The Anisotropy of Electron Scattering in Uniaxially Deformed N-Si Single Crystals with Radiation Defects

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Abstract

The tensoresistance at the uniaxial pressure along the crystallographic direction [100] for n-Si single crystals, which were irradiated by the different doses of gamma quants was investigated. On the basis of the theory of anisotropic scattering and experimental data of the tensoresistance the dependences of the parameter of mobility anisotropy on the uniaxial pressure for the data of single crystals are obtained. It has been shown that for unirradiated n-Si single crystals, the parameter of mobility anisotropy does not depend on uniaxial pressure since the alloying impurities of phosphorus will be completely ionized at T=77 K. For the gamma - irradiated n-Si single crystals the parameter of mobility anisotropy will decrease with an increase in exposure dose by reducing the screening effect. In this case, it is necessary to take into account the mechanisms of electron scattering on the impurity ions, impurity complexes, which consist of several ions of the impurity and on the fluctuation potential, which leads to the appearance of gradients of resistivity. The changing of relative contribution of these the scattering mechanismsat at the uniaxial pressure determines the obtained dependences of the parameter of mobility anisotropy and the tensoelectric properties of gamma-irradiated n-Si single crystals.

Introduction

The main materials for the production of the widest range of electronic devices and sensors of modern micro and nanoelectronics are many-valley semiconductors, among which silicon plays a leading role due to its unique properties, virtually unlimited natural resources, commercial availability, and growing technologies [1-4]. Physical properties of semiconductors depend essentially on defects and impurities that arise in the technological processes of their obtaining or exploitation. The change in the electrophysical properties of silicon single crystals in radiation irradiation is mainly determined by secondary defects - complexes of vacancies and interstitial atoms with each other, with atomic impurities (A-, E-centers, divacancies, and other defects) [5]. Such defects, as a rule, create deep energy levels in the band gap of silicon. The study of the impact of radiation on various physical properties of silicon is important from the point of view of studying the term of operation and changes of the performance of devices and measuring equipment manufactured on its basis, used in atomic reactors, accelerators of nuclear particles, aerospace industry, space, scientific research [6-10]. In particular, there is a significant demand for the radiation resistant pressure sensors for such areas of science and technology, whose manufacture in economically developed countries is about 60% among all other sensors of physical quantities.

Therefore, it is interesting both in the theoretical and practical terms to investigate the mechanisms of scattering of charge carriers in deformed silicon single crystals with radiation defects. At the temperature of sliquid nitrogen, the shallow levels will be completely ionized, and the deep are partially or completely non-ionized. Changing their degree of ionization by acting on silicon single crystals of various external physical-active fields (temperature, electrical, deformation, radiation) can significantly affect electrical, acousto-electrical, optical and other properties of silicon. The energy of ionization of the shallow level is well described by the approximation of the effective mass. Since the dependence of the effective mass on the deformation manifests itself even in the third approximation of the perturbation theory [11], we can assume that the ionization energy of the shallow level does not depend on the deformation. Therefore, shallow levels are practically not shifted relative to the corresponding extremes of the valence band or conductivity band of the semiconductor. According to experimental data and theoretical calculations, the rate of displacement of deep levels during deformation may differ significantly from the displacement velocity of the corresponding extremum C or V-zone [12]. This leads to a change of its degree of filling [13]. This, in turn, can lead to a change in the scattering conditions of charge carriers. This fact must be taken into account when analyzing kinetic effects in deformed single crystals of semiconductors with deep energy levels.

