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# SPECIFIC FEATURES OF DEFECT FORMATION IN THE n-SI <P> SINGLE CRYSTALS AT ELECTRON IRRADIATION

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***На основі вимірювань інфрачервоної Фур'є-спектроскопії, ефекту Холла та тензо-холл-ефекту була встановлена природа та визначена концентрація основних типів радіаційних дефектів в монокристалах n-Si <P>, опромінених різними потоками електронів з енергією 12 МеВ. Показано, що для досліджуваних монокристалів кремнію при електронному опромінені є досить ефективним утворення нового типу радіаційних дефектів, що належать комплексам VOiP (А-центр, модифікований домішкою фосфору). З розв'язків рівняння електронейтральності отримано залежності енергії активації для глибокого рівня E1=EC–0,107 еВ, що належить комплексу VOiP, від одновісного тиску вздовж кристалографічних напрямків [100] та [111]. За допомогою методу найменших квадратів одержані апроксимаційні поліноми для розрахунку даних залежностей. При орієнтації осі деформації вздовж кристалографічного напрямку [100] глибокий рівень E1=EC–0,107 еВ буде розщеплюватись на дві компоненти з різною енергією активації. Це пояснює нелінійні залежності енергії активації глибокого рівня E1=EC–0,107 еВ від одновісного тиску P≤0,4 ГПа. Для тисків P>0,4 ГПа розщеплення даного глибокого рівня буде значним і можна вважати, що глибокий рівень комплексу VOiP взаємодіятиме тільки з двома мінімумами зони провідності кремнію, а зміна енергії активації буде лінійною за деформацією. Для випадку одновісного тиску P≤0,4 ГПа вздовж кристалографічного напрямку [111] зміна енергії активації для комплексу VOiP описується квадратичною залежністю. Відповідно зміщення глибокого рівня E1=EC–0,107 еВ для даного випадку теж є квадратичною функцією за деформацією. Різні залежності енергії активації комплексу VOiP від орієнтації осі деформації відносно різних кристалографічних напрямків можуть свідчити про анізотропні характеристики даного дефекту. Встановленні особливості дефектоутворення в опромінених електронами монокристалах n-Si <P> можуть бути використані при розробці на основі даних монокристалів різних приладів функціональної електроніки***

***Ключові слова: монокристали кремнію, інфрачервона Фур'є-спектроскопія, ефект Холла, одновісний тиск, радіаційні дефекти, глибокі енергетичні рівні***

## 1. Introduction

Penetrating radiation is currently widely employed in various fields of science and technology and in many cases can act as an effective technological tool [1]. Specifically, the purposeful application of radiation in semiconductor materials science and electronics makes it possible to obtain high quality semiconductor materials, significantly improve the production, and reduce its cost, of many types of semiconductor instruments [2–5]. The most convenient and the most affordable semiconductor to form planar structures, which are the base of modern integrated electronics, is silicon, due to its unique properties, almost unlimited natural stocks, commercial availability, and cultivation technology [6–9]. Silicon is the base for constructing and improving super-large and ultra-fast integrated circuits, new elements for micro- and nanoelectronics of our time [6, 9–12]. silicon is the model semiconductor because electronic paramagnetic resonance (EPR) provided for the possibility to determine the atomic configuration and electron structure of radiation defects [13]. The use of radiation exposure in order to modify the properties of silicon and to obtain, based on it, the fundamentally new elements for functional electronics necessitates thorough studies into processes of defect formation. Establishing the patterns in such processes would make it possible to subsequently elucidate the progress of different



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kinetic and optical effects in silicon with radiation defects. Thus, it is a relevant task to investigate this direction, as the results to be obtained could be useful both for scientists and engineers who work in the field of semiconductor materials science. Undertaking such a research is important both in terms of scientific and applied significance when developing the fundamentals for the new radiation technologies of semiconductors and while studying the impact of irradiation on various devices in silicon electronics.

