INFLUENCE OF UNIAXIAL DEFORMATION ON THE FILLING OF THE LEVEL ASSOCIATED WITH A-CENTER IN n-Si CRYSTALS

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Single crystals of n-Si with the initial charge carrier concentration of 1.24×10^{14} cm^{-3} which were irradiated with Co^{60} γ-quanta to a dose of 3.8×10^{17} quantum/cm^2 have been studied. The piezoresistance of γ-irradiated n-Si crystals has been measured in the case where $X \parallel J \parallel [100]$ and $X \parallel J \parallel [110]$. The technique of calculations of the drift rate is presented, and the filling degree α of deep levels is estimated. The variation of the energy gap between the deep energy level $E_C - 0.17$ eV and the lower valleys in the conduction band in n-Si crystals induced by an uniaxial elastic deformation along the crystallographic directions [100] and [110] is calculated. The average value of the coefficient α is determined at various temperatures.

1. Introduction

The study of a behavior of deep centers at a crystal deformation can provide an important information on the character of relations between the local electron states at those centers and the nearest bands, the defect symmetry type, and the deformation degree of internal bonds in the lattice. Therefore, the issues concerning the structure and the energy spectrum of the centers of strong electron localization is challenging.

The behavior of deep states at a deformation cannot be analyzed so simply as that of shallow ones. At a deformation, the latter practically do not shift with respect to band edges, whereas the former drift with a high rate, and every such state is characterized by its own drift rate.

The study of features of the piezoresistance effect in the n-Si semiconductor, provided that its forbidden band includes deep energy levels belonging to radiation-induced defects, is of interest in both informative and practical aspects. As is known, the deep energy level $E_c - 0.17$ eV, which belongs to the A-center (the complex of a vacancy and an interstitial oxygen atom), is known to be a prevailing radiation-induced defect in γ-irradiated n-Si crystals with a high content of the oxygen impurity [1, 2].

2. Results and Their Discussion

To study the influence of radiation-induced defects on the piezoresistance of n-Si crystals under the conditions $X \parallel J \parallel [100]$ and $X \parallel J \parallel [110]$, we used specimens with the specific resistance $\rho_{300\ \mathrm{K}} = 30\ \Omega \times$ cm and the initial charge carrier concentration $n = 1.24 \times 10^{14}$ cm^{-3}, which were subjected to the irradiation with Co^{60} γ-quanta to a dose of 3.8×10^{17} quantum/cm^2(Figs. 1 and 2).

Figure 1 illustrates the measurement results for the longitudinal piezoresistance of γ-irradiated n-Si crystals at various fixed temperatures, provided $X \parallel J \parallel [100]$. In nonirradiated n-Si crystals (without deep states in the forbidden band), the piezoresistivity (at $X \parallel J \parallel [100]$) is governed by a migration of charge carriers from four valleys (with a higher mobility $\mu_\perp$) going up the en-

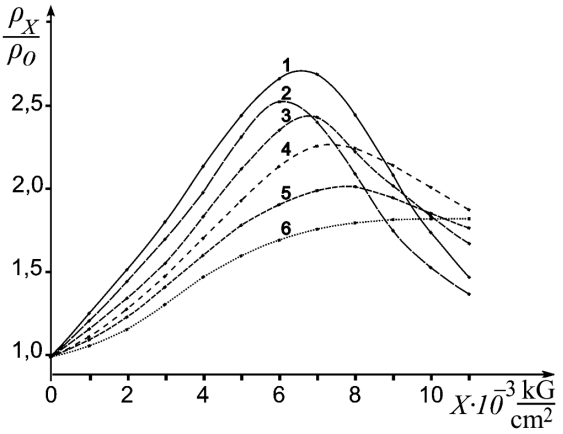

Fig. 1. Dependences $\frac{\rho_X}{\rho_0} = f(X)$ after the γ-irradiation of n-Si crystals to the dose $\Phi = 3.81 \times 10^{17}$ quantum/cm^2 for the case $X \parallel J \parallel [100]$ and at temperatures $T = 77.2$ (*1*), 120 (*2*), 135 (*3*), 170 (*4*), 200 (*5*), and 300 K (*6*)