Results and Discussion

In our work, the tensoresistance at T = 77 K for the uniaxially deformed n-Si single crystals along the crystallographic direction [100], doped by phosphorus impurities, with the concentration $n = 1{,}1 \cdot 10^{14} cm^{-3}$, after $\gamma-$ irradiation by different doses of gamma quants was investigated (Fig. 1).
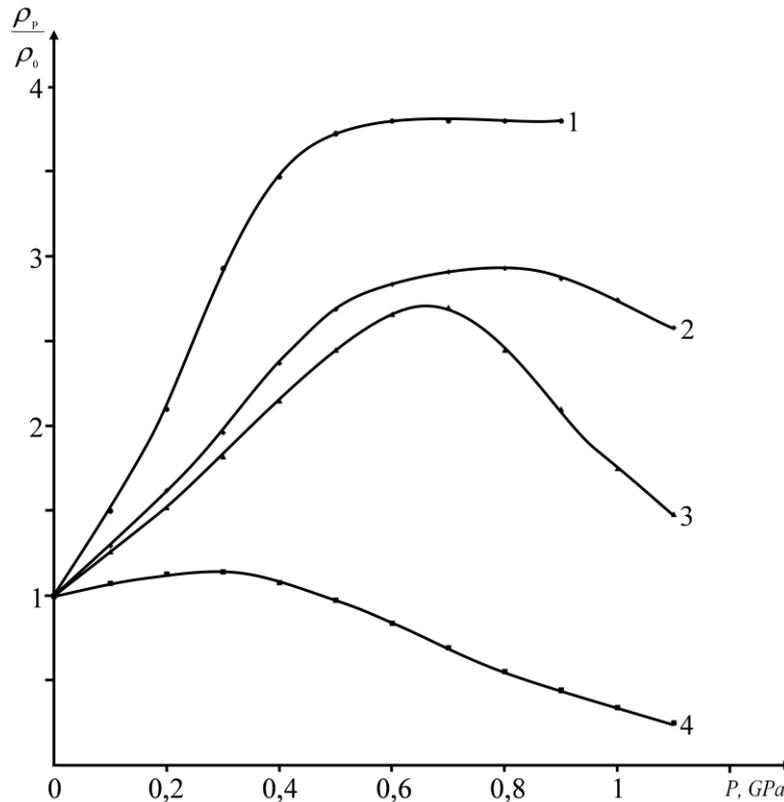
Fig.1 The dependence of tensoresistance $\frac{\rho_P}{\rho_0} = f(X)$ at $T = 77\,K$ for the uniaxially deformed n-Si single crystals along the crystallographic direction [100], irradiated by $\gamma-$ quants of different doses

$$\Phi \cdot 10^{-17}\frac{quants.}{sm^2}: 1\text{-}0;\ 2\text{-}1{,}9;\ 3\text{-}3{,}8;\ 4\text{-}9{,}5.$$

The main radiation defects that formed during irradiation of n-Si were A-centers (a complex of vacancies and an inter-atomic oxygen atom).

As shown in Fig. 1 (curves 2-4), the dependence $\frac{\rho_P}{\rho_0} = f(P)$ after $\gamma-$ irradiation is significant changing as quantitatively and as qualitatively, when A-centers with a compensating deep level $E_C - 0{,}17eB$ are formed in n-Si single crystals [14]. For unirradiated n-Si single crystals (without deep levels in the band gap), the presence of tensoresistance at the uniaxial pressure along the crystallographic direction [100] is due to the deformation redistribution of electrons between the four valleys with higher mobility $\mu_\perp$, which rise upwards, and two valleys with less mobility $\mu_\parallel$ that are lowered downwards, on the energy scale at the deformation [15].

This initially leads to an increase in the resistivity with the subsequent exit to saturation, when the redistribution of electrons between valleys at high pressures is completed (Fig. 1, curve 1). In the given conditions, for the $\gamma-$ irradiated n-Si single crystals (Fig. 1, curves 2-4), the course of the dependencies $\frac{\rho_P}{\rho_0} = f(P)$ can be explained by the presence of two mechanisms of change the resistivity with pressure [13]: 1) by the deformational redistribution of charge carriers between the valleys, which shifted on a scale of energies in opposite directions, as a result of which the resistivity increases; 2) by an increase in the total concentration of electrons in the C-zone due to the reduction of the energy of ionization of the deep level of

the A-center, which leads to a decrease in the resistivity when the magnitude of the uniaxial pressure increases.

In the case of an isoenergy surface, which is an ellipsoid of rotation, the mobility of charge carriers for an arbitrary crystallographic direction is determined from the ratio [11]:

$$\mu = \mu_\perp \sin^2 \theta + \mu_\| \cos^2 \theta, \qquad (1)$$

where θ - the angle between the considered direction and the main axis of the ellipsoid; $\mu_\perp$ and $\mu_\|$ - the mobility of current carriers across and along the axis of the ellipsoid.