## 2. Literature review and problem statement

It is known [14] that in the n-Si crystals in the process of irradiation at room temperature, mostly the A- and E-centers form, as well as divacancies ($V_2$), the complexes of $C_iO_i$, $C_iC_S$, multi-vacancy complexes with oxygen ($V_x$+$O_y$) ($x$, $y$=1, 2, 3). For the silicon single crystals, grown by the Czochralski method, with a small content of alloying additives, the main radiation defects are the A-centers, divacancies, and the $C_iO_i$ complexes [15]. The formation of the E-centers, divacancies, the $C_iC_S$ complexes is characteristic of the irradiated silicon, grown by the method of crucibleless zone melting [16]. The authors of work [17] demonstrated that the additional introduction, at the expense of chemical-mechanical polishing, of a copper additive to the silicon single crystals, irradiated by electrons with energy of 5 MeV, leads to the formation of a new complex CuVO. These complexes form at the expense of quasi-chemical reactions between the A-centers and intranodal atoms of copper. Paper [18] considered the mechanisms of configuration rearrangement of a trivacancy in silicon. It is shown that the probability of each possible configuration for a trivacancy depends on the energy of electron irradiation. Study [19] shows that during isothermal annealing, at temperature $t$=150 °C, of the silicon single crystals, irradiated by large fluxes of electrons, it is rather effective to capture the intranodal atoms of Si by the $C_iO_i$ defects with the formation of the $C_iO_i(Si_I)$ defects. Based on calculations using a density functional theory, it was shown that this defect has two configurations that differ in energy by 0.19 eV. Increasing the time of stable operation of silicon detectors, which are used to control the position and the flux of particles in experiments related to the high-energy physics necessitates studying the nature, properties, and stability of the defects formed during operation of such detectors [20]. In this case, it is quite important to investigate the processes of annealing radiation defects, as well as their impact on the electrical properties of the irradiated silicon detectors [21]. It is also known that in the silicon, irradiated by fast electrons with energy $E$>10 MeV, along with point defects, the clusters of defects start to form [22]. The presence of such clusters can significantly affect the mobility of current carriers in silicon single crystals [23].

However, the above studies leave almost unexplored the issue on the impact of concentration of a doping additive on the mechanisms that form the specified types of defects. This is primarily due to the complexity of constructing adequate theoretical models of defect formation involving alloying additives. Resolving this task requires many independent experimental and theoretical studies, which in many cases yield conflicting results. Thus, it remains interesting, both from theoretical and practical points of view, to investigate defect formation in silicon with the medium and strong levels of doping at energies of electron irradiation greater than 10 MeV. In this case, the concentration of a doping additive will significantly affect the efficiency of introduction at irradiation of both point and complex defects (clusters), as well as the probability to form new radiation defects [24].

## 3. The aim and objectives of the study

The aim of this study is to identify the impact of irradiation by different fluxes of fast electrons with energy 12 MeV on the mechanisms of defect formation in the n-Si single crystals, alloyed with an additive of phosphorus, concentration $N_d$=2.2·10$^{16}$ cm$^{-3}$.

To accomplish the aim, the following tasks have been set:

– to explore the nature of basic types of radiation defects in silicon, which formed at electron irradiation;

– to determine, based on the solutions to electroneutrality equations and study into the Hall effect, the concentration of formed defects, and their activation energy;

– to construct dependences of activation energy of the formed defects on the magnitude and orientation of uniaxial pressure relative to different crystallographic directions.

## 4. Experimental methods for identification of the nature of radiation defects in the n-Si <P> single crystals, irradiated by electrons with energy 12 MeV

### 4. 1. Studying the infra-red Fourier-spectroscopy and the Hall effect

Silicon single crystals were irradiated at room temperature at the microtron M-30, whose parameters make it possible to form the beams of accelerated electrons with energies in the range of 1–25 MeV with a monoenergy of 0.02 % and a current of up to 50 μA. Temperature control was executed using a copper-constantan differential thermocouple. During the irradiation, temperature of the silicon samples was regulated by blowing with vapors of liquid nitrogen. Fig. 1 shows absorption spectra for the n-Si single crystals, irradiated by a flux of electrons of 1·10$^{17}$ el/cm$^2$. The spectra were investigated in the temperature range from 10 K to 300 K.

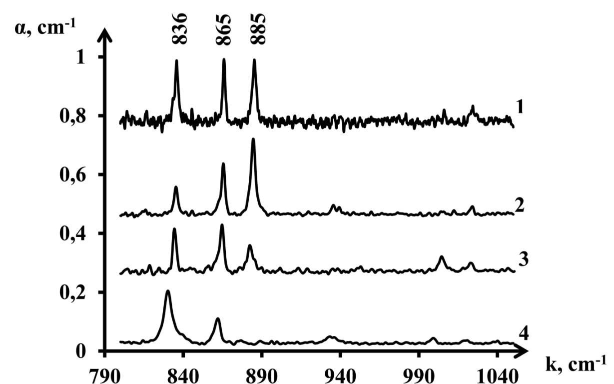


Fig. 1. Absorption spectra for the n-Si single crystals, irradiated by a flux of electrons of 1·10$^{17}$ el/cm$^2$, examined at different temperatures $T$, K: 1–10, 2–80, 3–150, 4–300

