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Investigation of Changes in Resistivity of n-Si with Temperature and Uniaxial Stress

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In this work the changes in resistivity of n-Si with temperature and uniaxial stress X , oriented both in $\langle 100 \rangle$ and in $[111]$ direction, were investigated. The value of the anisotropy parameter of mobility was obtained in the conditions of $\vec{J} \parallel \vec{X} \parallel [100]$ and $\vec{J} \perp \vec{X} \parallel [100]$ with using the experimental data concerning longitudinal and transverse tensor-resistance. The presence of the n-Si tensor-resistance was found in the conditions of $\vec{X} \parallel \vec{J} \parallel [111]$, i.e., in the absence of the interminimum redistribution of charge carriers. The physical explanation of the results was presented.

Keywords: silicon, resistivity, uniaxial elastic deformation, tensor-resistance, anisotropy parameter of mobility.

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Introduction

More than half a century the silicon and germanium remain the basic materials for the production of the widest class of the electronic devices in semiconductor electronics [1, 2]. Devices made on their basis are used both in research, and in industry [3-5]. The hard requirements in the engineering area concerning reliability in the work of semiconductor devices and their resistance to the various physical-active external influences encourage of researchers to use the methods which give the most accurate and unambiguous results in determining the basic parameters of the materials in a wide intervals of changing of the external condition [6, 7]. Application to the crystals the directed elastic deformation effects, that change both the interatomic distance, and the lattice symmetry, results in the significant changes of electronic subsystem in many-valley semiconductors [8, 9]. Therefore the study of tensor-effects in semiconductor crystals of high symmetry is important both in scientific, and in applied aspects [10, 11]. The significant informativity of such method allows studying the peculiarities of the band structure of many-valley semiconductors and defining its parameters and magnitudes that characterize the mechanisms of scattering of charge carriers, with high degree of certainty [9, 12, 13].

The deformation of semiconductor is the reason of appearance a number of effects caused by the interaction of electrons with the crystal lattice. The shift of the

energy levels of the semiconductor under the influence of deformation and the resulting change in the energy spectrum of the charge carriers, which causes a change in the electrical characteristics of the material, are the physical basis of the deformation effects [14]. In homogeneous semiconductors the displacement of energy levels leads to the dependence of resistivity on deformation, i.e., the tensor resistive effect appears, or the effect of tensor resistance. The uniaxial elastic deformation removes the degeneracy on energy of the equivalent minima in Ge and Si of n-type conductivity. The interminimum redistribution of electrons, which arising at this, leads to the change in resistivity, since the mobility of charge carriers in the isoenergetic ellipsoids of these crystals is the strongly anisotropic [8, 14].

All studies of tensor resistance can be conditionally divided into two groups: in linear and nonlinear approximations comparatively deformation. In the first case, the measurements are performed in the field of small deformations (which satisfy to condition of $\Xi_u \cdot u \ll kT$, where Ξ_u is the constant of deformation potential, $u = X / C^*$ is the deformation, C^* is the elastic constant), and their results are used to determine the numerical values of the coefficients of tensor-resistance. In the second case the change in electrical conduction of crystals is investigated at large deformations, when the energy gap $\Delta E \sim \Xi_u \cdot u$ between ascending and descending valleys is comparable with kT ($\Xi_u \cdot u \gg kT$). Therefore in many-valley semiconductors the nonlinear effects relatively deformation are beginning

to emerge. This, naturally, is reflected on the dependencies of changes in resistivity r_X/r_0 from the mechanical load X [$r_X/r_0=f(X)$], by which the mechanisms of the observed phenomena are identified.

