DEFORMATION POTENTIAL CONSTANTS Ξ_u AND Ξ_d IN n-Si DETERMINED WITH THE USE OF THE TENSORESISTANCE EFFECT

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On the basis of longitudinal piezoresistance measurements in the geometry $X \parallel J \parallel [100]$ and the theory of anisotropic scattering, the deformation potential constants Ξ_u and Ξ_d for γ-irradiated n-Si have been determined. It has been shown that, while determining the anisotropy of relaxation times for n-Si with the deep energy level $E_c - 0.17$ eV, the dependence of the concentration of deep ionized centers on the deformation must be taken into consideration.

1. Introduction

Deformation potential constants are important parameters characterizing the band structure of semiconductors. The development of methods aimed at their reliable determination is an important task of experimental physics of semiconductors. The corresponding values obtained experimentally are applied when calculating the energy shifts of corresponding extremes at various kinds of deformation and the transition probabilities at the scattering by acoustic lattice vibrations, which determine both the mobility of charge carriers and the peculiarities in the anisotropic characteristics of transport phenomena at such scattering [1–4]. The peculiarities of deformation effects in semiconductors, which are associated with the energy shifts of various extremes in the band spectrum and the reconstruction of the spectrum itself at the deformation [5], are governed by the deformation potential constants. A uniaxial elastic deformation, which reduces the initial symmetry of the crystal, eliminates the band spectrum degeneration. For instance, it may be a degeneration with respect to the energies of equivalent minima in the conduction band; and the magnitude of energy decoupling at the deformation is determined by the corresponding values of deformation potential constants.

It should be noted that, at the present development stage of the technology of semiconductor materials, the researches of electron transport phenomena in nanostructures demand that the reliable values for deformation potential constants, effective masses, relaxation time, as well as other important parameters, be known [6–8]. In particular, as was demonstrated in work [7], a reduction of the dimensionality of a system substantially affects the charge carrier mobility and the deformation potential constants in silicon nanoconductors.

Various external physically active influences – e.g., high radiation fields – can substantially affect the band parameters of semiconductor materials, in particular, the deformation potential constants. This circumstance should be taken into account while designing semiconductor-based sensors and devices. Silicon is one of the basic materials for functional electronics for today, and it will probably remain as such in the future. Therefore, it is expedient to continue the study of the physical properties of this material under various extreme conditions.

This work is aimed at determining the constants Ξ_u and Ξ_d of the deformation potential in the conduction band of γ-irradiated n-Si crystals, by using the tensoeffect, which manifests itself at a uniaxial elastic deformation. As a rule, the application of only one of the methods for the determination of deformation potential constants allows only either of them (Ξ_u or Ξ_d) or their combination to be determined. We succeeded in finding them separately, which is of importance from both the practical and theoretical aspects. Unlike germanium, for which the corresponding constants are known more or less reliably, the literature data for the deformation potential constants in silicon are rather scattered. Especially little information is available concerning the constant Ξ_d of the deformation potential in silicon. The absence of reliable data on the magnitudes of those constants does not allow precise calculations to be carried out for the value and the character of the conduction-band bottom shift in n-Si at a uniaxial elastic deforma-

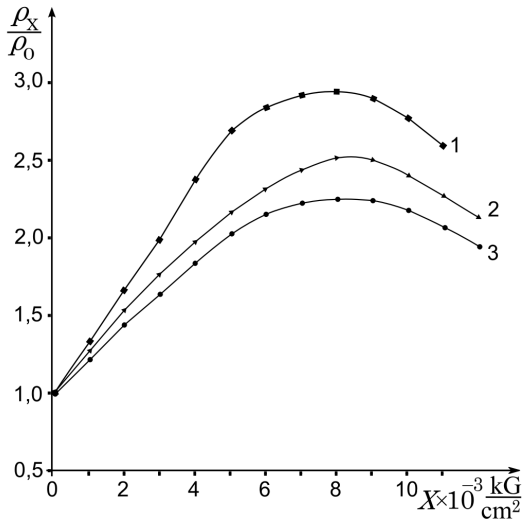

Fig. 1. Piezoresistance dependences $\frac{\rho_X}{\rho_0} = f(X)$ for n-Si γ-irradiated to a dose of 1.9×10^{17} quant/cm^2 measured in the geometry $X \parallel J \parallel [100]$ at various temperatures $T = 77$ (*1*), 110 (*2*), and 150 K (*3*)