Absorption lines with frequencies of 836 and 885 cm$^{-1}$ correspond to the A-center ($VO_i$ complex) [14]. The properties of this defect have been studied in detail [25]. The

defect introduces to the forbidden zone of silicon the deep acceptor level $E_C - 0{,}17$ and observed in the spectra of infrared absorption in both the neutral (absorption line 836 cm$^{-1}$) and the negatively charged (absorption line 885 cm$^{-1}$) states [26]. The A-center is annealed in the temperature range of 300–400 °C. Absorption line with a frequency of 865 cm$^{-1}$ corresponds to the $C_iO_i$ complex [27]. At radiation irradiation, carbon, in accordance with the exchange mechanism by Watkins, is pushed by its own internodes from nodes to the intranodal position thereby forming a stable defect ($C_i$) [28]. At diffusion in the lattice, intranodal carbon ($C_i$) effectively interacts with additives, thereby forming electrically active defects. In the silicon, grown by the Czochralski method, $C_i$ effectively interacts with intranodal oxygen ($O_i$), resulting in the formation of a $C_iO_i$ complex [29]. A given complex is stable to temperature $T$=600 K and forms in the forbidden zone of silicon a deep level of $E_V + 0{,}35$ eV [30]. The activation energy of radiation defects in silicon, irradiated by the flux of electrons $\Phi$=1·10$^{17}$ el/cm$^2$, determined based on the temperature dependences for the concentrations of electrons (Fig. 2, curve 3), proved to be equal to $E_A = E_c - (0{,}107 \pm 0{,}005)$ eV, which corresponds to the A-center, which was additionally modified by a phosphorus additive ($VO_iP$ complex) [13].

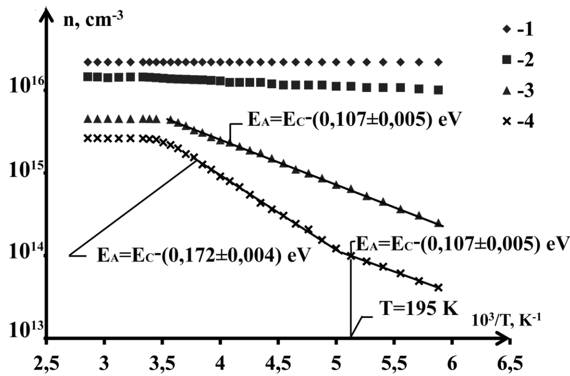


Fig. 2. Temperature dependences of electron concentration for the n-Si single crystals irradiated by different fluxes of electrons $\Phi$, el/cm$^2$: 1 — 0, 2 — 5·10$^{16}$, 3 — 1·10$^{17}$, 4 — 2·10$^{17}$

The silicon, irradiated by a flux of electrons $\Phi$= =2·10$^{17}$ el/cm$^2$, is characterized by a change in the inclination of temperature dependence of concentration at temperature $T$≈195 K (refer to Fig. 2, curve 4). At temperatures $T$<195, activation energy of the radiation defects formed in silicon, similar to the case when irradiated by flux $\Phi$=1·10$^{17}$ el/cm$^2$, corresponds to the $VO_iP$ complex, while at temperatures $T$>195 K – to the $VO_i$ complex. At temperatures $T$>290 K, the radiation defects belonging to A-centers will be fully ionized, since the electron concentration reaches saturation (Fig. 2, curves 2–4), and in the spectrum of absorption one observes the disappearance of line 885 cm$^{-1}$ (Fig. 1, curve 4), which corresponds to the negatively charged state of the A-center. The deep level $E_V + 0{,}35$ eB in this case will be completely filled with electrons, and, over the entire investigated range of temperatures, its ionization will not occur. In addition, an increase in the flow of electronic radiation will lead to an increase in the concentration of radiation defects that correspond to the $C_iO_i$ complexes. This explains the decrease in the concentration of electrons in the conduction zone of the irradiated silicon single crystals relative to unirradiated samples with an increase in the flow of electron irradiation at temperatures exceeding a room temperature.