The shortage of studies of effects that are linear with respect to the deformation consists in the shortage of information at explaining of the experimental results, especially in case, when the several mechanisms of tenso-effects are simultaneously appeared. In the linear theory of the tenso-resistance effects we usually do not take into account the change in the effective mass of the charge carriers in the conduction band due to the smallness of the interaction effect between the conduction and valence bands, since the forbidden band in these materials has a large width. In addition, as a rule, we also neglect the effects of intervalley scattering of charge carriers; it is believed that under conventional conditions at $T < 100$ K the intervalley scattering makes a negligible contribution into the relaxation time of the conduction electrons that determines the electrical conduction of crystals. However at higher temperatures ($T > 100$ K) in the nondegenerate n-Si crystals the intervalley scattering begins to appear both in the temperature dependence of mobility, and in tenso-resistance, since the deformation (under defined placements of the deformation axis relative to the crystal axes) can significantly change or completely exclude the transitions between the respective valleys [15, 16]. Thus, both effects will be manifested in the field of strong deformations.

To increase the amount of information that can be obtained about the properties of studied many-valley semiconductor in the field of strong deformations, the experimental measurements of longitudinal tenso-resistance (in condition of $\vec{J} \parallel \vec{X}$, where J is the current) it is desirable to supplement by the measurements of transversal tenso-resistance, despite the fact that in practice the study of tenso-effects at $\vec{J} \perp \vec{X}$ associated with the significant complexities. In addition to the data required for the calculation of the constant of deformation potential Ξ_u , such studies also provide the experimental data for the calculation of the anisotropy parameter of mobility K .

The aim of this study was to establish the laws of resistivity changes in n-Si single crystals depending on the mechanical load under the orientation of the current in the sample both along, and perpendicular to the axis of deformation, as well as depending on the temperature (both in absence of mechanical load, and at its application along different crystallographic directions).

I. Longitudinal tenso-resistance. Theoretical information

Let us consider the change of the n-Si resistivity under conditions of the directional compression at $\vec{X} \parallel \vec{J} \parallel [100]$. In the absence of mechanical stress (at $X=0$), the conductivity of the crystal is given by:

$$S_0 = 2n_0 e m_{\parallel} + 4n_0 e m_{\perp}, \quad (1)$$

or

$$S_0 = 2n_0 e m_{\parallel} (1+2K), \quad (2)$$

where n_0 is the concentration of electrons in the one minimum of undeformed crystal (at $X=0$), and m_{\parallel} and m_{\perp} are the mobilities of charge carriers along and across the long axis of the isoenergetic ellipsoid, respectively, e is the electron charge, $K = m_{\perp} / m_{\parallel}$ is the anisotropy parameter of mobility.

When application in silicon the mechanical stress along the crystallographic direction [100], two minima ([100] and [$\bar{1}00$]), disposed in this direction, will fall on the energy scale down, and the four remaining minima ([010], [0 $\bar{1}0$], [001], [00 $\bar{1}$]) will rise up, and that will lead to the redistribution of charge carriers between the minima. In this case, the conductivity of the deformed crystal will be the following

$$S_X = 2n_1 e m_{\parallel} + 4n_2 e m_{\perp}, \quad (3)$$

where n_1 and n_2 are the concentrations of electrons in the descending minimum and in the minimum, which rises on the scale of energy under the influence of uniaxial elastic deformation, respectively.

It should be noted that in the non-degenerate n-Si crystals the change of resistivity with increasing of the mechanical stress X (when $\vec{X} \parallel \vec{J} \parallel [100]$) was due to the fact that the carriers, moving from the ascending valleys into descending valleys, reduce their mobility from the m_{\perp} to m_{\parallel} .

When the charge carriers in samples are described by the Maxwell-Boltzmann statistics, the ratio n_2/n_1 can be represented as follows:

$$\frac{n_2}{n_1} = \exp\left(-\frac{\Delta E}{kT}\right) = C, \quad (4)$$

where ΔE is the energy gap between the energy minima in the deformed crystal, which is determined by the ratio

$$\Delta E = \Xi_u (S_{11} - S_{12}) X, \quad (5)$$

where S_{11} and S_{12} are the rigidity constants.