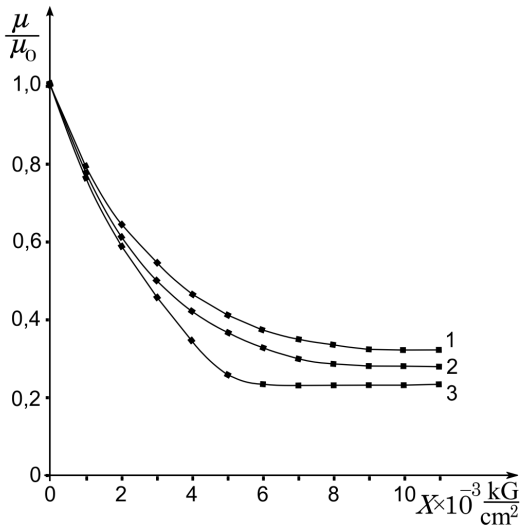

Fig. 2. Dependences $\frac{\mu}{\mu_0} = f(X)$ for n-Si γ-irradiated to a dose of 1.9×10^{17} quant/cm^2 measured in the geometry $X \parallel J \parallel [100]$ at various temperatures $T = 150$ (*1*), 110 (*2*), and 77 K (*3*)

tion, when the mechanical stress X is directed along the crystallographic direction [111]. The shift of the deep energy level under the given conditions cannot be calculated as well [9].

2. Experimental Part

In this work, we study the piezoresistance of γ-irradiated n-Si crystals with the initial concentration of charge carriers $n = 1.1 \times 10^{14}$ cm^{-3}and the deep energy level $E_c - 0.17$ eV in the geometry $X \parallel J \parallel [100]$. The deep energy level $E_c - 0.17$ eV belonging 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 with a high content of oxygen impurity [10].

In Fig. 1, the temperature dependences of the piezoresistance of γ-irradiated n-Si measured in the geometry $X \parallel J \parallel [100]$ are depicted. A reduction of the n-Si specific resistance in the maximum of the dependence $\frac{\rho_X}{\rho_0} = f(X)$ is explained by a reduction of the gap between the deep energy level $E_c - 0.17$ eV and the bottom of the conduction band [11].

The dependence of the charge carrier mobility on the deformation at a definite fixed temperature T_0 in the presence of deep energy levels is described by the formula [12]

$$\mu = \mu_0 \frac{\left\langle \frac{\rho_i}{\rho_{i+1}} \right\rangle^{-\frac{X}{\Delta X}}}{\frac{\rho(T_0, X)}{\rho(T_0)}}, \qquad (1)$$

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 $X_{i+1} > X'$, where X' is the mechanical stress, at which the dependence $\frac{\rho_X}{\rho_0} = f(X)$ has a maximum; and μ_0 is the mobility of electrons in the undeformed semiconductor at the temperature T_0. By applying expression (1) to experimental data exhibited in Fig. 1, we calculated the dependences of the charge carrier mobility on the deformation, $\frac{\mu}{\mu_0} = f(X)$, for n-Si with the deep energy level $E_c - 0.17$ eV at various fixed temperatures (see Fig. 2). Figure 2 demonstrates that the dependences $\frac{\mu}{\mu_0} = f(X)$ saturate at large X's, which can be explained by the complete migration of charge carriers from four valleys, which rise at a deformation of n-Si, when $X \parallel J \parallel [100]$, into two valleys falling at that. In this case, the deep level $E_c - 0.17$ eV exchanges charge carriers with only two valleys, which therefore govern the concentration and the mobility of charge carriers in n-Si at strong uniaxial deformations [13].