**4. 2. Calculation of concentration of radiation defects belonging to the $VO_i$, $VO_iP$, $C_iO_i$ complexes**

Based on the statistics about nondegenerate electron gas in semiconductors, we calculated the concentrations of the formed radiation defects corresponding to these complexes. Assume that in silicon with a concentration of donor additive $N_d$, $L_i$ types of different radiation defects form, with concentrations $N_i$. Then, at a temperature of absolute zero, all levels of defects will be filled, as well as part of donor levels. At temperatures lower than the room temperature, small donors of phosphorus will be completely ionized, while the energy levels that correspond to the $VO_i$ and $VO_i$ complexes – only partially. Only for the deep level $E_V + 0{,}35$ eB, which belongs to the $C_iO_i$ complex, its ionization will not occur over the entire investigated range of temperatures. Thus, for the examined case, it is possible to write the following equation of electroneutrality:

$$n_1 + n_2 + n = N_d - N_1, \qquad (1)$$

where $n_1$, $n_2$ are the concentrations of electrons at the energy levels that correspond to the $VO_iP$, $VO_i$ complexes, respectively; $n$ is the concentration of electrons in the conduction band; $N_1$ is the concentration of the $VO_iP$ complexes.

With respect to expressions for the corresponding concentrations [31]

$$n_1 = \frac{N_1}{2e^{\frac{E_1 - E_F}{kT}} + 1}, \quad n_2 = \frac{N_2}{2e^{\frac{E_2 - E_F}{kT}} + 1}, \quad n = N_c e^{\frac{E_F}{kT}}, \qquad (2)$$

equation (1) can be recorded in the following form:

$$\frac{N_1}{1 + \frac{2N_c}{n} e^{\frac{E_1}{kT}}} + \frac{N_2}{1 + \frac{2N_c}{n} e^{\frac{E_2}{kT}}} + n = N_d - N_1, \qquad (3)$$

where

$$N_c = \frac{(2m_n kT)^{3/2}}{4\pi^3 \hbar^3}$$

is the effective density of states of the conduction zone; $E_1 = E_C - 0{,}107$ eV and $E_2 = E_C - 0{,}172$ eV are the activation energies of the $VO_iP$ and $VO_i$ complexes, respectively; $N_2$ is the concentration of the $VO_i$ complexes; $E_F$ is the Fermi energy.

Because the isoenergetic surfaces in silicon are the ellipsoids of rotation, the effective mass of the states' density [31] is then

$$m_n = Z^{\frac{2}{3}} \left(m_\parallel m_\perp^2\right)^{\frac{1}{3}}, \qquad (4)$$

where $Z$ is the number of equivalent ellipsoid (minima), $m_\parallel$ and $m_\perp$ are the components of tensor of the effective mass of an electron along and across the long axis of the ellipsoid. For silicon in the non-deformed state, $Z = 6$, $m_\parallel = 0{,}9163 m_0$, $m_\perp = 0{,}1905 m_0$, $m_0$ is the mass of a free electron [32]. Then, in accordance with (4), $m_n = 1{,}062 m_0$,

In order to calculate the concentration of radiation defects belonging to the $VO_i$ and $VO_iP$ complexes, we record equation (3) for two different values for the concentration of electrons at temperatures $T_1$ and $T_2$, respectively. We obtain the following system of equations of electroneutrality:

$$\begin{cases} \dfrac{N_1}{1+\dfrac{2N_c(T_1)}{n(T_1)}e^{\frac{E_1}{kT_1}}}+\dfrac{N_2}{1+\dfrac{2N_c(T_1)}{n(T_1)}e^{\frac{E_2}{kT_1}}}+n(T_1)=N_d-N_1, \\ \dfrac{N_1}{1+\dfrac{2N_c(T_2)}{n(T_2)}e^{\frac{E_1}{kT_1}}}+\dfrac{N_2}{1+\dfrac{2N_c(T_2)}{n(T_2)}e^{\frac{E_2}{kT_1}}}+n(T_2)=N_d-N_1. \end{cases} \quad (5)$$

Considering the importance of effective mass of the states' density for electrons in the conduction band, the concentration of a phosphorus doping additive, as well as experimental values for the concentrations of electrons $n(T_1)$ and $n(T_2)$ for the assigned flux of electron irradiation (Fig. 2, curves 2–4), can be derived from the concentration of radiation defects that correspond to the $VO_i$ and $VO_iP$ complexes. As noted above, at temperatures $T$>290 K, energy levels $E_1=E_C-0{,}107$ eV and $E_2=E_C-0{,}172$ eV will be completely ionized. For this case, the equation of electroneutrality will then take the form:

$$N_3+n=N_d-N_1, \quad (6)$$

where $N_3$ is the concentration of radiation defects belonging to the $C_iO_i$ complexes. The result of the performed calculations is the obtained values for the concentration of formed radiation defects $N_1$, $N_2$ and $N_3$ for the n-Si single crystals, irradiated by different fluxes of electrons (Table 1).