From the constancy of the total concentration of electrons in the conduction band (c-band), we obtain

$$2n_1 + 4n_2 = 6n_0, \quad (6)$$

and with using Eq. (4) we find

$$n_1 = \frac{3n_0}{1+2C}, \quad n_2 = \frac{3n_0 C}{1+2C}. \quad (7)$$

On the basis of Eqs. (7) and (3), we can write in the general form

$$S_X = 6n_0 e m_{\parallel} \frac{(1+2CK)}{(1+2C)} \quad (8)$$

or we obtain tenso-resistance of n-Si, which appears under directional compression at $\vec{X} \parallel \vec{J} \parallel [100]$ and is described by the relation:

$$r_X = r_0 \frac{(1+2K)(1+2C)}{3(1+2CK)}, \quad (9)$$

where r_0 is the resistivity of undeformed crystal.

However, since under these conditions at a sufficiently high deformation all electrons will move into two valleys, the conductivity will be determined as follows:

$$s_{\infty} = 6n_0 e m_{\parallel}. \quad (10)$$

Substituting (10) into (8), we obtain the connection between r_X and r_{∞} :

$$r_X = r_{\infty} \frac{1+2C}{1+2CK}, \quad (11)$$

where $r_{\infty} = \lim_{X \rightarrow \infty} r(X)$ is the value of resistivity with deformation X , which provides a complete migration of charge carriers into the energy minima, that located in the direction of the axis of strain.

Thus, in the case of n-Si, we can calculate the resistivity of the crystal for any value of X , using the measured values r_0 or r_{∞} with known values of K and C , based on Eqs. (9) and (11). Furthermore, knowing the relationship r_{∞}/r_0 , we also can get from Eq. (11) the anisotropy parameter of mobility K (at $X=0$, $C=1$):

$$\frac{r_{\infty}}{r_0} = \frac{1+2K}{3}. \quad (12)$$

From Eq. (12) for n-Si under conditions of $\vec{X} \parallel \vec{J} \parallel [100]$, we will obtain the following relation

$$K \frac{\vec{r}}{J} \frac{\vec{r}}{X} \parallel [100] = \frac{3}{2} \frac{r_{\infty}}{r_0} - \frac{1}{2}, \quad (13)$$

Considering (by analogy with n-Si) the change in resistivity of n-Ge depending on the applied mechanical stress X where $\vec{X} \parallel \vec{J} \parallel [111]$, we can obtain the equation similar to Eq. (13), but for germanium crystals:

$$K \frac{\vec{r}}{J} \frac{\vec{r}}{X} \parallel [111] = \frac{3}{2} \frac{r_{\infty}}{r_0} - \frac{1}{2}, \quad (14)$$

The obtained relationships (13) and (14) for n-Si and n-Ge are similar in appearance, but differ in the fact that

in case of n-Si $\frac{r_{\infty}}{r_0} \equiv \frac{r_{\infty}^{[100]}}{r_0}$, and for n-Ge

$$\frac{r_{\infty}}{r_0} \equiv \frac{r_{\infty}^{[111]}}{r_0}.$$

Equations (13) and (14) allow to determine with high accuracy the anisotropy parameters of mobility on basis of measurements only longitudinal tenso-resistance, but at condition of the full migration of electrons into the minimum(ma), which is (are) descended under deformation. Furthermore, these equations give the possibility to reliably determine the anisotropy parameter of scattering $K_t = \langle t_{\parallel} \rangle / \langle t_{\perp} \rangle$ (energy averaging was denoted by broken brackets), because,

$$K = \frac{m_{\perp}}{m_{\parallel}} = \frac{K_m}{K_t} = \frac{m_{\parallel}}{m_{\perp}} \frac{\langle t_{\perp} \rangle}{\langle t_{\parallel} \rangle}, \quad \text{where } K_m = m_{\parallel} / m_{\perp} \text{ is}$$

the anisotropy parameter of effective mass; m_{\parallel} and m_{\perp} are the cyclotron effective masses of charge carriers along and across the long axis of isoenergetic ellipsoid,

respectively; t_{\parallel} and t_{\perp} are the components of the relaxation time tensor in the absence of a magnetic field in the linear approximation, respectively.

