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Abstract

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PHYSICS

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A POSSIBLE MECHANISM FOR THE FORMATION OF COMPLEX RADIATION DEFECTS IN SILICON INTRODUCED BY ELECTRON IRRADIATION

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As a result of bombardment of silicon single crystals by electrons with energy exceeding a certain threshold, structural disturbances arise. It is known (1) that primary defects (a vacancy, an interstitial atom) are unstable at room temperature, and the observed centers (for example, by their influence on the recombination characteristics of the material) are secondary formations—associations of primary defects either with impurity atoms or with one another. In the present work an attempt will be made to consider some possible mechanisms of formation of secondary defects in silicon and the dependence of the efficiency of introducing associations on the electron energy.

The concentration of isolated defects introduced by electron irradiation is calculated in the usual way (2). The differential cross section for the interaction of a relativistic electron (kinetic energy $E = (m - m_0)c^2$) with an atom (mass M , charge number Z), when energy in the range from T to $T + dT$ is transferred to the atom, is equal to (3,4)

$$d\sigma = AB \left[1 - \beta(\beta + \alpha) \frac{T}{T_m} + \alpha\beta \sqrt{\frac{T}{T_m}} \right] \frac{T_m}{T^2} dT. \quad (1)$$

In this expression

$$A = \pi Z^2 \left(\frac{e^2}{m_0 c^2} \right)^2; \quad B = \frac{1 - \beta^2}{\beta^4}; \quad \alpha = \frac{\pi Z}{137};$$

e and m_0 are the charge and rest mass of the electron;

$$\beta^2 = \frac{v^2}{c^2} = \frac{\mathcal{E}(\mathcal{E} + 2)}{(\mathcal{E} + 1)^2}, \quad \text{where } \mathcal{E} = \frac{E}{m_0 c^2};$$

c is the speed of light,

$$T_m = \frac{2m_0}{M} m_0 c^2 \mathcal{E}(\mathcal{E} + 2)$$

is the maximum energy that an electron can transfer to an atom ($\hat{4}$). According to the model of Kinchin and Pease ($\hat{5}$), an atom having energy T can produce $g(T)$ displacements:

$$g(T) = \begin{cases} 0, & 0 \leq T \leq E_d, \\ 1, & E_d \leq T \leq 2E_d, \\ T/2E_d, & 2E_d \leq T \leq T_m, \end{cases} \quad (2)$$

where E_d is the threshold energy for displacement of an atom from a lattice site to an interstitial position. The form of $g(T)$ adopted by us is, for all values of T , close in magnitude to $g(T)$ proposed by other authors ($\hat{4}, \hat{7}$), and permits the integration to be carried out to the end. The concentration of isolated displacements in a thin specimen ($\hat{2}$)

$$n_d = n_0 \sigma_d \overline{g(T)} \Phi, \quad (3)$$

where n_0 is the number of atoms per unit volume of the solid; σ_d is the integral displacement cross section, Φ is the integral flux of fast electrons, and

$$\sigma_d \overline{g(T)} = \int_{E_d}^{T_m} g(T) \left(\frac{d\sigma_d}{dT} \right) dT.$$

It may be assumed that, independently of the detailed mechanism of formation of associations of isolated displacements with impurity atoms, their concentration is proportional to n_d .

Let us consider possible pathways for the formation of another class of complex defects, which consist of two primary defects; we shall call them bound pairs. It may be assumed that, for small n_d , formation of a complex defect from two single defects introduced as a result of the collision of two different electrons with lattice atoms is unlikely, since the mean distance between them is sufficiently large. In this case one should take into account the interaction $g(T)$ of vacancies and $g'(T)$ of interstitial atoms formed as a result of a single collision of an electron with an atom. A bound pair may be formed from two homogeneous (divacancy, two interstitial atoms) or two heterogeneous (a complex consisting of a vacancy and an interstitial atom) structural disturbances; this process may proceed in different ways. For homogeneous disturbances, one of the possible paths is the association of each of the g disturbances with any of the $(g - 1)$ neighbors, which gives $g(g - 1)/2$ ways of forming a bound pair; another path is

the association of each only with its nearest neighbor, which gives, as is easily shown, $(g-1)$ ways of forming a pair ^(6,7). An intermediate path is undoubtedly also possible, but we shall consider only these limiting cases. For bound pairs consisting of heterogeneous disturbances, these two possibilities also exist, and as a result one obtains g^2 and $(2g-1)$ ways of forming a pair, respectively. Thus the concentration n_c of the enumerated types of complex defects is expressed as

$$n_c \sim n_0 \sigma_d \overline{f(g)} \Phi, \quad (4)$$

where

$$f(g) = \begin{cases} g(T) & \text{(a),} \\ g(g-1)/2 & \text{(b),} \\ (g-1) & \text{(c),} \\ g^2 & \text{(d),} \\ (2g-1) & \text{(e);} \end{cases} \quad (5)$$

$$\sigma_d \overline{f(g)} = \int_{E_d}^{T_m} f[g(T)] \left(\frac{d\sigma}{dT} \right) dT. \quad (6)$$