Table 1

Concentration of radiation defects in the n-Si <P> single crystals, irradiated by different fluxes of electrons with an energy of 12 MeV

| Flux of electron radiation Φ, el/cm$^2$ | Concentration of radiation defects $N_i$, cm$^{-3}$ | | |
|---|---|---|---|
| | $N_1$ | $N_2$ | $N_3$ |
| $5\cdot10^{16}$ | $3.7\cdot10^{15}$ | $4.4\cdot10^{13}$ | $3.8\cdot10^{15}$ |
| $1\cdot10^{17}$ | $1\cdot10^{16}$ | $2.5\cdot10^{14}$ | $7.4\cdot10^{15}$ |
| $2\cdot10^{17}$ | $1.04\cdot10^{16}$ | $1.8\cdot10^{15}$ | $9\cdot10^{15}$ |

Table 1 shows that increasing the flux of electronic radiation increases the concentration of radiation defects of all three types. The largest concentration corresponds to the $VO_iP$ complexes; it is practically not changed when increasing the flow from $1\cdot10^{17}$ to $2\cdot10^{17}$ el/cm$^2$ because there is a limit for the concentration of a phosphorus doping additive, which is included in the composition of these complexes. The concentration of the $VO_i$ complexes, when increasing the flux of electrons, is monotonically increasing, which is explained by the active generation of vacancies that enter the quasi-chemical reactions with the intramodal atoms of oxygen, thereby forming the $VO_i$ complexes.

**4. 3. Studying the tensor hall-effect for the uniaxially deformed n-Si <P> single crystals with radiation defects**

The highly informative method of tensor effects under a uniaxial elastic deformation renders a high degree of reliability to studying the patterns in a zonal structure of multivalley semiconductors, making it possible to properly define its parameters and the magnitudes that characterize the mechanisms of current carriers scattering. Specifically, investigating the behavior of deep centers under deformations yields important information about the nature of relationship between the local electron states of these centers and the closest regions, indicating the type of symmetry of a defect, the deformation degree of inner bonds in the lattice. The behavior of deep levels under deformation does not lend itself to such a simple analysis as does the behavior of shallow levels. Shallow levels almost do not move under deformation relative to the edges of zones, while the deep ones move at a great speed, and each of these levels is characterized by its own displacement rate [32]. Thus, we also measured the tensor hall-effect at $T$=200 K for the n-Si single crystals irradiated by flux $\Phi=1\cdot10^{17}$ el/cm$^2$ of electrons with an energy of 12 MeV (Fig. 3).

It follows from Fig. 3 that when silicon is deformed along the different crystallographic directions one observes a growth in the concentration of electrons. Only at uniaxial pressure along the crystallographic direction [111] does the concentration of electrons increases to the pressure of P≈0.4 GPa, followed by the saturation. We derive from the solutions to equation (3)

$$E_1=kT\ln\left(\frac{n}{2N_c}\left(\frac{N_1}{N_d-N_1-n-\dfrac{N_2}{1+2\dfrac{N_c}{n}e^{\frac{E_2}{kT}}}}-1\right)\right). \quad (7)$$

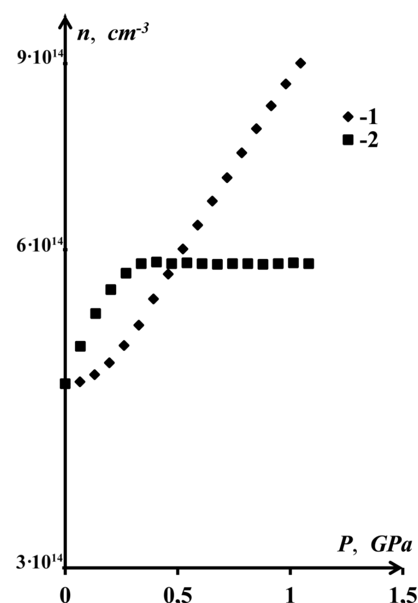


Fig. 3. Dependences of electron concentration on the uniaxial pressure for the n-Si <P> single crystals, irradiated by the flux of electrons $\Phi=1\cdot10^{17}$ el/cm$^2$ at $T$=200 K, under condition that the axis of deformation is aligned along different crystallographic directions: 1 – [100]; 2 – [111]

