RADIATION-INDUCED REARRANGEMENT OF DEFECTS IN SILICON CRYSTALS

B.V. PAVLYK, R.M. LYS, A.S. HRYPA, D.P. SLOBODZYAN, I.O. KHVYSHCHUN, I.A. SHYKORYAK, R.I. DIDYK

Ivan Franko Lviv National University
(107, Tarnavskyi Str., Lviv 79019, Ukraine; e-mail: `lys_r@ukr.net`*)*

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Physical and mathematical models of the radiation-induced ordering of a defect structure in silicon crystals are proposed. These models involve an increase of the diffusion coefficient of interstitial silicon in the irradiation field and a reduction of the defect lifetime at irradiation doses below 260 Gy. Free surfaces of crystals, phase interfaces, and dislocations are considered to be effective defect sinks.

1. Introduction

The main factors leading to the degradation of elements of semiconductor electronics are the processes of generation, evolution, and migration of structural defects of a crystal lattice, both the growth ones and those formed under the action of external factors (surface treatment of crystals, temperature, ionizing fields, *etc.*).

One of the methods used to improve the most defective near-surface region of crystals is low-dose ionizing irradiation. Such an action of ionizing fields is accompanied by several factors — formation of radiation-induced defects, their interaction with biographical ones, annihilation and accumulation of defects. Depending on which process plays the dominant role, the electrophysical characteristics of materials and devices produced on their basis can either improve or worsen.

In the scientific literature, the processes of radiation-induced defect formation in semiconductor crystals are described rather exhaustively [1–3]. The physics of processes related to the improvement of characteristics of crystals and devices under the action of low-radiation doses ("low-dose effect") is studied incompletely, though this effect is already used in the practical technology of production of devices of semiconductor electronics. That is why researches in this field represent an urgent task.

The "low-dose effect" manifests itself especially clearly when studying radiation-induced processes in surface-barrier structures (SBS). The reasons for a deviation of parameters of MOS-transistors and diodes (mobilities of charge carriers and threshold voltages) from theoretically calculated values in the presence of structural defects were studied in many works [4, 5].

The physical nature of such processes is analyzed with regard for several factors:

- the action of irradiation is accompanied by the generation of Frenkel defects in crystals; interacting with recombination-active impurities, they change their charge state and carrier capture cross-section;
- a recombination impurity passes from a site of the crystal lattice to an interstice due to the interaction with an interstitial atom of the matrix;
- an interstitial recombination center (I) interacts with a radiation-induced vacancy (V), which is accompanied by their annihilation;
- semiconductor and oxide are separated by a strongly defective layer several hundred angstroms in thickness that contains a large part of fast centers, among which there are Frenkel pairs, their associates with oxygen and a doping agent, and divacancies.

The radiation-induced decrease of the concentration of a recombination-active impurity in silicon crystals is explained by the effects of internal gettering of the impurity and doping atoms by surfaces of oxygen precipitates and dislocations formed under a technological treatment of crystals [6].

In [3–5], it was shown that, on the initial stage of irradiation, the efficiency of radiation-induced changes in the parameters of semiconductor structures tends to the saturation, which also correlates well with data of works [3, 6, 7].

The analysis of scientific publications and the experimental results obtained in our studies of peculiarities of the radiation-induced evolution of a defect structure in silicon crystals serve as a basis for the construction of physical and mathematical models of the radiation-induced improvement of characteristics of surface-barrier structures based on p-Si crystals.

2. Experimental Results and Their Discussion

Figure 1 shows the dose dependences of a variation of the capacity-voltage characteristics (CVC) of Bi–Si–Al structures under the action of X-rays (Cu, 50 kV, 10 mA).