3. Results of Calculations and Their Discussion

If the isoenergetic surface is an ellipsoid of revolution, the mobility of charge carriers in an arbitrary direction is determined by the relation [5]

$$\mu = \mu_\perp \sin^2\theta + \mu_\parallel \cos^2\theta, \tag{2}$$

where θ is the angle between the considered direction and the principal axis of the ellipsoid, and $\mu_\perp$ and $\mu_\parallel$ are the mobilities of charge carriers across and along the ellipsoid axis, respectively. For n-Si, if $X \parallel [100]$, the ellipsoids are at mutually perpendicular axes. Therefore, taking Eq. (2) into account, we obtain

$$\mu_1 = \mu_\parallel, \quad \mu_2 = \mu_\perp. \tag{3}$$

The specific electroconductance of the n-Si crystal at the deformation $X \parallel [100]$ looks like

$$\sigma_X = 2en_1(X)\mu_\parallel + 4en_2(X)\mu_\perp = en(X)\mu(X), \tag{4}$$

where $n_1(X)$ and $n_2(X)$ are the concentrations of charge carriers in the valleys that rise and fall, respectively, at the deformation, and $n(X)$ is the total charge carrier concentration in the conduction band at the deformation.

Since the concentration of ionized centers with the level $E_c - 0.17$ eV depends on the mechanical stress X, the anisotropy parameter of relaxation times, K_τ, evidently also depends on X. Therefore, it is impossible to determine K_τ for n-Si with the deep energy level $E_c - 0.17$ eV from the measurements of the longitudinal piezoresistance, as it was done in work [14] for shallow levels, where the necessary conditions are a constant concentration of charge carriers in the conduction band and the absence of intervalley scattering, which actively reveals itself at $T > 100$ K.

Let us write down expression (4) for two mechanical stresses X_1 and X_2, which differ a little from each other. In so doing, we may consider that, when the deformation X varies from X_1 to X_2, the concentration of ionized centers with the level $E_c - 0.17$ eV remains constant. Hence,

$$\sigma_{X_1} = 2en_1(X_1)\mu_\parallel + 4en_2(X_1)\mu_\perp = en(X_1)\mu(X_1), \tag{5}$$

$$\sigma_{X_2} = 2en_1(X_2)\mu_\parallel + 4en_2(X_2)\mu_\perp = en(X_2)\mu(X_2). \tag{6}$$

In addition, we may write down

$$\begin{cases} 2n_1(X_1) + 4n_2(X_1) = n(X_1) \\ 2n_1(X_2) + 4n_2(X_2) = n(X_2) \end{cases}, \quad \begin{cases} \frac{n_2(X_1)}{n_1(X_1)} = e^{-\frac{\Delta E_1}{kT}} = a_1, \\ \frac{n_2(X_2)}{n_1(X_2)} = e^{-\frac{\Delta E_2}{kT}} = a_2, \end{cases} \tag{7}$$

where ΔE_1 and ΔE_2 are the values of energy gaps that arise between two falling and four rising valleys at different values (X_1 and X_2, respectively) of deformation in n-Si along the crystallographic direction [100]. Taking Eqs. (5)–(7) into account, we obtain

$$\frac{\mu(X_1)}{\mu(X_2)} = \frac{\mu_\parallel + 2\mu_\perp a_1}{\mu_\parallel + 2\mu_\perp a_2} \frac{1+2a_2}{1+2a_1} \tag{8}$$

or

$$\frac{\mu(X_1)}{\mu(X_2)} = \frac{1+2Ka_1}{1+2Ka_2} \frac{1+2a_2}{1+2a_1}, \tag{9}$$

where $K = \dfrac{\mu_\perp}{\mu_\parallel}$ is the parameter of charge carrier mobility anisotropy. From Eq. (9), we determine the quantity K,

$$K = \frac{(1+2a_2)\mu(X_2) - (1+2a_1)\mu(X_1)}{2a_2(1+2a_1)\mu(X_1) - 2a_1(1+2a_2)\mu(X_2)}, \tag{10}$$

$$K = \frac{K_m}{K_\tau}, \tag{11}$$

where K_m is the parameter of effective mass anisotropy, and K_τ is the parameter of relaxation time anisotropy.