It should be noted that expression (7) holds only for the case of a uniaxial pressure along the crystallographic direction [111] when six minima in the silicon conduction band

are displaced synchronously [33]. In this case, there is no any deformation redistribution between the minima along the upward energy scale. At uniaxial pressure along the crystallographic direction [100], the silicon's two minima in the conduction band will descend along the energy scale by magnitude [33]

$$\Delta E_1 = -\left(\Xi_d + \frac{1}{3}\Xi_u\right)(S_{11} + 2S_{12})P - \frac{2}{3}\Xi_u(S_{11} - S_{12})P, \qquad (8)$$

and the other four minima would ascend by magnitude

$$\Delta E_2 = -\left(\Xi_d + \frac{1}{3}\Xi_u\right)(S_{11} + 2S_{12})P + \frac{1}{3}\Xi_u(S_{11} - S_{12})P. \qquad (9)$$

As a result, the activation energy of the deep level under the applied uniaxial pressure may vary in different ways data relative to these minima. Therefore, in this case, on can argue only about the effective value for the activation energy of the deep level in the A-center; calculations must account for a shift in the respective minima under deformation.

If one assumes that $n_1$ is the concentration of electrons in the minima that descend, and $n_2$ – in those minima that ascend at uniaxial pressure, the total concentration of electrons in the silicon conduction band is then

$$n = n_1 + n_2. \qquad (10)$$

For nondegenerate electron gas [32]

$$n_1 = 2\left(\frac{2\pi m_1 kT}{\hbar^2}\right)^{3/2} e^{\frac{E_F - \Delta E_1}{kT}},$$

$$n_2 = 2\left(\frac{2\pi m_2 kT}{\hbar^2}\right)^{3/2} e^{\frac{E_F - \Delta E_2}{kT}}, \qquad (11)$$

where $m_1$, $m_2$ are the effective masses of states' density in these minima, whose values are easily derived from expression (4).

Then, with respect to expressions (2), (10) and (11), we find from electroneutrality equation (3) that

$$E_1 = kT\ln\left(\frac{n}{2\left(N_{c_1}e^{\frac{-\Delta E_1}{kT}} + N_{c_2}e^{\frac{-\Delta E_2}{kT}}\right)}\cdot\left(\frac{N_1}{N_d - N_1 - n - \dfrac{N_2}{1 + 2\dfrac{N_c}{n}e^{\frac{E_2}{kT}}}} - 1\right)\right), \qquad (12)$$

where

$$N_{c_1} = 2\left(\frac{2\pi m_1 kT}{\hbar^2}\right)^{3/2},$$

$$N_{c_2} = 2\left(\frac{2\pi m_2 kT}{\hbar^2}\right)^{3/2}.$$

Based on expressions (7) and (12), it becomes possible to derive the dependences of activation energy on uniaxial pressure along the crystallographic directions [111] and [100] for the $VO_iP$ complex.

## 5. Results of studying the influence of uniaxial pressure on activation energy of the $VO_iP$ complex

In order to calculate activation energy of the $VO_iP$ complex in the uniaxially deformed silicon single crystals, it is necessary to take into consideration the values for constants of deformational potential $\Xi_u = 9{,}23$ eV and $\Xi_d = -2{,}12$ eV [34], rigidity constants $S_{12} = -0{,}21\cdot10^{-11}$ $Pa^{-1}$, $S_{11} = 0{,}77\cdot10^{-11}$ $Pa^{-1}$ [33], the concentration of a phosphorus doping additive $N_d$=2.2·$10^{16}$ $cm^{-3}$, values for the concentrations of radiation defects $N_1$ and $N_2$ (refer to Table 1), experimental data from measuring the tensor hall-effect (Fig. 3), as well as effective value for the activation energy of A-center (the $VO_i$ complex) in the uniaxially deformed silicon single crystals. This parameter was derived earlier in papers [35, 36]. The magnitude of change in the energy slit between the deep level of A-center and the bottom of the n-Si conduction band (pressure coefficient for the effective value of activation energy of A-center) at uniaxial pressure along the crystallographic direction [100] calculated per every $10^8$ Pa, proved to be equal to (2.45±0.10)·$10^{-3}$ eV [35], and at uniaxial pressure along the crystallographic direction [111] – to (0.68±0.03)·$10^{-3}$ eV [36]. Fig. 4 shows the results of such calculations. The analytical dependences of activation energy for the $VO_iP$ complex on uniaxial pressure were constructed using the method of least squares.