As one can see from the given dependences, the increase of the absorbed irradiation dose to 260 Gy results in a reduction of the amplitude of the characteristic CVC maximum caused by the charge accumulation in the dielectric near-surface layer of the semiconductor under the formation of a SBS. The structural defects generated due to the irradiation represent recombination centers. On the initial stage of irradiation ($D < 260$ Gy), the dominant role in the SBS is played by recombination processes, whereas the further rise of the irradiation dose results in the prevalence of the processes of generation and accumulation of new radiation-induced defects. In this case, one already observes the worsening of the electrophysical characteristics of the studied SBSs rather than their improvement.

It is also found out [6, 8] that the irradiation affects the lifetime of electrically active defects and minor charge carriers. On the initial stages of the irradiation of Si crystals, the lifetime of minor carriers τ grows by a factor of 2–4 and then starts to decrease. The annealing favors the growth of τ at least to 250° C.

Such a dependence of the lifetime is explained by the action of two processes:

1. decrease of the number of recombination-active centers of the chemical nature (Au, Cu, and others), which results in the growth of τ.

2. decrease of τ due to the continuous rise of the number of radiation-induced recombination centers with increase in the dose, as well as the localization of electrically-active impurities at vacancies.

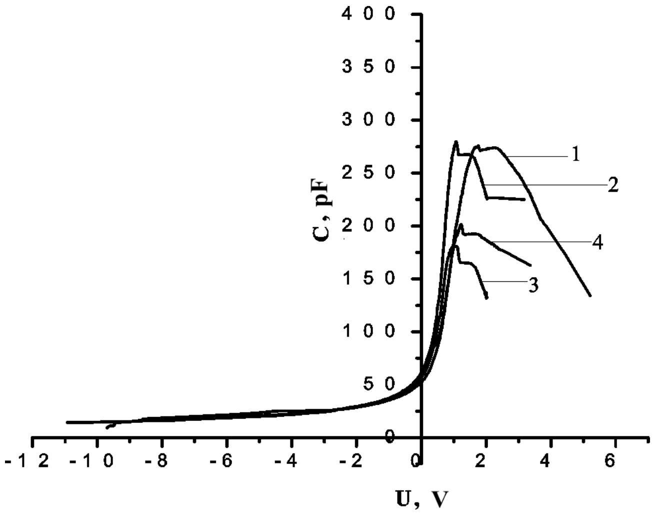

Fig. 1. Capacity-voltage characteristics of Bi–Si–Al structures: non-irradiated (*1*) and irradiated with doses of 130 Gy (*2*), 260 Gy (*3*), and 390 Gy (*4*) at T=100 K and a modulation frequency of 5 kHz

It is possible that process 1 slows down at certain doses, while process 2 saturates much later.

The above processes were described using the modified equation for the diffusion of interstitial silicon under irradiation:

$$\frac{\partial N(x,t)}{\partial t} = D^* \frac{\partial^2 N(x,t)}{\partial x^2} - \frac{N(x,t)}{\tau(t)} + G. \tag{1}$$

Here, $N(x,t)$ is the concentration distribution of interstitial silicon (Si_i), D^* is the diffusion coefficient of Si_i in the irradiation field, G is the rate of generation of Si_i, and $\tau(t)$ is its lifetime.

In Eq.(1), the radiation-induced variation of the diffusion coefficient is taken into account by introducing the quantity D^*. Due to the irradiation, the latter appears two orders of magnitude larger as compared with the diffusion coefficient at the same temperature [1].

In order to solve this equation, it is necessary to choose the initial and boundary conditions. With regard for the fact that effective sinks for Si_i can be dislocations, free surfaces, and dielectric–semiconductor or metal–semiconductor interfaces, the boundary conditions can be presented in the form

