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DEFECT CONCENTRATION IN CLUSTERS, CREATED BY FAST-PILE NEUTRONS IN n-Si (FZ, Cz)

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The dependence of concentration of defects on doping level for average cluster in n-Si was calculated. It was shown that in the framework of the Gossick's model the concentration of defects for the average cluster is in inverse proportion to the square of a cluster radius. One obtains the size distribution of defect clusters created by fast neutrons of WWR-M reactor, by the transformation of energy spectrum of the primary knock-on atom in n-Si (FZ, Cz). Threshold energy of defect clusters formation 4.7 keV by comparing n-Si crystals irradiated by deuterons and fast-pile neutrons was calculated.

The principal possibility to describe the properties of defects clusters is determined by the condition that in cluster the total number of defects is significantly more than one. Such requirement provides the possibility of statistical description of the aggregate of point defects, which form a cluster. The objectives of the work are:

(i) to calculate the size distribution of clusters and on this basis to define the defect concentration in average defect cluster, which is formed in silicon by the fast-pile neutron irradiation;

(ii) to describe on the basis of cluster model the dependence of the effective concentration of carriers in high-resistance n-type silicon on fluence of irradiation by fast-pile neutrons and 24 GeV protons.

It is known that the fast-pile neutrons (n^o) create regions in n-Si with the high concentration of defects, named as clusters. From a condition of an charge neutrality of cluster one follows

$$N_1\left(r_1^3-r_0^3\right)=N_2\left(r_2^3-r_1^3\right), \qquad (1)$$

where N_1 is the concentration of defects in cluster; N_2 is the doping impurity concentration; r_1, r_0, r_2 are the radiuses of defect cluster, neutral region and extension of a space-charge region of cluster, accordingly.

In the special case of Gossick's model [1], when $V=\dfrac{4\pi\varepsilon\varepsilon_o r_1\Psi_p}{eN_2}$ is in approximation of $r_0\sim r_1$; $(r_1-r_0)\sim L_{D1}=\dfrac{1}{e}\cdot\sqrt{\dfrac{kT\varepsilon\varepsilon_o}{N_1}}$ and under condition (1) the concentration of defects in clusters should be not less

$$N_1=\frac{\varepsilon\varepsilon_0\psi_p^2}{kT\,r_1^2}, \qquad (2)$$

where ε, ε_o are the relative dielectric constants of a material and vacuum, accordingly; Ψ_p is the height of a potential barrier of cluster; e is the electron charge; k is Boltzmann's constant; T is the absolute temperature.

In the high-resistance n-Si with resistivity $\rho\geq 40$ Ω·cm the clusters can be considered as condensers of the spherical form. The charge of such condenser is directly proportional to radius of the defect cluster, and the number of the charged defects is directly proportional to energy, spent by primary knock-on atom (PKA) of silicon on elastic collisions (E_{sp}). Then

$$r_1=\beta\cdot E_2\cdot\left(1-f_E\right), \qquad (3)$$

where E_2 is the energy of the silicon PKA; f_E is the part of energy relating to ionization losses; β is the factor of proportionality.

The spectrum of the silicon PKA created by fast-pile neutrons is presented in [2] and the method of calculation of average cluster radius is proposed in [3]. The carried out calculations have shown, that the silicon PKA created by fast-pile neutrons on the average spend on elastic collisions 26 keV in cascades and create clusters with the average size $r_1=90$ Å and $r_1=70$ Å in n-Si grown by a floating-zone method (FZ) and Czochralskii method (Cz), accordingly.

The coefficient of proportionality, according to (3), is $\beta=3.5$ Å·keV^{-1} for n-Si (FZ) and $\beta=2.7$ Å·keV^{-1} in the case of n-Si (Cz). Such difference may be due to the recombination of vacancies and interstitial silicon atoms on oxygen atoms, which are the well-known recombination centers. Under interactions of nuclear particles with silicon atoms it is not essential how the energy is transmitted to lattice atoms, therefore the found meaning β is correct and in the case of irradiation of silicon by deuterons.