It should be noted, however, that the reasonable use of Eqs. (13) and (14) is possible only if some values is not significantly change with deformation (such as: the energy spectrum of electrons, the phonon spectrum of lattice vibrations; the constants of deformation potential Ξ_u), and the deformative redistribution of electrons between the valleys (while maintaining its overall concentration in the conduction band: $4n_0 = const$ in the case of n-Ge and $6n_0 = const$ for n-Si) has the determining role in the forming of tenso-resistance effect.

The dependence on the deformation of the probability of f-transitions between the valleys located on mutually perpendicular axes is one of the factors that violates these conditions in the case of n-Si (this factor changes the relative contribution between the individual mechanisms of tenso-resistance under deformation) (Fig. 1). That is why, for the reliable determination of the anisotropy parameter of mobility $K = m_{\perp} / m_{\parallel}$, in n-Si at $T > 100$ K (when the intervalley scattering becomes significant) we must experimentally study not only the longitudinal tenso-resistance r_X^{\parallel} / r_0 (at $\vec{J} \parallel \vec{X}$), but also to carry out the measurements of transversal tenso-resistance r_X^{\perp} / r_0 (at $\vec{J} \perp \vec{X}$). Such measurements allow expanding the information about properties of the investigated many-valley semiconductors. This, for example, is manifested in the experiments with silicon crystals with impurity concentrations of $N_d > 10^{15} \text{ cm}^{-3}$, when in the low temperature range the deformation dependence of the degree of ionization of impurity centers becomes apparent and also, as noted, in the temperature region, when the intervalley scattering becomes significant.

It should be noted that in the study of the effect of transversal tensoresistance the physical picture of phenomenon is the same as that in the study of longitudinal tensoresistance. The uniaxial elastic deformation, changing of the crystal lattice symmetry,

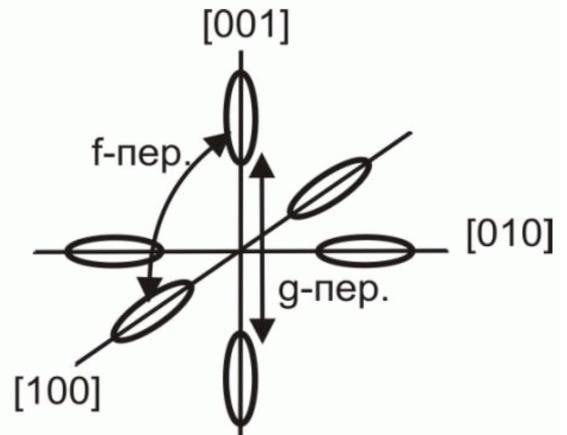


Fig. 1. Intervalley scattering of electrons in the n-Si [16].

leads to the removal of degeneracy on energy of the equivalent minima. According to [14], for n-Si under application of the mechanical stress X in conditions of $\vec{J} \perp \vec{X} \parallel [100]$, we obtain the expression for calculating the anisotropy parameter of mobility:

$$K \frac{\mathbf{r}}{J \perp \vec{X} \parallel [100]} = \frac{1}{3 \frac{r_{\infty}}{r_0} - 2} = \left(3 \frac{r_{\infty}}{r_0} - 2 \right)^{-1}, \quad (15)$$

II. Results and discussion

In the study of changes in resistivity of many-valley semiconductors such as n-Si and n-Ge under the influence of directional (uniaxial) pressure usually it was used the assumption that such pressure only shifts the isoenergetic ellipsoids in the energy scale without changing appreciably their shape [14]. Given the importance of this assumption, the aim of this work was the need to obtain additional evidence of its acceptability within the bounds of experiments, which were conducted specifically for this. Thus, we would have one more reason to believe that the named above assumption corresponds to the realities and the appearance of any doubts would be inappropriate at the practical use of this assumption.