$$N(x,0) = N_0 = f(x),$$

$$N(0,t) = N_0 \exp(\alpha t) = g(t),$$

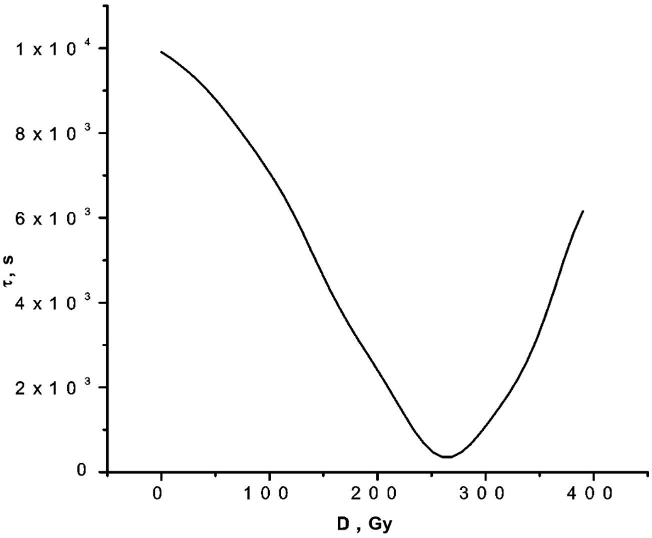

Fig. 2. Lifetime of silicon in the interstitial state as a function of the irradiation dose

$$N(l,t) = N_0 \exp(\beta t) = q(t),$$

where $N(0,t)$ and $N(l,t)$ are the concentrations of Si_i defects at the sample surface, l is the sample thickness, N_0 is the mean concentration of interstitial silicon, and $\alpha = \beta = 2.7 \times 10^{-4}$ are constants. The initial distribution can be chosen as the Gaussian one.

Based on the analysis of the literature data from [1, 9, 10], we chose the following initial parameters for the modeling of defect diffusion in silicon crystals: the diffusion coefficients $D = 10^{-16}$ m^2/s under normal conditions and $D^* = 10^{-14}$ m^2/s under irradiation; defect generation rate in the semiconductor under irradiation $G = 10^{13}$ m^{-3}/s; mean lifetime of defects in the crystal without irradiation $\tau = 10^4$ s; mean concentration of interstitial silicon $N_0 = 10^{17}$ m^{-3}; and sample thickness $l = 5\times 10^{-4}$ m. The experiment lasted for 90 min, which corresponds to a dose of 360 Gy.

The analysis of our previous studies and literature data [1, 3, 6, 8–10] allowed us to construct a function $\tau(D)$ in the form of the curve presented in Fig. 2. One can see two regions in this curve:

1. region, where the defect lifetime decreases on the initial stage of irradiation starting from the value τ_0 (corresponding to the lifetime before the irradiation) to its minimum value characterized by the equal efficiencies of the processes of defect gettering and recombination, on the one hand, and their generation, on the other hand.

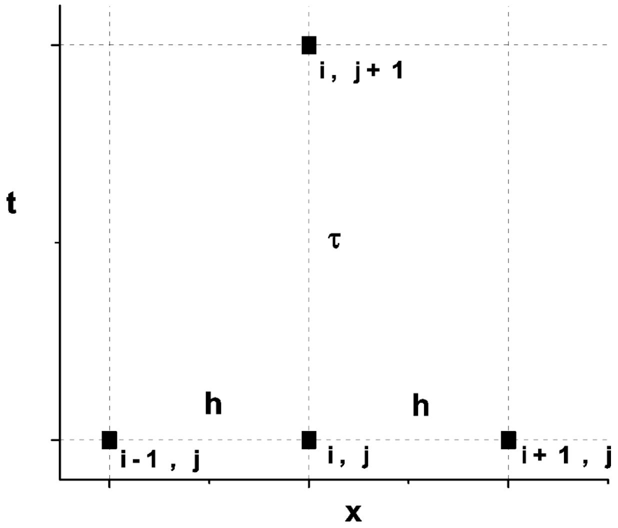

Fig. 3. Rectangular network of the explicit difference scheme

2. region characterized by the considerable prevalence of the process of defect generation in the irradiation field.

In order to avoid difficulties when solving the diffusion equation, we tabulated the function $\tau(D)$ and considered the value of τ instantaneous.