The cross-section of the formation of defect clusters created by fast-pile neutrons (Σ = 0.15 cm^{-1}) weakly depend on threshold energy of their formation ($\breve{E}_2$) and in the case of irradiation by deuterons it is in inverse proportion to the energy transmitted to a silicon atom. Trying to obtain the constancy of the factor β under irradiation by fast-pile neutrons and deuterons with average energy $\breve{E}_D = 10.5$ MeV the average radius of defect clusters were calculated for the different values of the threshold energy $\breve{E}_2$ of defect cluster creation. The obtained value $\breve{E}_2 = 4.7$ keV well agrees with the theoretical and experimental estimations of Vinetskii [4] and Ivanov [5]. It is shown that under the irradiation of n-Si (FZ) by deuterons the $E_{sp} = 9$ keV ($\bar{r}_1 = 32$ Å) and for irradiation by fast neutrons with energy 14.5 MeV the $E_{sp} = 43$ keV ($\bar{r}_1 = 150$ Å) [6].

Only the neutrons with energy $E_n \geq 36$ keV are able to transmit the energy to the silicon atom more than 4.7 keV and to form defect cluster with size more than 28 Å in the lattice of n-Si (FZ). Then the average radius of clusters created by neutrons with energy $E_n \geq 36$ keV in n-Si (FZ) can be calculated by equation

$$\bar{r}_1 = 54.3 \cdot \log \frac{E_n\,(\text{keV})}{20}\,[\overset{\circ}{\text{A}}]. \qquad (4)$$

The high-resistance n-Si samples with resistivity near 2.5 · 10^3 Ω·cm, grown by FZ method and OFZ/G with oxygen enrichment, were investigated before and after irradiation by 24 GeV protons up to fluence ~10^{14} p·cm^{-2}. Under such high energy the proton and neutron shifts are roughly separated by Coulomb contribution in single interaction act in silicon. This difference is very small in comparison with nuclear interaction of particles with such high energies. Thus, 24 GeV protons are identical to neutrons with the same energy. Then, according to (4), it is possible that 24 GeV protons form the defects clusters with average radius $\bar{r}_1 = 330$ Å in silicon.

The dependence of carrier concentration on fluence is determined first of all by the introduction rate of defect clusters and then by introduction rate of defects into the conducting matrix. For the theoretical description of the dose dependence of the effective carrier concentration the temperature dependence of the defect recharges both in conducting matrix of n-Si and in the space-charge regions of defect clusters is required to know. According to [7] the effective concentration of carriers (N_{ef}) depending upon irradiation dose (Φ) and temperature (T) is equal to

$$N_{ef}(T,\Phi) = N(T,\Phi)\cdot(1 - f(T,\Phi)), \qquad (5)$$

with $f(T,\Phi) = 1 - \exp(-\Sigma V \Phi)$, where $N(T,\Phi)$ is a carrier concentration in the conducting matrix of n-Si; $f(T,\Phi)$ is a volume fraction occupied by clusters; $V = \frac{4}{3}\pi r_2^3$ is a volume of defect cluster of radius r_2.

Proceeding from Gossick`s model for the volume and according to (5) we obtain

$$N_{ef}(T,\Phi) = N(T,\Phi)\times$$

$$\times\exp\left[-\frac{4\pi\varepsilon\varepsilon_o \Sigma r_1 \Phi}{N_2(T,\Phi)\cdot e^2}\cdot\left(F - kT\ln\frac{N_c(T)}{N_2(T,\Phi)}\right)\right], \qquad (6)$$

where $N_2(T,\Phi)$ is a concentration of screening centers in the space-charge regions of defect clusters; F is the Fermi level position in the center of the cluster relative to the bottom of the conduction band; $N_c(T)$ is an effective state density in the conduction band.

We know that the Fermi level is connected to thermodynamic character of a system. Therefore we can define F and $kT\ln\frac{N_c(T)}{N_2(T,\Phi)}$ as an increment of a free energy of a system (cluster and conducting matrix) at adding to it one electron under condition of a constancy of volume and temperature. Then $\frac{e^2 N_2(T,\Phi)}{4\pi\varepsilon\varepsilon_o r_1 \Sigma\Phi}$ we can define as a diminution of a free energy of all system at formation of $\Sigma\Phi$ clusters in unit of silicon specimen volume. The divacancy, as is known, is a multi-charge center. In intrinsic silicon the Fermi level will place at a neutral level of the divacancy (E_V + 0.52 eV) on our evaluations. At capture of free electron (supplied by ionization of dopants) the energy of a center will increase on 0.165 eV. Therefore with increase dopant concentration the Fermi level in a cluster (F) will be displaced to the conduction band (E_c). At a high injection of holes through p-n transition, the cluster core has been depicted as p-type because of the acceptor-like behaviour of the TSC (Thermally Stimulated Current) peak [8]. In our opinion, a divacancies after capture of holes pass in a neutral charge state and, therefore, the Fermi level in clusters becomes equal E_V + 0.52 eV.