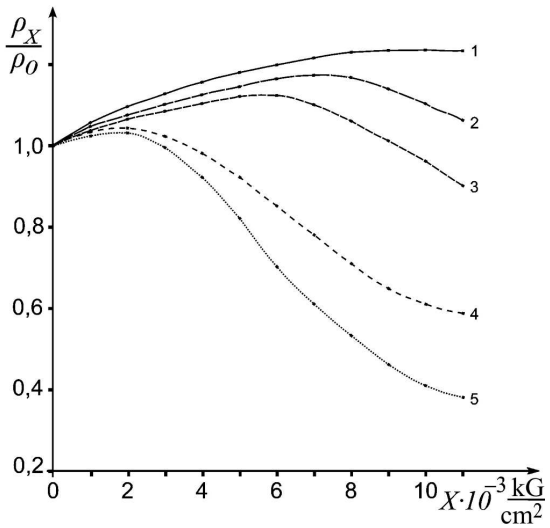

Fig. 2. Dependences $\frac{\rho_X}{\rho_0} = f(X)$ after γ-irradiation of n-Si crystals to the dose $\Phi = 3.81 \times 10^{17}$ quantum/cm^2 for the case $X \parallel J \parallel$ [110] and at temperatures $T = 300$ (*1*), 160 (*2*), 140 (*3*), 120 (*4*), and 77 K (*5*)

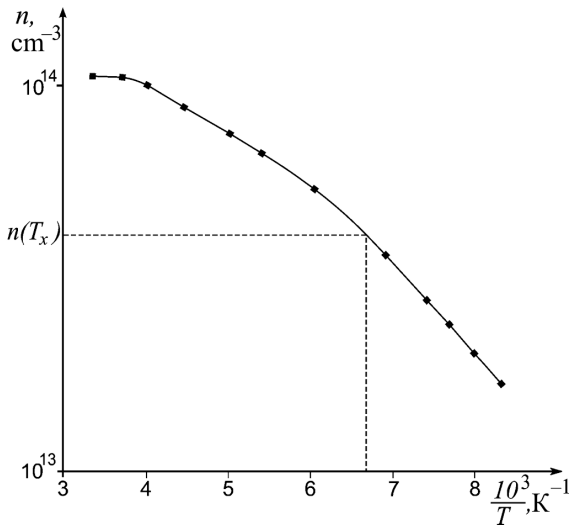

Fig. 3. Temperature dependence of the charge carrier concentration in an n-Si crystal γ-irradiated to the dose $\Phi = 3.81 \times 10^{17}$ quantum/cm^2

ergy scale to two valleys (with the mobility $\mu_\parallel < \mu_\perp$) going down. This process results firstly in the growth of the specific resistance, followed by its saturation [3]. In our case, such a dependence was observed only at $T = 300$ K (Fig. 1, curve *6*), when the deep center with the level $E_c - 0.17$ eV was completely ionized. As the temperature fell down, and the level of radiation-induced defects started to manifest itself, the dependences $\rho_X/\rho_0 = f(X)$ had a peculiarity, namely, they passed through a maximum with a subsequent reduction of the specific resistance, when mechanical stresses increased (Fig. 1, curves *1–5*).

Qualitatively similar dependences $\rho_X/\rho_0 = f(X)$ were obtained at various fixed temperatures for γ- irradiated n-Si crystals under the condition $X \parallel J \parallel$ [110] (Fig. 2). But, in contrast to the previous case (Fig. 1), only a weak growth of the $\rho_X/\rho_0 = f(X)$-dependences was observed (Fig. 2, curves *1–3*) and only at extremely high temperatures. It can be explained by the charge carrier migration from two valleys going up to four valleys going down the energy scale at a crystal deformation.

The profiles of the $\rho_X/\rho_0 = f(X)$-dependences obtained in those experiments for both crystallographic directions in n-Si crystals can be explained by the action of two mechanisms of specific resistance response to a change of the pressure:

– a redistribution of charge carriers among valleys that drift under the action of a deformation in opposite directions along the energy scale;

– an increase of the total charge carrier concentration in the C-band owing to a strain-induced reduction of the energy gap between the deep level $E_c - 0.17$ eV and the bottom of the conduction band, which brings about a decrease of the specific resistance, as X grows.