Taking Eqs. (10) and (11) into account, we obtain

$$K_\tau = K_m \frac{2a_2(1+2a_1)\mu(X_1) - 2a_1(1+2a_2)\mu(X_2)}{(1+2a_2)\mu(X_2) - (1+2a_1)\mu(X_1)}. \tag{12}$$

Let us determine the quantity K_τ in the framework of the anisotropic scattering theory [15],

$$K_\tau = \frac{\langle \tau_\parallel \rangle}{\langle \tau_\perp \rangle}, \tag{13}$$

where

$$\langle \tau_\parallel \rangle = \int_0^\infty dx x^{3/2} e^{-x} \tau_\parallel, \quad \langle \tau_\perp \rangle = \int_0^\infty dx x^{3/2} e^{-x} \tau_\perp. \tag{14}$$

Under the mixed scattering conditions, the expressions for $\tau_\parallel$ and $\tau_\perp$ look like

$$\tau_\parallel = \frac{a_\parallel}{\sqrt{k_B T^{3/2}}} \frac{x^{3/2}}{x^2 + b_0}, \quad \tau_\perp = \frac{a_\perp}{\sqrt{k_B T^{3/2}}} \frac{x^{3/2}}{x^2 + b_1}, \tag{15}$$

where

$$a_\parallel = \frac{\pi c_{11} \hbar^4}{k_B \Xi_d^2 \sqrt{2m_\parallel m_\perp^2}} \frac{1}{\Phi_{0a}},$$

$$a_\perp = \frac{\pi c_{11}\hbar^4}{k_{\rm B}\Xi_d^2\sqrt{2m_\parallel m_\perp^2}}\,\frac{1}{\Phi_{1a}}, \tag{16}$$

$$\Phi_{0a} = 1 + 1{,}645\frac{\Xi_u}{\Xi_d} + 1{,}03\frac{\Xi_u^2}{\Xi_d^2},$$

$$\Phi_{1a} = 1 + 0{,}818\frac{\Xi_u}{\Xi_d} + 0{,}688\frac{\Xi_u^2}{\Xi_d^2}, \tag{17}$$

$$b_0 = \frac{a_\parallel \Phi_{0i}}{\sqrt{k_{\rm B}}T^{3/2}\tau_{0i}(kT)}, \quad b_1 = \frac{a_\perp \Phi_{1i}}{\sqrt{k_{\rm B}}T^{3/2}\tau_{0i}(kT)}, \tag{18}$$

$$\tau_{0i}(k_{\rm B}T) = \frac{\sqrt{2}m_\perp\varepsilon_0^2(k_{\rm B}T)^{3/2}}{\pi n e^4\sqrt{m_\parallel}}, \tag{19}$$

n is the concentration of ionized centers, ε_0 is the dielectric permeability, e is the electron charge,

$$\Phi_{0i} = \frac{3}{2\beta^3}\left[\left(\frac{\beta}{1+\beta^2} - a\right)\ln\gamma^2 - a\ln\left(1+\beta^2\right) + 2L(a) + \right.$$

$$\left. + \frac{\beta\gamma^2}{2}\left(\frac{\beta^2-1}{\beta^2+1} + \frac{a(\beta^2+1)}{\beta}\right)\right],$$

$$\Phi_{1i} = \frac{3}{4\beta^3}\left[((1-\beta^2)a - \beta)\ln\gamma^2 + 2(\beta^2-1)L(a) - 2\beta^2 a - \right.$$

$$\left. - (\beta^2-1)a\ln(1+\beta^2) + \frac{\gamma^2}{2}(\beta(1+3\beta^2) + a(3\beta^4+2\beta^2-1))\right], \tag{20}$$

$\beta^2 = \frac{m_\parallel - m_\perp}{m_\perp}$, $a = \arctan\beta$, $L(a) = -\int\limits_0^a \ln\cos\varphi d\varphi$ is the Lobachevskii function, $\gamma^2 = \frac{\pi\hbar^2 e^2}{2m_\parallel\varepsilon_0 k_{\rm B}^2}\cdot\frac{n}{T^2 x}$, and $x = \frac{\varepsilon}{k_{\rm B}T}$. In view of Eqs. (16) and (19), expressions (18) can be rewritten as follows:

$$b_0 = \frac{nA\Phi_{0i}}{\Xi_d^2\Phi_{0a}}, \quad b_1 = \frac{nA\Phi_{1i}}{\Xi_d^2\Phi_{1a}}, \tag{21}$$