Such verification can be realized by selecting some concrete (important in the cognitive sense) parameter that is used to describe the various (or related) physical phenomena and the correlation between them. The anisotropy parameter of mobility K in many-valley semiconductors was chosen as such parameter. The parameter K can be calculated from the results of experiments on tenso-resistance using different equations, namely: (13) and (15) (in the case of n-Si). Eq. (13) is used for treatment of measurement results of tenso-resistance in n-Si under conditions of $\vec{J} \parallel \vec{X} \parallel [100]$. Eq. (15) is suitable for treatment of the results obtained also in the study of tenso-resistance in n-Si, but in conditions that meet the mutually perpendicular arrangement of the vectors of current \vec{J} and mechanical stress \vec{X} , i.e., when $\vec{J} \perp \vec{X} \parallel [100]$.

Fig. 2 shows a typical shape and dimensions of samples for research of tenso-effects along and across of the deforming force axis.

In this paper, the necessary measurements were performed at $T = 77.4$ K on n-Si crystals with resistivity of $r_{300K} \cong 100$ Ohm·cm, and the results of these measurements are shown by corresponding curves in Fig. 3.

The utilization of the experimentally obtained results in the field of saturation on the investigated dependencies (Fig. 3) provide the obtaining of the data concerning the anisotropy parameter of mobility K in accordance with Eq. (13) and curve 1

$$K \frac{\mathbf{r}}{J \parallel \vec{X} \parallel [100]} = \frac{3 r_{\infty}}{2 r_0} - \frac{1}{2} \cong 5.8; \quad (16)$$

and in accordance with Eq. (15) and curve 2 of the same

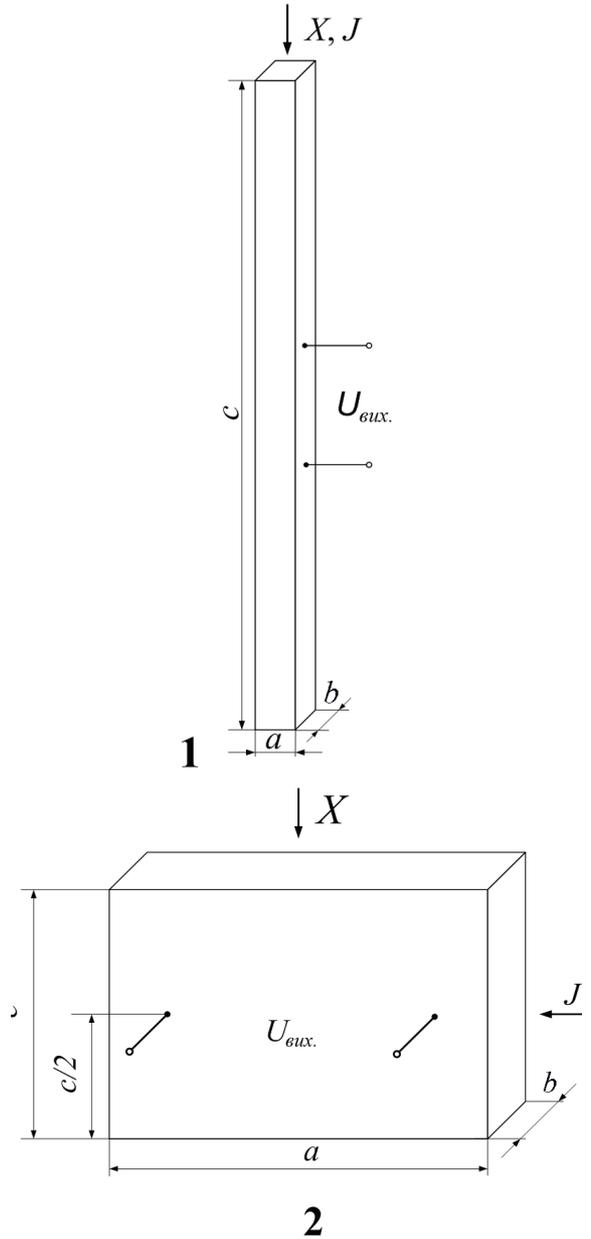


Fig. 2. A typical form of the samples and their sizes ($a \times b \times c$) for measurements of the longitudinal and transverse tenso-resistance: 1 – $\vec{J} \parallel \vec{X}$ ($0.7 \times 0.5 \times 10$ mm); 2 – $\vec{J} \perp \vec{X}$ ($2.2 \times 0.5 \times 2.0$ mm).