In work [7] theoretically and experimentally is shown as taking into account the recharges of defects in the region of the space-charge of defect cluster and conducting matrix. Thus, we deviate from a pure Gossick's model, namely: by showing that the position of a Fermi level in the cluster (F) relative to the conduction band depends on dopant concentration in silicon; the screening center concentration (the donors) in the space-charge region is defined by the recharges of acceptor defects.

Samples of n-Si with resistivity $\sim 2.5 \cdot 10^3$ Ω cm grown by the method of the floating-zone in vacuum (FZ), in argon atmosphere (Ar) and received by the method of neutron-transmutation doping (NTD) are investigated before and after irradiation by various doses of fast-pile neutrons. Measured at room temperature the dose dependence of the effective concentration of the charge carriers is presented in Fig. 1. After the radiation dose equal to $2 \cdot 10^{13}$ n°· cm^{-2} the Fermi level position in clusters and in the conducting matrix is leveled relative to the bottom of the conduction band reaching the value (E_c - 0.528 eV) in n-Si (FZ), (E_c - 0.523 eV) in n-Si (Ar) and (E_c - 0.511 eV) in n-Si (NTD). The average radius (r_1) of defect cluster equal to $r_1 = 92$ Å (n-Si, FZ) and $r_1 = 76$ Å (n-Si, Ar, NTD).

The similar account of dose dependence of effective carrier concentration in n-Si, irradiated by 24 GeV protons, which create of defect clusters of average radius $\overline{r}_1 = 330$ Å has shown, that macroscopic cross-section of defect cluster introduction is $\Sigma = 5 \cdot 10^{-3}$ cm^{-1} (Fig. 2).

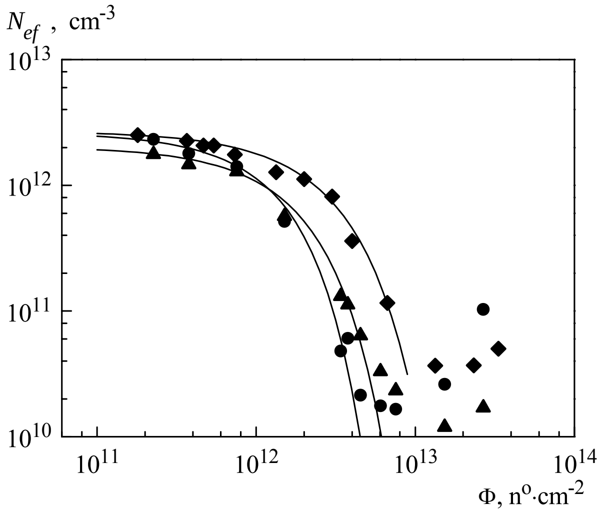

Fig. 1. The dependence of effective concentration of electrons at room temperature on the fluence of fast-pile neutrons in: ● – n-Si (FZ), ▲ – n-Si (Ar), ♦ – n-Si (NTD). The average concentration of carriers ($\overline{n}_o$) in n-Si for: (FZ) – 2.65·10^{12}; (Ar) – 2.04·10^{12}; (NTD) - 2.69·10^{12} cm^{-3}.

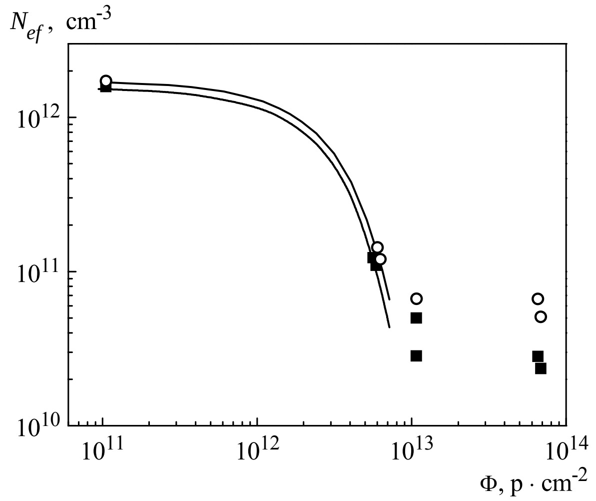

Fig. 2. The dependence of effective concentration of electron in the samples of n-Si (FZ) (■) and n-Si (OFZ/G) (○) on fluence (Φ) of protons with energy 24 GeV.