where $A = \frac{\pi^2 c_{11}\hbar^4 e^4}{2k_{\rm B}^3 m_\perp^2 T^3\varepsilon_0^2}$. According to Eqs. (12)–(21), we obtain

$$\frac{\Phi_{1a}}{\Phi_{0a}}\,\frac{\int\limits_0^\infty dx(x^3e^{-x})/(x^2 + \frac{nA\Phi_{0i}}{\Xi_d^2\Phi_{0a}})}{\int\limits_0^\infty dx(x^3e^{-x})/(x^2 + \frac{nA\Phi_{1i}}{\Xi_d^2\Phi_{1a}})} =$$

$$= K_m\frac{2a_2(1+2a_1)\frac{\mu(X_1)}{\mu_0} - 2a_1(1+2a_2)\frac{\mu(X_2)}{\mu_0}}{(1+2a_2)\frac{\mu(X_2)}{\mu_0} - (1+2a_1)\frac{\mu(X_1)}{\mu_0}}. \tag{22}$$

Differentiating Eq. (4) with respect to X, we obtain

$$\frac{d\sigma}{dX} = e\left(\mu\frac{dn}{dX} + n\frac{d\mu}{dX}\right) \tag{23}$$

or

$$-\frac{1}{\rho^2}\frac{d\rho}{dX} = e\left(\mu\frac{dn}{dX} + n\frac{d\mu}{dX}\right). \tag{24}$$

The concentration of electrons in a deformed semiconductor in the presence of a deep energy level is determined by the formula [16]

$$n = n_0 e^{-\frac{\Delta E}{\alpha kT}}, \tag{25}$$

where ΔE is the change of the energy gap between the deep level and the conduction band bottom at a deformation, α is a coefficient that varies from 1 to 2 depending on the degree of deep level filling, and n_0 is the concentration of electrons in the undeformed semiconductor. With regard for Eq. (25), we obtain

$$\frac{d\rho}{dX} = -en\rho^2\frac{d\mu}{dX} + \frac{\rho}{\alpha kT}\frac{d(\Delta E)}{dX}. \tag{26}$$

Since the dependence $\frac{\rho_X}{\rho_o} = f(X)$ has a maximum at $X = X_0$ (see Fig. 1, curve *1*), this means that $\left.\frac{d\rho}{dX}\right|_{X=X_0} = 0$.

At strong uniaxial deformations, $\Delta E = \frac{d(\Delta E)}{dX}X$ [9]. Then, in accordance with Eqs. (25) and (26), we obtain

$$\frac{\ln\left(en_0\mu(X_0)\rho(X_0)\right)}{X_0} = \frac{1}{\mu(X_0)}\left.\frac{d\mu}{dX}\right|_{X=X_0}. \tag{27}$$

If the mechanical stress along the crystallographic direction [100] $X \geq X_0$, the specific electric conductance of n-Si is determined only by two valleys with the charge carrier mobility $\mu = \mu_\parallel$. In view of the relation

$$\mu_\parallel = \frac{e}{m_\parallel}\langle\tau_\parallel\rangle, \tag{28}$$

and expressions (14)–(20), Eq. (27) can be written down in the form

$$\frac{\ln\left(en_0\mu(X_0)\rho(X_0)\right)}{X_0} =$$

$$= \frac{1}{\mu(X_0)}\frac{e\pi c_{11}\hbar^4}{(k_{\rm B}T)^{3/2}\Xi_d^2\sqrt{2m_\parallel^3 m_\perp^2}}\times$$

$$\times \frac{d}{dX}\left[\int\limits_0^\infty dx \frac{x^3 e^{-x}}{x^2 + \frac{nA\Phi_{0i}}{\Xi_d^2}\Phi_{0a}}\right]\Bigg|_{X=X_0}, \quad (29)$$

or

$$B\int\limits_0^\infty dx \frac{x^3 e^{-x}}{\left(x^2 + \frac{A\Phi_{0i}}{e\mu(X_0)\rho(X_0)\Xi_d^2\Phi_{0a}}\right)^2} = e\mu^2(X_0)\rho(X_0), \quad (30)$$

where $B = \frac{A\Phi_{0i}\pi c_{11}\hbar^4 e}{(k_B T)^{3/2}\Xi_d^4\Phi_{0a}\sqrt{2m_\parallel^3 m_\perp^2}}$.