For n-Si at the deformation along the crystallographic direction [100], the ellipsoids are located on mutually perpendicular to the axes, therefore, taking (1) into account, we obtain:

$$\mu_1 = \mu_\| \ , \mu_2 = \mu_\perp . \qquad (2)$$

Then the electrical conductivity for a $n - Si$ single crystal in such conditions is:

$$\sigma_P = \frac{1}{\rho_P} = 2en_1(P)\mu_\| + 4en_2(P)\mu_\perp, \qquad (3)$$

$n_1(P)-$ concentration of electrons in valleys, which lowered downwards, and $n_2(P)-$ in the valleys, which rise on the scale of energy at the deformation.The total concentration of electrons in the conduction band n-Si and the ratio between the charge carrier concentrations in the valleys can be written as follows:

$$2n_1(P) + 4n_2(P) = n(P), \qquad \frac{n_2(P)}{n_1(P)} = e^{-\frac{\Delta E}{kT}} = A, \qquad (4)$$

where $\Delta E = \dfrac{\Xi_u P}{C_{11} - C_{12}} -$ the energy gap that occurs between two valleys that are lowered and the four that rise at the deformation, Ξ_u - displacement constant of the deformation potential, C_{11} and C_{12} - elastic constants [15].

Then (3), considering (4), will be:

$$\sigma_P = \frac{1}{\rho_P} = \frac{en(P)\mu_\|}{2A+1} + \frac{2eAn(P)\mu_\perp}{2A+1} \qquad (5)$$

For unirradiated n-Si single crystals, the electron concentration doesn't depend on the magnitude of the uniaxial pressure P, so $2n_1(P) + 4n_2(P) = N_D = const$. $N_D -$ concentration of the shallow impurity phosphorus in the studied single crystals.

Components of mobility $\mu_\|$ and $\mu_\perp$ for the electrons on the basis of the theory of anisotropic scattering on acoustic phonons and impurity ions have the form [16]:

$$\mu_\| = \frac{e}{m_\|}\langle \tau_\| \rangle = \frac{4ea_\|}{3\sqrt{\pi k}m_\| T^{\frac{3}{2}}} \int_0^\infty \frac{x^3 e^{-x}dx}{x^2 + b_0}, \ \mu_\perp = \frac{e}{m_\perp}\langle \tau_\perp \rangle = \frac{4ea_\perp}{3\sqrt{\pi k}m_\perp T^{\frac{3}{2}}} \int_0^\infty \frac{x^3 e^{-x}dx}{x^2 + b_1}, \qquad (6)$$

where
$$a_{\parallel} = \frac{\pi c_{11}\hbar^4}{k\Xi_d^2\sqrt{2m_{\parallel}m_{\perp}^2}} \cdot \frac{1}{\Phi_{0a}}, \quad a_{\perp} = \frac{\pi c_{11}\hbar^4}{k\Xi_d^2\sqrt{2m_{\parallel}m_{\perp}^2}} \cdot \frac{1}{\Phi_{1a}}, \tag{7}$$

$$\Phi_{0a} = 1 + 1{,}645\frac{\Xi_u}{\Xi_d} + 1{,}03\frac{\Xi_u^2}{\Xi_d^2}, \quad \Phi_{1a} = 1 + 0{,}818\frac{\Xi_u}{\Xi_d} + 0{,}688\frac{\Xi_u^2}{\Xi_d^2}. \tag{8}$$

$$b_0 = \frac{a_{\parallel}\Phi_{0i}}{\sqrt{k}T^{\frac{3}{2}}\tau_{0i}(kT)}, \quad b_1 = \frac{a_{\perp}\Phi_{1i}}{\sqrt{k}T^{\frac{3}{2}}\tau_{0i}(kT)}. \tag{9}$$

$$\tau_{0i}(kT) = \frac{\sqrt{2}m_{\perp}\varepsilon_0^2(kT)^{\frac{3}{2}}}{\pi N e^4\sqrt{m_{\parallel}}}, \tag{10}$$

where $N-$ concentration of impurity ions, $n-$ concentration of screening charge carriers (electrons), $\varepsilon_0 -$ dielectric permeability, Ξ_u and $\Xi_d -$ constants of deformation potential, $e-$ electron charge.