figure

$$K \frac{\mathbf{r}}{J \perp \vec{X} \parallel [100]} = \left(3 \frac{r_{\infty}^{\perp}}{r_0} - 2 \right)^{-1} \cong 5.3, \quad (17)$$

Thus, the results obtained for the n-Si by passing a current along the deformation direction [100] and perpendicular to it were quite close to each other, so that we can consider them as approximate to coincident (taking into account the accuracy of experiments). From this it follows directly that the equations, intended for the obtaining of values of the anisotropy parameter of mobility K , in both cases discussed above adequately describe the change of resistivity in many-valley semiconductor under the influence of the directional (uniaxial) pressure. Therefore, the isoenergetic ellipsoids

in many-valley semiconductors only are shifted in the energy scale, meanwhile do not practically change their shape (or little change).

The many-valley n-Si ⟨P⟩ ($r_{300K} \cong 0.02$ Ohm·cm) behaves somewhat differently at its deformation under the conditions of a possible manifestation of the shear deformation that occurs at $\vec{J} \parallel \vec{X} \parallel [111]$ (i.e., in the condition of symmetrical arrangement of the deformation axis with respect to all isoenergetic ellipsoids when the interminimum redistribution of charge carriers is absent).

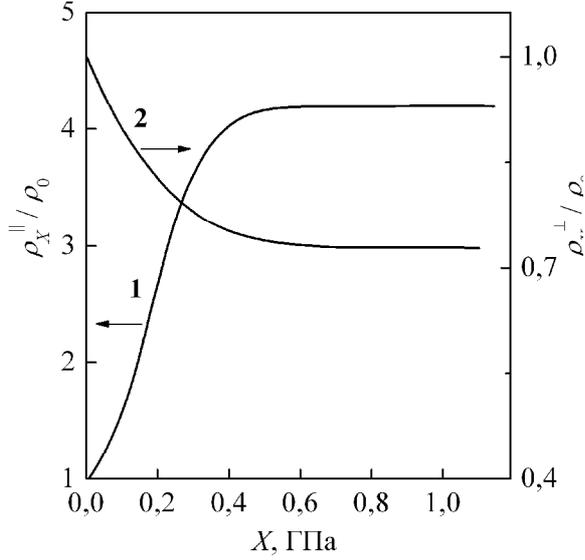


Fig. 3. Dependencies $r_{X}^{\parallel} / r_0 = f(X)$ and $r_{X}^{\perp} / r_0 = f(X)$ for n-Si ($r_{300K} \cong 100$ Ohm·cm) at $T = 77.4$ K and $\vec{X} \parallel [100]$: 1 – $\vec{J} \parallel \vec{X}$; 2 – $\vec{J} \perp \vec{X}$.