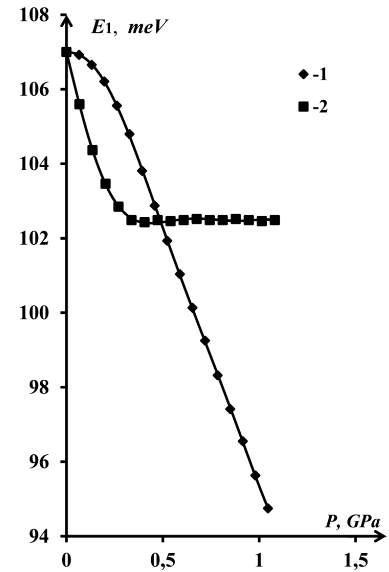


Fig. 4. Dependence of activation energy of the level $E_1$=$E_C$–0.107 eV, belonging to the $VO_iP$ complex, on uniaxial pressure provided the axis of deformation is aligned along different crystallographic directions: 1 – [100]; 2 – [111]. Solid curves are the theoretical calculations based on the approximation polynomials, given in Table 2

The approximation polynomials for the calculation of activation energy of the $VO_iP$ complex in the uniaxially deformed n-Si single crystals are given in Table 2. Calculation of coefficients for these polynomials was performed using the system of computer algebra MathCad 14.

It follows from Table 2 that the dependence of activation energy of the $VO_iP$ complex on uniaxial pressure $P \le 0{,}4$ GPa

for both orientations of the uniaxial pressure is the quadratic function for deformation.

Table 2

Approximation polynomials for the calculation of activation energy of the $VO_iP$ complex in the uniaxially deformed n-Si <P> single crystals

| Orientation of uniaxial pressure relative to different crystallographic directions | Dependence of activation energy $E_1$ (meV) on uniaxial pressure $P$ (GPa) |
|---|---|
| Uniaxial pressure along crystallographic direction [100] | $E_1(P)=\begin{cases}-20{,}73P^2-0{,}02P+107, P\le 0{,}4,\\ -13{,}56P+109, P>0{,}4.\end{cases}$ |
| Uniaxial pressure along crystallographic direction [111] | $E_1(P)=\begin{cases}30{,}37P^2-23{,}65P+107, P\le 0{,}4,\\ 102{,}48, P>0{,}4.\end{cases}$ |

## 6. Discussion of results of studying the defect formation in the n-Si <P> single crystals under electron irradiation

As noted above, the silicon, irradiated by fast electrons with an energy of E>10 MeV, along with point defects, could potentially form the clusters of defects whose nuclei consist of divacancies or multi-vacancy complexes [23]. However, in the case under consideration, the energy levels of such defects (for example, divacancies that form the core of a disarrangement area) were not observed over the investigated range of temperatures in the absorption spectra and at Hall measurements. This relates to that the concentration of the formed clusters of defects could probably be much less than the concentration of point defects, which belong to the $VO_i$, $VO_iP$, and $C_iO_i$ complexes. As shown by calculations in Fig. 4, an increase in the magnitude of a uniaxial pressure along the crystallographic direction [100] leads to a decrease in activation energy of the $VO_iP$ complex over the entire range of the investigated pressures, while at uniaxial pressure along the crystallographic direction [111] – only for uniaxial pressures $P\le 0{,}4$. When the axis of deformation is aligned along the crystallographic direction [100], the deep level $E_1=E_C-0{,}107$ eV, which belongs to the $VO_iP$ complex, will be decomposed into two components with a different activation energy. One component will be associated with the two minima in the silicon conduction band, which would descend, while a second component will be associated with the four minima that would ascend along the energy scale under deformation. This explains the resulting non-linear dependences of effective activation energy of the deep level $E_1=E_C-0{,}107$ eV (averaged for the specified minima) on uniaxial deformation along the crystallographic direction [100] under uniaxial pressures $P\le 0{,}4$ GPa (Fig. 4, curves 1). At high uniaxial pressures $P>0{,}4$ GPa, decomposition of the deep level $E_1=E_C-0{,}107$ eV will be significant and, accordingly, the intensity of transitions of electrons from this deep level to the four minima in the silicon conduction band, which ascend, will be far less than the intensity of transitions to the two minima, which descend along the energy scale under deformation. Thus, we can assume that at such high uniaxial pressures the deep level of the $VO_iP$ complex interacts only with the two minima in the silicon conduction band. It is known [35] that a change in the magnitude of activation energy of a deep level under deformation is determined both from the displacement of the level itself and the minima relative to the bottom of conduction band in the non-deformed state. Displacements of minima in the silicon conduction band are the linear functions of pressure. Therefore, a shift of the deep level $E_1=E_C-0{,}107$ eV at uniaxial pressure $P>0{,}4$ GPa along the crystallographic direction [100] will also be linear, but with a lower rate than the displacement speed of two minima in the conduction band, which descend along the energy scale under deformation. This explains the linear reduction of activation energy for the $VO_iP$ complex under such pressures. The displacement of six minima in the silicon conduction band at uniaxial pressure along the crystallographic direction [111], in accordance with [33], is