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

$$\Phi_{1i} = \frac{3}{4\beta^3}[((1-\beta^2)a - \beta)\ln\gamma^2 + 2(\beta^2-1)L(a) - 2\beta^2 a - (\beta^2-1)a\ln(1+\beta^2) + \tag{11}$$

$$+ \frac{\gamma^2}{2}(\beta(1+3\beta^2) + a(3\beta^4 + 2\beta^2 - 1))],$$

where $\beta^2 = \dfrac{m_{\parallel} - m_{\perp}}{m_{\perp}}$, $a = arctg\beta$, $L(a) = -\int\limits_0^a \ln\cos\varphi\, d\varphi -$ function of Lobachevsky,

$\gamma^2 = \dfrac{\pi\hbar^2 e^2}{2m_{\parallel}\varepsilon_0 k^2} \cdot \dfrac{n}{T^2 x}$, $x = \dfrac{E}{kT}$.

Taking into account expressions (7) and (10), expressions (9) can be written as follows:

$$b_0 = \frac{NB\Phi_{0i}}{\Xi_d^2\Phi_{0a}}, \quad b_1 = \frac{NB\Phi_{1i}}{\Xi_d^2\Phi_{1a}}, \tag{12}$$

where $B = \dfrac{\pi^2 c_{11}\hbar^4 e^4}{2k_Б^3 m_{\perp}^2 T^3\varepsilon_0^2}$.

Then expression (5) for the electrical conductivity of the deformed single crystal $n-Si$

$$\sigma_P = \frac{1}{\rho_P} = \frac{4e^2 n}{3\sqrt{\pi k}m_{\parallel}T^{\frac{3}{2}}(2A+1)}\left[\frac{a_{\parallel}}{m_{\parallel}}\int\limits_0^\infty \frac{x^3 e^{-x}dx}{x^2 + \frac{NB\Phi_{0i}}{\Xi_d^2\Phi_{0a}}} + \frac{2Aa_{\perp}}{m_{\perp}}\int\limits_0^\infty \frac{x^3 e^{-x}dx}{x^2 + \frac{NB\Phi_{1i}}{\Xi_d^2\Phi_{1a}}}\right] \tag{13}$$

For such semiconductors as silicon and germanium, in addition to the anisotropy of effective masses, the anisotropy of relaxation times is also characteristic. A rather detailed theoretical analysis, which was made by Harring in [17], showed that the use of scalar relaxation time can only be used in the first approximation to describe the scattering mechanisms on the neutral impurities and optical phonons. In the case of scattering on the acoustic phonons and especially on the impurity ions, the approach of the scalar time of relaxation is not applicable. In this case, it is necessary to take into account its anisotropy. In general, the degree of scattering anisotropy characterizes the parameter of the anisotropy of the mobility of charge carriers [16]

$$K = \frac{\mu_\perp}{\mu_\parallel} = \frac{K_m}{K_\tau}, \tag{14}$$

where K_m − parameter of anisotropy of effective masses (for silicon $K_m = \frac{m_\parallel}{m_\perp} = 4{,}81$), $K_\tau = \frac{\langle \tau_\parallel \rangle}{\langle \tau_\perp \rangle}$ −

parameter of anisotropy of relaxation times.

According to the expression (6),

$$K = \frac{a_\perp}{a_\parallel} K_m \frac{\displaystyle\int_0^\infty \frac{x^3 e^{-x} dx}{x^2 + \frac{NB\Phi_{1i}}{\Xi_d^2 \Phi_{1a}}}}{\displaystyle\int_0^\infty \frac{x^3 e^{-x} dx}{x^2 + \frac{NB\Phi_{0i}}{\Xi_d^2 \Phi_{0a}}}}. \tag{15}$$