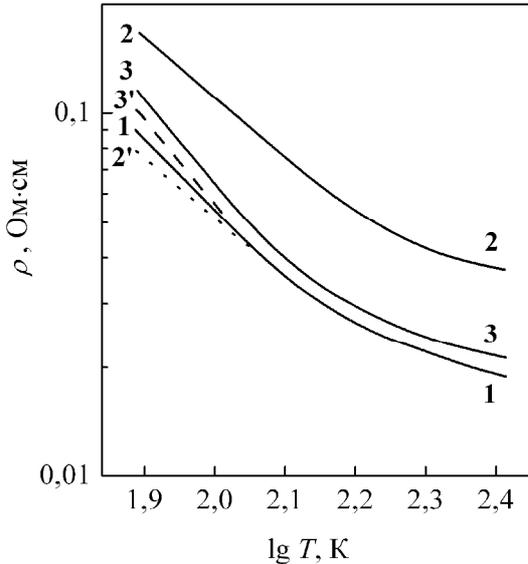


Fig. 4. Dependencies $r = f(\lg T)$ in double logarithmic scale for low-resistance n-Si ⟨P⟩ ($n_e \approx 3.44 \cdot 10^{17} \text{ cm}^{-3}$): 1 – $X = 0$; 2 – $\vec{J} \parallel \vec{X} \parallel [001]$ and 3 – $\vec{J} \parallel \vec{X} \parallel [111]$ at $X = 1.2$ GPa. Dashed lines 2' and 3' correspond to the parallel shift of the curves 2 and 3, respectively.

It is characteristic that in the latter case, as shown in Fig. 4, the temperature changes $r = f(T)$ in the undeformed and uniaxially elastically deformed crystals along different crystallographic directions were significantly different, as you might expect. Moreover, as shown in Fig. 4, the mentioned differences were particularly noticeable in the field of the predominantly impurity scattering (i.e., at low temperatures). In this temperature range at $\vec{J} \parallel \vec{X} \parallel [111]$, despite the absence of interminimum redistribution of charge carriers, the presence of the resistivity changes in the n-Si crystals was revealed.

Fig. 4 shows that the slope of resistivity increase with decreasing of T at liquid nitrogen temperature in the undeformed crystal (curve 1) is significantly higher than in the deformed crystal at $\vec{J} \parallel \vec{X} \parallel [001]$ (curves 2 and 2' of the same figure). The increase of slope $r = f(T)$, which is observed under deformation of n-Si along the [111] direction (Fig. 4, curves 3 and 3') compared with the undeformed crystal (curve 1), indicates that in the case of $\vec{X} \parallel [111]$ the energy gap between the bottom of the conduction band and the level of impurity occurrence is not reduced with increasing X (as was in the case of $\vec{X} \parallel [001]$), but growing.

The ionization energy of the phosphorus impurity in the n-Si (~ 0.045 eV) is about 4 times higher than in n-Ge (~ 0.012 eV). Therefore, other conditions being equal, the complete "depletion" of donor centers (in this case, the impurity phosphorus atoms) in moderately and heavily doped n-Si crystals (but not degenerate), unlike the n-Ge, even at room temperature is not reached (not to mention the lower T). Thus, the study of the resistivity changes in these experiments was conducted under conditions of incomplete "depletion" of the impurity centers. This led (at $T = const$) to the appearance of the specific tenso-resistance effect associated with the deformative "freezing-out" of charge carriers from the conduction band. The resulting effect is not related with interminimum redistribution of charge carriers, which can not be in n-Si at $\vec{X} \parallel [111]$, in principle.

It should be noted that the following experimental fact is one more proof of authenticity of data, which are obtained at $\vec{J} \perp \vec{X}$, but (in contrast to the experiments described above) in the absence of interminimum redistribution of charge carriers. The tenso-resistance value of n-Si samples deformed in the direction of [111], which is symmetrical with respect to all isoenergetic ellipsoids, is practically independent on measuring of resistivity r along or across the deformation axes (Fig. 5). This fact is also true, when in the latter case we conduct the research not in one, but in two mutually perpendicular directions of the electric current passing through the sample.