Figure 3 demonstrates the temperature dependence of the charge carrier concentration in n-Si crystals γ-irradiated to a dose of 3.8×10^{17} quantum/cm^2. The characteristic feature of the dependence $n = f\left(10^3/T\right)$ (Fig. 3) is the transition from a "full-slope" drift mode of the level $E_c - 0.17$ eV at temperatures $T \le T_X$ to a "half-slope" one at $T > T_X$. According to Fig. 3, the characteristic transition temperature is $T_X = 148$ K, and the corresponding charge carrier concentration is $n(T_X) \approx 4 \times 10^{13}$ cm^{-3}.

Let us determine a variation of the energy gap between the deep level $E_c - 0.17$ eV and the bottom of the conduction band in n-Si crystals under the conditions $X \parallel J \parallel$ [100] and $X \parallel J \parallel$ [110]. We use a method, which was applied in work [4], when studying the same n-Si crystals, but at $X \parallel J \parallel$ [111]. The electron concentration in the conduction band depends on the deformation according to the formula [4, 5]

$$n_\varepsilon = n \exp\left(-\frac{\Delta E}{\alpha k T}\right), \qquad (1)$$

where n is the electron concentration in a nondeformed semiconductor, α is a coefficient that changes from 1 to 2 depending on the deep level filling degree [5, 6], and ΔE is a variation of the energy gap between the deep

energy state and the bottom of the conduction band at a deformation. Let us differentiate expression (1) with respect to X:

$$\frac{dn_\varepsilon}{dX} = -\frac{n}{\alpha kT}\exp\left(-\frac{\Delta E}{\alpha kT}\right)\frac{d(\Delta E)}{dX}. \tag{2}$$

According to the results of works [2, 4–6],

$$\frac{d(\Delta E)}{dX} = \text{const}. \tag{3}$$

Since the derivative $\frac{dn_\varepsilon}{dX}$ at some point X_1 is equal to the slope of the tangent line to the plot of the function $n_\varepsilon = f(X)$ at this point, it can be written down as follows:

$$\left.\frac{dn_\varepsilon}{dX}\right|_{X_1} = \tan\beta_1. \tag{4}$$

According to Eqs. (1), (2), and (4), we have

$$\frac{d(\Delta E)}{dX} = -\frac{\alpha_1 kT}{n_\varepsilon(X_1)}\tan\beta_1. \tag{5}$$

Taking Eq. (3) into account, we obtain that, for two different X_1 and X_2,

$$\frac{\alpha_1\tan\beta_1}{n_\varepsilon(X_1)} = \frac{\alpha_2\tan\beta_2}{n_\varepsilon(X_2)}. \tag{6}$$

In works [2, 7], the charge carrier concentration at temperatures $T > T_X$ was shown to look like $n \sim \exp\left(-\frac{E_0}{2kT}\right)$. In the low-temperature case $T \le T_X$, the argument of the exponential function includes the total energy of level activation ($\alpha = 1$ at $T \le T_X$). According to Eq. (6),

$$\frac{\alpha_1\tan\beta_1}{n_\varepsilon(X_1)} = \frac{\tan\beta_0}{n_\varepsilon(X_0)}, \tag{7}$$

where $\tan\beta_0$ is the slope of the tangent line to the plot of the function $n_\varepsilon = f(X)$ at the point X_0, where $n_\varepsilon(X_0) = n(T_X)$. In view of Eqs. (5) and (7), the change of the energy gap between the deep level E_ε and the lower valleys in the conduction band at a deformation (and provided $T = \text{const}$) is equal to

$$\frac{d(\Delta E)}{dX} = -\frac{kT}{n_\varepsilon(X_0)}\tan\beta_0. \tag{8}$$

Now, from Eq. (7), the coefficient α at $X = X_1$ can be determined as

$$\alpha_1 = \frac{n_\varepsilon(X_1)\tan\beta_0}{n_\varepsilon(X_0)\tan\beta_1}. \tag{9}$$