According to Eqs. (22) and (30), we obtain the following system of two equations for the desired deformation potential constants Ξ_u and Ξ_d:

$$\begin{cases} \frac{\Phi_{1a}}{\Phi_{0a}} \frac{\int\limits_0^\infty \frac{x^3 e^{-x} dx}{x^2 + \frac{nA\Phi_{0i}}{\Xi_d^2\Phi_{0a}}}}{\int\limits_0^\infty \frac{x^3 e^{-x} dx}{x^2 + \frac{nA\Phi_{1i}}{\Xi_d^2\Phi_{1a}}}} = K_m \frac{2a_2(1+2a_1)\frac{\mu(X_1)}{\mu_0} - 2a_1(1+2a_2)\frac{\mu(X_2)}{\mu_0}}{(1+2a_2)\frac{\mu(X_2)}{\mu_0} - (1+2a_1)\frac{\mu(X_1)}{\mu_0}}, \\ B\int\limits_0^\infty \frac{x^3 e^{-x} dx}{\left(x^2 + \frac{A\Phi_{0i}}{e\mu(X_0)\rho(X_0)\Xi_d^2\Phi_{0a}}\right)^2} = e\mu^2(X_0)\rho(X_0). \end{cases} \quad (31)$$

This system has two pairs of solutions: (1) $\Xi_u = 9.23$ eV and $\Xi_d = -2.12$ eV, and (2) $\Xi_u = -66$ eV and $\Xi_d = 29$ eV. The second pair must be rejected because of the following reasons.

1. At a deformation, four valleys would have to fall on the energy scale. However, this result contradicts the reliable experimental and theoretical regularities established in the Smith–Herring piezoresistance effect.
2. The shift rate for the deep level of the A-center in n-Si at a uniaxial deformation turns out considerably overestimated for all crystallographic directions.
3. The value of charge carrier mobility in n-Si crystals calculated in the framework of the anisotropic scattering theory is much lower than the experimental one.

The reliability of the results obtained is confirmed by the fact that the value of deformation potential constant $\Xi_u = 9.23$ eV calculated in this work is rather close to the value $\Xi_u = 9.3$ eV obtained earlier for pure silicon crystals, mainly under phonon scattering conditions [17], and for silicon crystals irradiated at small doses [18]. The method used in works [17, 18] to determine the deformation potential constant Ξ_u has restrictions by the temperature and the impurity concentration. The corresponding constant in silicon can be determined precisely enough on the basis of this method only if the piezoresistance at a uniaxial deformation is created by a redistribution of charge carriers between the valleys. However, if the concentration of radiation-induced defects – e.g., A-centers – at the γ-irradiation attains values, at which the variation in their filling degree at a deformation can appreciably affect the concentration of charge carriers in the conduction band, the application of this method is impossible.

4. Conclusions

To summarize, first, the method proposed in this work allows both constants of the deformation potential, Ξ_u and Ξ_d, to be determined at a simultaneous action of various mechanisms giving rise to the piezoresistance. Second, it enables the corresponding constants to be determined at an arbitrary concentration of both shallow and deep centers in silicon crystals, which is important at the manufacturing of various kinds of pressure transducers and sensors with given parameters. The method proposed for the determination of the deformation potential constants could be approbated to determine the relevant constants for such technically important multivalley semiconductors, as Ge, GaAs, GaSb, CdSb, and others.

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КОНСТАНТИ ДЕФОРМАЦІЙНОГО ПОТЕНЦІАЛУ Ξ_u та Ξ_d У n-Si, ВИЗНАЧЕНІ МЕТОДОМ ТЕНЗОРЕЗИСТИВНОГО ЕФЕКТУ

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Р е з ю м е

На основі вимірювань поздовжнього п'єзоопору для випадку, коли $X//J//[100]$, і теорії анізотропного розсіяння визначено константи деформаційного потенціалу Ξ_u та Ξ_d в γ-опроміненому n-Si. Показано, що при визначенні параметра анізотропії часів релаксації для n-Si з глибоким енергетичним рівнем $E_c - 0,17$ еВ необхідно враховувати залежність концентрації іонізованих глибоких центрів від деформації.