These experiments were performed at $T = 4.2$ K in the heavily doped n-Si ⟨As⟩ crystals ($r_{300K} \cong 0.43 \cdot 10^{-2}$ Ohm·cm, $n_{e300K} \approx 1.07 \cdot 10^{17} \text{ cm}^{-3}$) grown in the crystallographic direction ⟨111⟩ by the Czochralski method. Samples were cut in the same direction with an accuracy of the orientation deducing not worse of 15' by the conventional X-ray method. Tenso-resistance

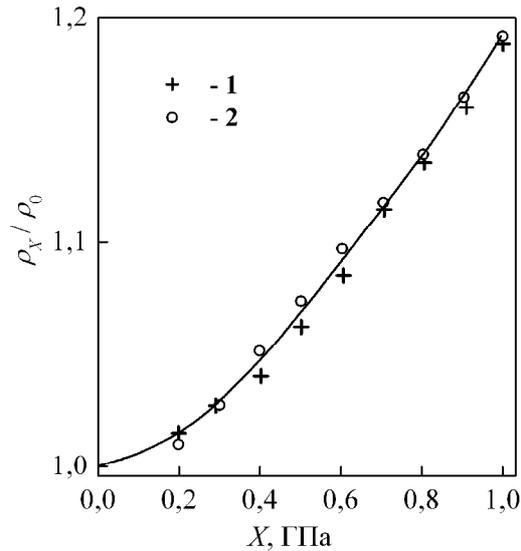


Fig. 5. Tensio-resistance of heavily doped n-Si ($r_{300K} \cong 0.43 \cdot 10^{-2}$ Ohm·cm) at liquid helium temperature under the conditions: 1 (+) – $J \parallel X \parallel [111]$; 2 (o) – $J \perp X \parallel [111]$.

measurements were performed under passing a current both along the deforming load X , and perpendicular to it, that is, in conditions $J \parallel X \parallel [111]$ and $J \perp X \parallel [111]$. It was also revealed that under low-temperature measurements the resolving power of the measurement results of the effect of relative increasing of resistivity for low-resistance n-Si crystals is raised in the conditions of the application of mechanical stress at $X \parallel [111]$.

Conclusions

1. The changes in resistivity of the n-Si single crystals ($r_{300K} \cong 100$ Ohm·cm) were experimentally investigated both at $J \parallel X \parallel [100]$, and at condition when the current in the sample was oriented perpendicularly to the deformation axis, i.e., at $J \perp X \parallel [100]$. The values obtained for the anisotropy parameter of mobility when the current passes along the direction of deformation ($K_{J \parallel X \parallel [100]}^{\mathbf{r}} \cong 5.8$) and perpendicular to it ($K_{J \perp X \parallel [100]}^{\mathbf{r}} \cong 5.3$) proved to be close to each other.

2. In n-Si (P) crystals ($r_{300K} \cong 0.02$ Ohm·cm) the dependencies of resistivity on the temperature $r = f(T)$ were investigated both under condition $X = 0$, and under $J \parallel X \parallel [001]$ and $J \parallel X \parallel [111]$ (where $X = 1.2$ GPa), and the differences between these dependencies were identified in the region of predominantly impurity scattering (at low temperatures from the using range). The presence of tensio-resistance in n-Si under symmetrical arrangement of the deformation axis with respect to all isoenergetic ellipsoids was revealed, when the interminimum redistribution of charge carriers is absent, in principle.

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Г.П. Гайдар

Дослідження змін питомого опору n-Si з температурою і направленим тиском

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У роботі досліджено зміни питомого опору кристалів n-Si з температурою і направленим тиском X , орієнтованим як у напрямку $\langle 100 \rangle$, так і в напрямку $[111]$. За експериментальними даними поздовжнього і поперечного тензоопору одержано значення параметра анізотропії рухливості для умов $\overset{\uparrow}{J} \parallel \overset{\uparrow}{X} \parallel [100]$ та $\overset{\uparrow}{J} \perp \overset{\uparrow}{X} \parallel [100]$. Виявлено наявність тензоопору в n-Si за умов $\overset{\uparrow}{X} \parallel \overset{\uparrow}{J} \parallel [111]$, тобто, при відсутності міжмінімумного перерозподілу носіїв заряду. Наведено фізичне обґрунтування одержаних результатів.

Ключові слова: кремній, питомий опір, направлена пружна деформація, тензоопір, параметр анізотропії рухливості.