The problem was solved numerically using the explicit difference scheme. For this purpose, we constructed a uniform rectangular (Fig. 3) network with the help of the coordinate lines:

$$x_i = ih, \quad i = (\overline{0, I}),$$

$$t_j = j\tau, \quad j = (\overline{0, J}),$$

where h and τ are the network steps in the x and t axes, respectively.

The values of $N(x,t)$ in the network nodes will be denoted by N_i^j, i.e. $N_i^j = N(x_i, \tau_j)$. We approximate N_i^j by the value of n_i^j and use the explicit scheme.

Applying finite differences, the following difference scheme is obtained:

$$\begin{cases} \dfrac{n_i^{j+1} - n_i^j}{\tau} = A\dfrac{n_{i+1}^j - 2n_i^j + n_{i-1}^j}{h^2} + Bn_i^j + C, \\ \quad i = (\overline{1, I-1}), i = (\overline{0, J}), \\ n_0^j = g(t_j), \\ n_I^j = q(t_j), \\ n_i^0 = f(x_i). \end{cases} \qquad (2)$$

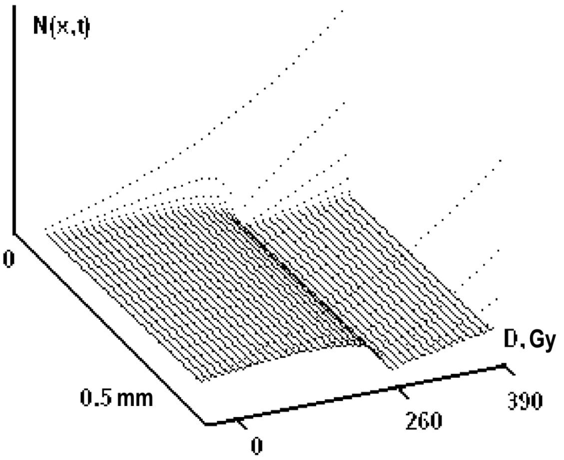

Fig. 4. Mean defect concentration in the bulk of silicon in various cross sections of the crystal as a function of the absorbed irradiation dose

The values of the constants substituted into Eq.(2) are as follows:

$A = D; \quad B = -1/\tau_0; \quad C = G.$

Taking into account that $h = l/I$, we obtain $x_i = ih = il/I$ and $\tau_j = j\tau$ (l is the sample thickness).

Applying the explicit network method, we search for n_i^j ($i = \overline{0, I}$; $j = \overline{0, J}$) and put their values into the array $n[i, j]$. After that, we plot the pointwise specified surface obtained in this way (Fig. 4).

The formulation of our equation and its solution with the help of the network method were performed in the mathematical environment Maple [11].

In the physical model of radiation-induced diffusion of silicon defects, we assume that the following processes run on the initial stages of the irradiation:
- generation of radiation-induced structural defects;
- abrupt increase of the diffusion coefficient of interstitial silicon (by 2–4 orders of magnitude), which can lead to the decrease of the concentration of intrinsic structural defects by 1-2 orders of magnitude [1];
- gettering of defects (interstitial silicon) at dislocations, free surfaces, and interfaces;
- recombination processes, whose efficiency is related to the mobility of components.

The results of calculations are demonstrated in Figs. 4–6. In these dependences, one can clearly distinguish several characteristic regions:
- On the initial stage of irradiation ($D < 200$ Gy), the concentration of structural defects changes relatively little (±20%) (Fig. 5, 6), which testifies to the close efficiencies of the processes of defect generation and annihilation;