In the general case for an arbitrary mechanical stress $X = X_n$ and an arbitrary temperature $T_1 \le T_X$ (provided $T = \text{const}$), we obtain

$$\alpha_n = \begin{cases} \dfrac{n_\varepsilon(X_n)\,\mathrm{tg}\,\beta_0}{n_\varepsilon(X_0)\,\mathrm{tg}\,\beta_n}, & \text{if} \quad X_n \neq X_0, \\ 1, & \text{if} \quad X_n = X_0. \end{cases} \tag{10}$$

In the case $T_2 > T_X$ ($T_2 = \text{const}$) in accordance with Eqs. (3) and (5),

$$\alpha_n = \frac{T_1}{T_2}\frac{n_\varepsilon(X_n, T_2)\tan\beta_0}{n_\varepsilon(X_0, T_1)\tan\beta_n}. \tag{11}$$

If the axis of a deformation is arranged asymmetrically with respect to the isoenergetic ellipsoids in n-Si crystals, the charge carriers practically stop their redistribution between the valleys at mechanical stresses of about $X \approx 7000$ kG/cm^2. So that, at higher X-values, only the second of the above-mentioned piezoresistance mechanisms survives. From the slopes of curves $\ln\rho = f(X)$, it is possible to determine the variation of the energy gap between the deep level $E_c - 0.17$ eV and the lower valleys in the conduction band [6]:

$$\frac{d(\Delta E)}{dX} = \frac{(\Delta\ln\rho)\alpha kT}{1.6\times10^{-19}\Delta X}, \tag{12}$$

where α is a coefficient that changes from 1 to 2 depending on the deep level filling degree.

As was shown in work [2], if the piezoresistance dependences, even in the range of strong uniaxial elastic deformations, are solely used in calculations, the latter cannot give rise always to correct results for a variation of the deep level position. The errors stem from the dependence of the charge carrier effective mobility on the degree of homogeneity of crystals and a slight modification of the relaxation time. Since the character and the magnitude of a pressure-induced level shift depend rather weakly on the temperature [8], only the correct account of the numerical coefficient α can bring us to true values of the gap variation at various fixed temperatures.

A variation of the energy gap between the deep level and the bottom of the conduction band can be described as follows:

$$\Delta E = \frac{d(\Delta E)}{dX}X. \tag{13}$$

Then, with regard for Eqs. (12) and (13), expression (1) for the electron concentration n_ε in the deformed semiconductor with deep energy states takes the form

$$n_\varepsilon = n\left(\frac{\rho_i}{\rho_{i+1}}\right)^{\frac{X}{\Delta X}}, \tag{14}$$

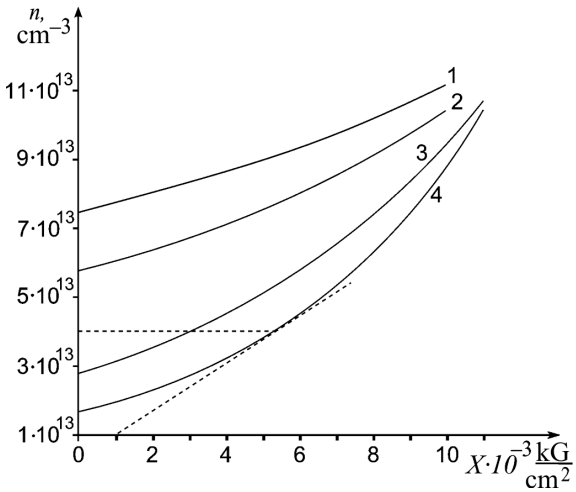

Fig. 4. Dependences $n_\varepsilon = f(X)$ after the γ-irradiation of n-Si crystals to the dose $\Phi = 3.81 \times 10^{17}$ quantum/cm^2 for the case $X \parallel J \parallel [100]$ and at temperatures $T = 200$ (*1*), 170 (*2*), 135 (*3*), and 120 K (*4*)