Taking into account the value of elastic constants $C_{11} = 1{,}674 \cdot 10^{11} Pa$ and $C_{12} = 0{,}649 \cdot 10^{11} Pa$, component of the tensor of effective masses $m_\parallel = 0{,}916 m_0$ and $m_\perp = 0{,}19 m_0$ [16], the constants of deformation potential $\Xi_u = 9{,}23\ eV$ and $\Xi_d = -2{,}12\ eV$ [18] and experimental results of measurements of the tensoresistance (Fig. 1), the concentration of electrons in uniaxially deformed (gamma-irradiated) n-Si single crystals has been determined on the basis of solutions of equation (12). It allowed to obtain the dependence of the parameter of mobility anisotropy on the uniaxial pressure on the basis of expression (15) (Fig. 2).
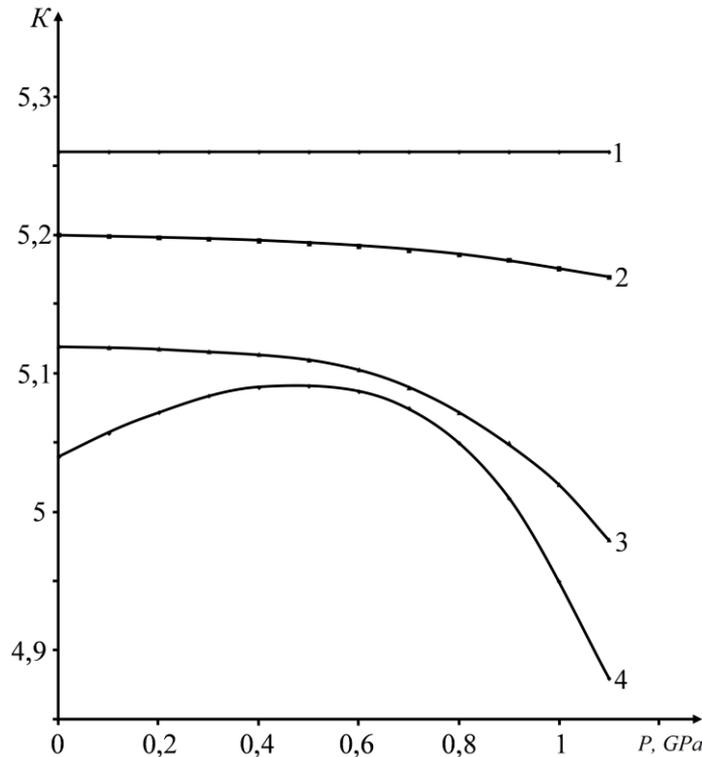
Fig.2. The dependence of the parameter of mobility anisotropy $K = f(P)$ at $T = 77\,K$ for the uniaxially deformed along the crystallographic direction [100] of n-Si single crystals, irradiated by $\gamma-$quants of different doses $\Phi \cdot 10^{-17} \dfrac{quants.}{sm^2}$: 1-0; 2-1,9; 3-3,8; 4-9,5.

As can be seen from Fig. 2, the parameter of mobility anisotropy for undeformed n-Si single crystals decreases with increasing dose of the $\gamma-$irradiation, which can be explained by the growth of the role of impurity scattering (by reducing the effect of screening) and the scattering efficiency on the fluctuation potential, which leads to the appearance of gradients of resistivity with increasing of degree of the compensation of irradiated samples [14]. Also, with the increase in the screening radius, along with the scattering of electrons on single ions, it is necessary to take into account scattering on the ion clusters in the form of impurity complexes, which consist of several ions of the impurity [16]. Since the probability of electron scattering is proportional to the square of the charge of the scattering center, that the presence of such complex defects in the volume of the semiconductor can make a significant contribution to the scattering of charge carriers and influence the magnitude of the parameter of mobility anisotropy. For unirradiated n-Si single crystals (Fig. 2, curve 1), the parameter of mobility anisotropy does not depend on uniaxial pressure, since the concentration of ionized shallow impurities of phosphorus in these conditions is constant and does not depend on deformation. The growth of the electron concentration for $\gamma-$irradiated n-Si single crystals with an increase of magnitude of the uniaxial pressure leads to a change in the relative contribution of the scattering mechanisms under consideration and, accordingly, explain the peculiarities of the obtained dependencies (Fig. 2, curves 2-4).

Conclusions

The creation of radiation defects in n-Si single crystals by means of the $\gamma-$irradiated significantly affects their tensoelectric properties. The magnitude of the tensoresistance of n-Si single crystals after irradiation will depend on the nature of the deformation rearrangement of the structure of the conduction band of silicon and the change in the electron concentration due to the ionization of a deep level of the A-center at the

uniaxial pressure. Reducing the degree of filling deep levels of $\gamma-$radiation defects belonging to the A–centers, with increasing the magnitude of the uniaxial pressure, reduces the effect of screening. This, in turn, affects the change in the relative contribution of various scattering mechanisms that will determine the electrical and tensoelectric properties of $\gamma-$irradiated n-Si single crystals. The obtained results should be taken into account when designing n-Si pressure sensors or stressed nanostructures (Si quantum dots, SiGe heterostructures) that will function in fields of high radiation.

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