Under the interaction with silicon atoms the neutrons with energy 1 MeV spend on elastic and inelastic collisions 29.2 keV for the scattering cross-section 3.22 b. Then the hardness factor (D) for 1 MeV neutrons is equal to 94 MeV·mb. In review [9] the hardness factor of 1 MeV neutrons is assumed equal to 95 MeV·mb. It is usually supposed that each scattered 1 MeV neutron forms single defect cluster. In silicon monocrystals the neutrons with energy 14.5 MeV form the defect clusters with macroscopic cross-section $\Sigma = 0.15$ cm^{-1} and, consequently, their hardness factor is equal to 130 MeV · mb. Therefore, at each scattering act of 14.5 MeV neutrons on the silicon atoms it is formed 1.5 defect clusters, at average. Based on the data of review [9] it is possible to determine that the hardness factor of 14.5 MeV neutrons is near 150 MeV · mb.

Let us suppose that $\beta = 3.5$ Å·keV^{-1} keeps its value also under the irradiation of n-Si (FZ) by 24 GeV protons. Then to form the cluster with radius 330 Å it is necessary to spend the energy E_{sp} = 94.3 keV for the displacement collisions. In n-Si (FZ) the hardness factor of 24 GeV protons will be equal 9.43 MeV·mb, i.e. 0.1 with respect to 1 MeV neutrons. In [9] for 24 GeV protons values 0.5 and 0.9 with respect to 1 MeV neutrons are given.

On the assumption that the macroscopic cross-section ($\Sigma = 0.15$ cm^{-1}) of cluster formation by fast-pile neutrons should remain constant, the spectrum of PKA was transformed into the size distribution of defect clusters in n-Si (Fig. 3), according to (3).

The concentration of defects in clusters was determined by different methods [10, 11]. The scattering cross-section of carriers per one acceptor in cluster was calculated. Although the task was solved in the Born's approximation, its formal application gives correct results. Mobility caused by the scattering on the defect clusters is equal [11]

$$\mu_k = \frac{9\varepsilon^2}{2(2\pi m)^{1/2}}\cdot\left(\frac{2}{\pi e}\right)^3\cdot\frac{(kT)^{3/2}}{N\cdot(N_1+N_2)\cdot r_1^6\cdot B(\alpha)},$$

$$B(\alpha)\cong 8\cdot(\ln\alpha/4+5/6)\,,\alpha = r_2/r_1, \qquad (7)$$

where $N=\Sigma\Phi$ is the concentration of defect clusters; Φ is the fluence of neutrons.

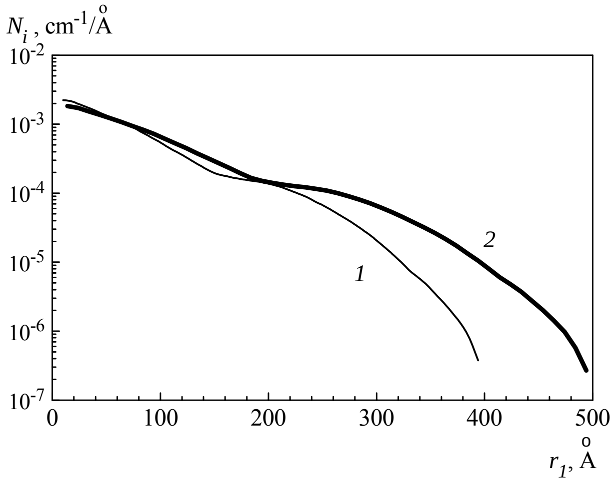

Fig. 3. The size distribution of defect clusters in n-Si (Cz) (*1*) and n-Si (Fz) (*2*).

The calculations show that only under low temperatures the free path of carriers becomes more than the extension of cluster space-charge and the concentration of defects in clusters can be determined in accordance with (7). Thus it is necessary to take into account the size distribution of clusters (see Fig. 3) with using of criterion (2). It was shown that

$$\sum_i N^{(i)}\cdot\left(N_1^{(i)}+N_2\right)\cdot r_1^{(i)6} = N\cdot\left(N_1+N_2\right)\cdot\overline{r_1^6}\,, \qquad (8)$$

where $N^{(i)}$ is the concentration of clusters with size $r_1^{(i)}$; $\overline{r_1}$ is the average radius of defect clusters in which the concentration of charged centers is equal N_1.