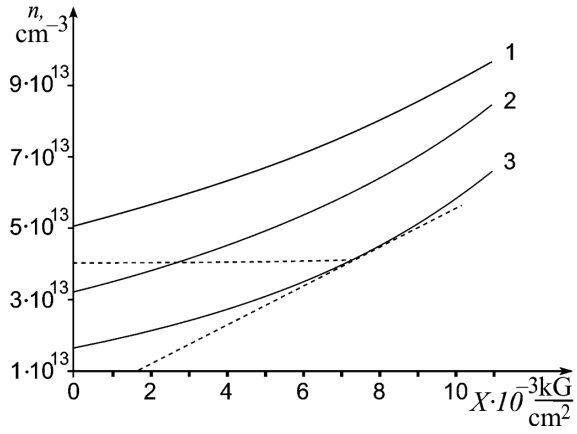

Fig. 5. Dependences $n_\varepsilon = f(X)$ after the γ-irradiation of n-Si crystals to the dose $\Phi = 3.81 \times 10^{17}$ quantum/cm^2 for the case $X \parallel J \parallel [110]$ and at temperatures $T = 160$ (*1*), 140 (*2*), and 125 K (*3*)

where ρ_i and ρ_{i+1} are the specific resistances at the mechanical stresses X_i and X_{i+1}, respectively, with both X_i and X_{i+1} being larger that the mechanical stress X', at which the dependence $\rho = f(X)$ has a maximum.

After the corresponding treatment of experimental dependences $\rho_X/\rho_0 = f(X)$ in the range $X >$7000–8000 kG/cm^2, Eq. (14) yields the dependence of the charge carrier concentration $n_\varepsilon = f(X)$ in γ-irradiated n-Si crystals at various temperatures under the conditions $X \parallel J \parallel [100]$ (Fig. 4) and $X \parallel J \parallel [110]$ (Fig. 5).

3. Conclusions

The stress-induced variation of the energy gap between the deep level $E_c - 0.17$ eV and the bottom of the conduction band in n-Si turned out to be $(2.45 \pm 0.10) \times 10^{-3}$ eV and $(1.42 \pm 0.06) \times 10^{-3}$ eV per every 10^3 kG/cm^2 for crystallographic directions [100] and [110], respectively.

The average values of the coefficient α calculated by formulas (10) and (11) for crystallographic directions [100] and [110] in uniaxially deformed n-Si crystals with the deep energy level $E_c - 0.17$ eV at various fixed temperatures T are quoted in the Table. As the calculations show, the average values of the coefficient α grow with the temperature for both crystallographic directions [100] and [110]. It can be explained by a reduction of the filling degree of the deep level $E_c - 0.17$ eV in n-Si. At low mechanical stresses ($X <$7000–8000 kG/cm^2), when the intervalley electron redistribution is still possible, the deep state $E_c - 0.17$ eV exchanges charge carriers with six valleys in the n-Si conduction band and, at strong uniaxial deformations, with those valleys that turn out lower by energy, which also affects the coefficient α.

[100]	T, K	120	135	170	200
	α	1.43	1.73	1.91	1.98
[110]	T, K	120	140	160	–
	α	1.12	1.35	1.77	–

The given method in the combination with longitudinal piezoresistance measurements allows one to study the behavior of deep energy states of both radiation and technological origins at any uniaxial pressure X and temperature T. The presence of deep energy states in crystals – e.g., n-Si ones – allows the tensosensitivity of multivalley semiconductors to be controlled in a wide range. Therefore, the results obtained can be applied to the development of tensosensors.

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ВПЛИВ ОДНОВІСНОЇ ДЕФОРМАЦІЇ НА ЗАПОВНЕННЯ РІВНЯ, ПОВ'ЯЗАНОГО З А-ЦЕНТРОМ, У КРИСТАЛАХ n-Si

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Р е з ю м е

Досліджено монокристали n-Si з вихідною концентрацією носіїв струму $1,24 \cdot 10^{14}$ см$^{-3}$, опромінені γ-квантами Co^{60} дозою $3,8 \cdot 10^{17}$ кв/см^2. Досліджено п'єзоопір γ-опромінених кристалів n-Si за умови, коли $X \| J \| [100]$ та $X \| J \| [110]$. Представлено метод розрахунку швидкості зміщення і оцінено ступінь заповнення α глибоких рівнів. Обчислено величину зміни енергетичної щілини між глибоким енергетичним рівнем E_C-0,17 еВ і нижніми долинами зони провідності n-Si при одновісній пружній деформації вздовж кристалографічних напрямків [100] і [110]. Визначено середнє значення коефіцієнта α (ступінь заповнення глибоких енергетичних рівнів) для різних температур.