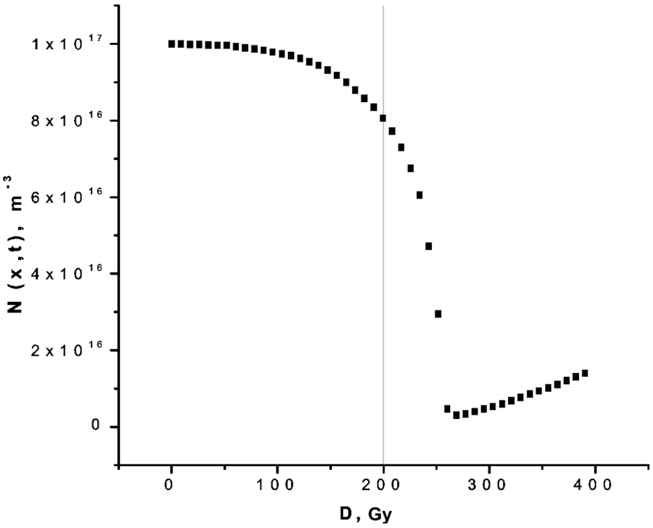

Fig. 5. Mean defect concentration in the bulk of silicon ($x = 0.25$ mm) as a function of the irradiation dose

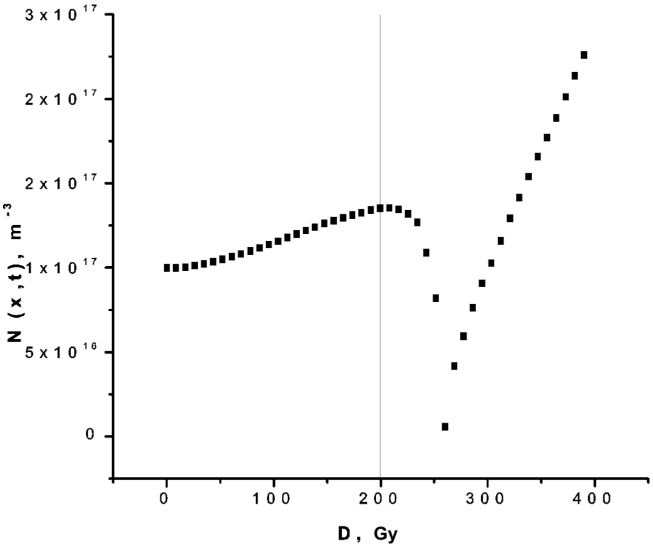

Fig. 6. Mean defect concentration in the near-surface region of silicon ($x = 10^{-5}$ m) as a function of the irradiation dose

- The region of the abrupt decrease of the concentration in the bulk and in the near-surface layer at $D = 260$ Gy is caused by the dominance of the processes of radiation-induced gettering and recombination of defects over the processes of their generation, which corresponds to the maximum of the radiation-induced ordering effect;
- In the region with $D > 260$ Gy, the process of generation of defects prevails over their radiation-induced ordering. Moreover, the effectiveness of the processes of generation and accumulation of radiation-induced de-

fects in the near-surface layer is much larger than that in the bulk of the sample.

3. Conclusions

The analysis of experimental and calculation data gives grounds to state that, on the initial stage of the irradiation, the effect of radiation-induced ordering in p-Si crystals is more pronounced in the more defect near-surface region (as compared to the bulk of the sample).

The proposed physical model of the process of radiation-induced rearrangement of the defect structure correlates well with experimental results.

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РАДІАЦІЙНО-СТИМУЛЬОВАНА ПЕРЕБУДОВА ДЕФЕКТІВ У КРИСТАЛАХ КРЕМНІЮ

Б.В. Павлик, Р.М. Лис, А.С. Грипа, Д.П. Слободзян, І.О. Хвищун, Й.А. Шикоряк, Р.І. Дідик

Резюме

Запропоновано фізичну та математичну моделі процесу радіаційно-стимульованого впорядкування дефектної структури кристалів кремнію. У даній моделі враховано збільшення коефіцієнта дифузії міжвузловинного кремнію в полі дії радіації, зменшення часу життя дефектів при дозах опромінення до 260 Гр. Ефективними стоками дефектів вважали вільні поверхні кристалів, межі поділу фаз, дислокації.