$$\Delta E_{[111]}=-\left(\Xi_d+\frac{1}{3}\Xi_u\right)\left(S_{11}+2S_{12}\right)P=-3{,}348\cdot 10^{-12}P. \quad (13)$$

The minus sign indicates that these minima are displaced in line with a linear law down the energy scale under deformation. In this case, the deep level $E_1=E_C-0{,}107$ eV is not decomposed under deformation. Since a change in the activation energy for the $VO_iP$ complex at uniaxial pressures $P\le 0{,}4$ GPa along the crystallographic direction [111] is described by a quadratic dependence (refer to Table 2), the displacement of the deep level $E_1=E_C-0{,}107$ eV for this case is also a quadratic function for deformation. Under uniaxial pressures $P>0{,}4$ GPa (refer to Fig. 4, curve 2), activation energy for the $VO_iP$ complex does not depend on the deformation. This means that the displacements of deep level $E_1=E_C-0{,}107$ eV under deformation occurs along the same direction and at the same rate as the six minima in the silicon conduction band.

Undertaking such an integrated research has made it possible to establish the relative share of defects with different nature in the defect formation in the single crystals of silicon under electronic irradiation. Earlier studies, which, for instance, addressed tensor effects in the single crystals of silicon and germanium, considered in calculations the effect on the tensor resistance of these crystals exerted only by a single type of a radiation defect, which could have contributed to additional errors [35, 36]. In addition, studying the tensor hall-effect, in contrast to investigating the tensor resistance, makes it possible to separately assess the impact of pressure on the concentration and mobility of current carriers. The derived approximation polynomials for calculating the dependences of activation energy of the deep level $E_1=E_C-0{,}107$ eV in the $VO_iP$ complex on uniaxial pressure could be applied in the theoretical description of various kinetic and optical effects in the uniaxially deformed n-Si <P> single crystals and strained nanostructures based on them, in the presence of such deep centers.

Interpretation of the defect formation processes is seriously complicated when there are clusters of defects that might form amorphous regions in silicon, metallic or dielectric inclusions. In this case, examining the Hall effect and the tensor hall-effect will yield information only about effective (averaged) values for conductivity, concentration, and mobility of current carriers. This requires additional research into processes of annealing of radiation defects, measuring the gradients of specific resistance, concentration and mobility of current carriers along a sample, electron microscopy.

## 7. Conclusions

1. It was established based on studying the infra-red Fourier-spectroscopy that the main radiation defects in the silicon single crystals, irradiated by electrons with an energy of 12 MeV, doped by a phosphorus additive with a concentration of $N_d$=2,2·10$^{16}$ cm$^{-3}$, are the A-centers (the $VO_i$ complexes) and the complexes that contain the intranodal carbon (the $C_iO_i$ complexes).

2. It is shown by employing additional measurements of the Hall effect and the tensor hall-effect that for the examined silicon single crystals at electron irradiation it is fairly effective to form a new type of radiation defects, which belong to the $VO_iP$ complexes (A-center, modified with a phosphorus additive). An analysis of the performed theoretical calculations reveals that the concentration of these complexes for the irradiated silicon single crystals is the largest relative to the concentration of the $VO_i$ and $C_iO_i$ complexes. However, an increase in the flux of electron radiation from 1·10$^{17}$ to 2·10$^{17}$ el/cm$^2$ almost does not change the concentration of the $VO_iP$ complexes, because there is limit to the degree of doping the silicon single crystals by a phosphorus additive.

3. It was established that activation energy of the $VO_iP$ complex at increasing the uniaxial pressure to 0.4 GPa, both under conditions of asymmetrical and symmetrical alignment of deformation axis relative to the isoenergetic ellipsoids in silicon, decreases in line with a quadratic law. Different dependences of activation energy for a given complex on the orientation of a deformation axis relative to different crystallographic directions might indicate the anisotropic characteristics of such a defect in silicon.

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