Let us introduce the following notation:

$$y = T_m/2E_d,$$

$$P_1 = B[y - \beta(\beta + \alpha) \ln 2 + 2\alpha\beta\sqrt{y}(\sqrt{2} - 1)],$$

$$P_2 = B[(y-1) - \beta(\beta + \alpha) \ln y + 2\alpha\beta(\sqrt{y} - 1)], \quad (7)$$

$$P_3 = By[\ln y - \beta(\beta + \alpha)(1 - 1/y) + 2\alpha\beta(1 - 1/\sqrt{y})],$$

$$P_4 = By^2[(1 - 1/y) - \frac{1}{2}\beta(\beta + \alpha)(1 - 1/y^2) + \frac{2}{3}\alpha\beta(1 - 1/y^{3/2})].$$

In this notation, after integrating (6) we obtain

$$\sigma_d = A(P_1 + P_2), \quad \sigma_d \bar{g} = A(P_1 + P_3), \quad \sigma_d \frac{\overline{g(g-1)}}{2} = \frac{A}{2}(P_4 - P_3),$$

$$\sigma_d \overline{(g-1)} = A(P_3 - P_2), \quad \sigma_d \overline{g^2} = A(P_1 + P_4), \quad (8)$$

$$\sigma_d \overline{(2g-1)} = A(P_1 + 2P_3 - P_2).$$

Table 1 gives the values of $P_1 \div P_4$ for silicon ($Z = 14$, $A = 28$) at various energies of fast electrons—from 0.5 to 40 MeV; the value of E_d was taken equal to 12.9 eV ⁽⁸⁾.

The values we have calculated for the quantity $\sigma_d \overline{f(g)}$ reflect the energy dependence of the concentration of defects of a given kind introduced by irradiation of the specimen with a unit integral electron flux (Fig. 1). It is obvious that the energy dependence of the functions (8) reflects the energy-

[Figure 1]

Fig. 1. Energy dependence of $\lg[\sigma_d f(g)/A]$ for various mechanisms of bound-pair formation. The numbering of the curves corresponds to the numbering of $f(g)$ in expression (5).

...energy dependence of the concentration not only of bound pairs, but also of associations of these pairs with an impurity atom (such as, for example, the K -center—a complex consisting of a vacancy, an interstitial atom, and an impurity atom ⁽⁹⁾). Indeed, the probability of formation of an association of a bound pair with an impurity atom is proportional to the product n_c and to the impurity concentration, which is independent of irradiation.

We have compared the calculations presented above with experimental data available in the literature on the efficiency of radiation damage to the lifetime in silicon. Under irradiation of silicon, defects of various types apparently form; nevertheless, it may be assumed that in many cases one type of center is decisive (for example, the A -center in n -silicon with a high oxygen content). Comparison of the energy dependences of the damage coefficients of n - and p -silicon with the curves in Fig. 1 reveals close agreement with the energy dependences of $\sigma_d g$ and $\sigma_d(g-1)$, respectively (see, for example, ⁽¹⁰⁾).

Table 1

E (MeV)	$B = \left[\frac{g+1}{g(g+2)} \right]^{0.776} g \times$	$y = (g+2)$	P_1	P_2	P_3	P_4
0.5	0.462	2.26	0.878	0.327	0.451	0.654
0.75	0.236	3.94	0.860	0.468	0.761	1.421
1.0	0.146	6.04	0.851	0.549	1.040	2.355
1.5	0.0737	11.28	0.830	0.652	1.431	4.61
2.0	0.0450	18.0	0.810	0.686	1.760	7.53
3.0	0.0221	35.84	0.806	0.736	2.260	15.19
5.0	0.00875	89.4	0.7967	0.7696	2.960	38.51
7.0	0.00468	166.2	0.7900	0.7800	3.435	71.0
10.0	0.00236	328.3	0.78705	0.78338	3.950	140.8

E (MeV)	$B = \left[\frac{g+1}{g(g+2)} \right]^{0.776g \times y}$	$y = (g+2)$	P_1	P_2	P_3	P_4
15.0	0.001083	716	0.78354	0.78423	4.57	307
20.0	0.000619	1252	0.78177	0.78375	5.00	537
30.0	0.000281	2770	0.78030	0.78220	5.62	1187
40.0	0.000159	4880	0.77894	0.78122	6.06	2095

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