen temperature at irradiation: solid circles – experimental data, lines – the data calculated according to expression (3) for the cases where the parameter ρ includes different terms: *1* – $1/\rho = 1/\rho_0$; *2* – $1/\rho = A\ n^A + 1/\rho_0$; *3* – $1/\rho = A\ n^A + B\ n^O + 1/\rho_0$

In other words,

$$\frac{1}{\rho} \sim A\langle n^A\rangle + B\langle n^O\rangle + \frac{1}{\rho_0}, \quad (4)$$

where

$$\langle n^A\rangle \sim T^3 \int_0^{T_{\rm D}/T} \frac{x^2 dx}{e^x - 1},$$

$$x = \frac{h\omega^A}{kT}, \quad \langle n^O\rangle \sim \frac{1}{e^{T_{\rm D}/T} - 1}. \quad (5)$$

After substitution of (4) and (5) into (3), we obtain a formula for λ_V. The fitting parameters are the constants A and B reflecting the interaction of "hot" atoms with acoustical and optical phonons, respectively. Curve *2* in Fig. 1 represents the result of the approximation of experimental data in the case where the term caused by the interaction of atoms with acoustical phonons is added to the temperature-independent one $1/\rho_0$. Curve *3* in the same figure shows the result of the approximation which additionally accounts for the interaction with optical phonons. As is seen from the figure, the correct description of the experimental data can only be achieved when all three constituents are taken into account.

Figure 2 shows the relative contributions of these three mechanisms to the efficiency of the deceleration of "hot" atoms. For T<300 K, the main contribution originates from the temperature-independent mechanism. At T>400 K, the deceleration

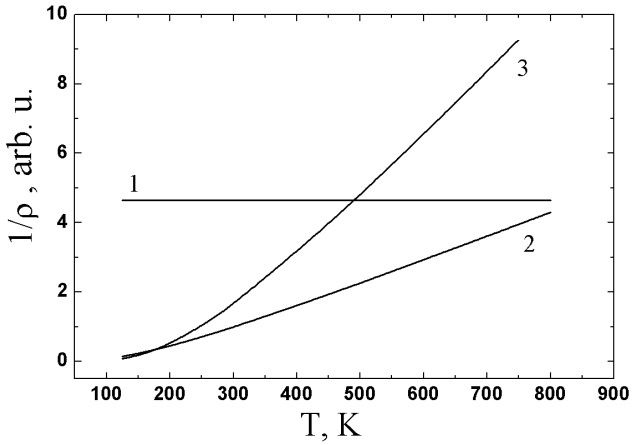

Fig. 2. Relative contributions of various mechanisms to the efficiency of the "hot" atom deceleration: *1* – temperature independent mechanism; *2* – scattering on acoustical phonons; *3* – scattering on optical phonons

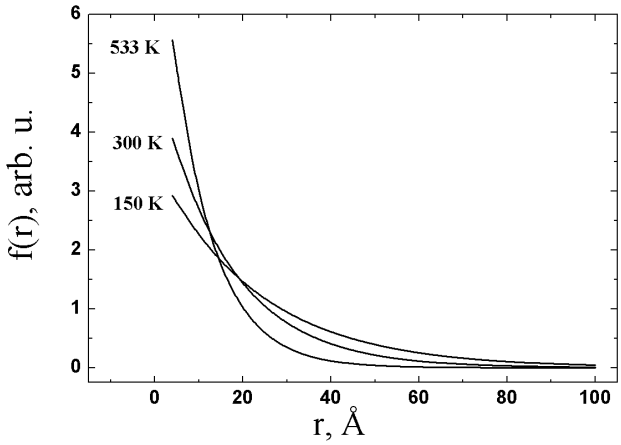

Fig. 3. Temperature change of the function of the FP distribution on the distance between a vacancy and an interstitial atom

occurs mainly due to the interaction of the "hot" atoms with phonons.

Consider how the function of the FP distribution in distances between a vacancy and interstitial atom, $f(r)$, changes with temperature. According to the results obtained in work [1],

$$f(r) = \frac{\exp(-r/\rho)}{\rho[1-\exp(-r_{\max}/\rho)]}. \quad (6)$$

Figure 3 shows $f(r)$ for three temperatures. It is seen that the curve steepness increases with temperature, as was required.

The above results raise the question: what is the mechanism of the "hot" atom deceleration? We have three hints.

1. The velocity of "hot" atoms is near 10^6 cm/s. The distance that the atoms pass before the thermalization occurs is a few tens of angstroms. This means that the time elapsed before the atom thermalization is of order 10^{-12} s. During this time, the atom should radiate up to 10^3 phonons, which seems to be unlikely.

2. The constants of the interaction of "hot" atoms with phonons, A and B, have the dimensionality of area and the order of magnitude (after the substitution of all known constants) 10^{-16} cm^2, which corresponds to the cross-section of the scattering of phonons on defects.

3. The efficiency of the deceleration of "hot" atoms is proportional to the number of equilibrium phonons.

Accounting for the above statements, it is pertinent to assume that there is an elastic interaction of "hot" atoms with the phonon oscillations of lattice atoms. As this occurs, the atoms don't loss the energy, but only change the direction of their motion in a crystal. As a result of multiple interactions with phonons, the atom changes the direction of motion in such a way that it approaches a vacancy. This manifests itself in the decrease in ρ, whose value is responsible for the steepness of the function of the FP distribution in distances between a vacancy and an interstitial atom (see Eq. (6)). In other words, one should say not about the process of deceleration of the "hot" atoms by phonons, but about the scattering process. The loss of energy by the "hot" atoms should occur due to the temperature-independent deceleration mechanism which becomes apparent in the pure form at $T<200$ K.

The physics of the processes occurring when the "hot" atoms pass through a crystal lattice requires the additional studies.

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Received 02.03.07.
Translated from Ukrainian by A.I. Tovstolytkin

ТЕМПЕРАТУРНА ЗАЛЕЖНІСТЬ ЕФЕКТИВНОСТІ ГЕНЕРАЦІЇ ВАКАНСІЙ В n-Si ПРИ ОПРОМІНЕННІ ЕЛЕКТРОНАМИ З ЕНЕРГІЄЮ 1 МеВ

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Р е з ю м е

Експериментально отримано температурну залежність ефективності генерації вільних вакансій (частини пар Френкеля (ПФ), які розпались на незалежні компоненти – вакансії та міжвузловинні атоми) в n-Si при його опроміненні електронами з енергією 1 МеВ у діапазоні температур 100 – 633 К. Встановлено, що ця залежність є зростаючою функцією в діапазоні 100–300 К з тенденцією до насичення при T>300 К. Показано, що зміна ефективності генерації вільних вакансій визначається функцією розподілу ПФ за відстанями між компонентами, крутизна якої зростає зі збільшенням температури зразків при опроміненні. Показано також, що зміна крутизни функції розподілу ПФ спричинена додатковим розсіянням "гарячих" міжвузловинних атомів, які утворюються в процесі опромінення, фононними коливаннями ґратки.