The mobility (μ_{dI}) caused by the scattering on clusters (μ_k) and charged centers (μ_p) can be founded as

$$\mu_{dI}^{-1} = \mu_p^{-1}+\mu_k^{-1}. \qquad (9)$$

The calculation of mobility resulting from the scattering on charged centers was carried out according to Brooks - Herring's formula. The mixed scattering due to the contributions of lattice scattering and scattering on defects and their clusters can be expressed only via drift mobility [12]

$$\mu_d = \mu_{dL}\left[1+x^2\left\{C_{ix}\cos x+S_{ix}\sin x-\frac{\pi}{2}\sin x\right\}\right],$$

$$x^2 = 6\,\mu_{dL}/\mu_{dI}\,, \qquad (10)$$

where μ_{dL} is the drift mobility resulting from lattice scattering.

Under small irradiation doses the changing of Hall factor can be neglected. So, in accordance with expressions (7) - (10) the changing of electron mobility was calculated at temperature of liquid nitrogen after small irradiation doses of n-Si by fast-pile neutrons and thus the concentration of defects in average cluster was determined. The concentration of defects in average cluster depending on doping level and growth method of n-Si is shown in Fig. 4.

The decrease of defect concentration in clusters at the increasing of doping level of n-Si is connected, apparently, with growth of number of negatively charged vacancies in cascades, and it gives rise to the reinforcement of the recombination of primary Frenkel pairs.

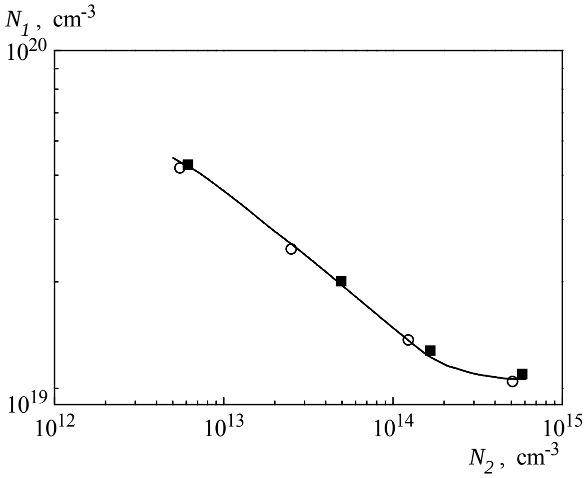

Fig. 4. The dependence of defect concentration in the average cluster on doping level of n-Si (Cz) (○) and n-Si (FZ) (■) samples.

It was obtained the distribution of defect clusters, created by the fast-pile neutrons, on sizes at the description of defect accumulation in the form of condensers of spherical shape. It was proved the possibility of statistical description of defect clusters due to the condition that total number of defects in clusters is significantly more than one. For n-type silicon the dose dependence of effective carrier concentration on the irradiation fluence of fast-pile neutrons and 24 GeV protons were described.

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КОНЦЕНТРАЦІЯ ДЕФЕКТІВ У КЛАСТЕРАХ, УТВОРЕНИХ ШВИДКИМИ НЕЙТРОНАМИ РЕАКТОРА В n-Si (FZ, Cz)

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Розраховано залежність концентрації дефектів від рівня легування для середньостатистичного кластера в n-Si. Показано, що в рамках моделі Госсіка концентрація дефектів для такого кластера обернено пропорційна квадрату його радіуса. Отримано розподіл за розмірами кластерів дефектів, утворених швидкими нейтронами реактора ВВР-М, шляхом перетворення енергетичного спектра первинно-вибитих атомів в n-Si (FZ, Cz). Розраховано граничну енергію утворення кластерів, яка становить 4,7 кеВ, порівнюючи кристали n-Si, опромінені дейтронами та швидкими нейтронами реактора.

КОНЦЕНТРАЦИЯ ДЕФЕКТОВ В КЛАСТЕРАХ, СОЗДАННЫХ БЫСТРЫМИ НЕЙТРОНАМИ РЕАКТОРА В n-Si (FZ, Cz)

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Рассчитана зависимость концентрации дефектов от уровня легирования для среднестатистического кластера в n-Si. Показано, что в рамках модели Госсика концентрация дефектов для такого кластера обратно пропорциональна квадрату его радиуса. Получено распределение по размерам кластеров дефектов, созданных быстрыми нейтронами реактора ВВР-М, путем преобразования энергетического спектра первично-выбитых атомов в n-Si (FZ, Cz). Вычислена пороговая энергия образования кластеров, которая составляет 4,7 кэВ, сравнивая кристаллы n-Si, облученные дейтронами и быстрыми нейтронами реактора.

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