LONGITUDINAL MAGNETORESISTANCE OF UNIAXIALLY DEFORMED *p*-SILICON AT J || B || [001]

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The influence of uniaxial pressure on the longitudinal magnetoresistance of pure *p*-Si crystals at the temperature $T = 77.4$ K and in the magnetic field $B = 45$ T has been studied. The results are discussed making allowance for negative effective masses of holes. A reduction of magnetoresistance with increase in the external pressure confirms the reduction of effective hole masses.

1. Introduction

The bands of heavy and light holes in silicon are known to be degenerate at the extremum point $\mathbf{k} = 0$, with the third band – due to spin-orbit interaction – being split from them by the energy $\Delta = 0.04$ eV. Such a small value of Δ brings about a non-parabolic dispersion law for the heavy- and light-hole bands. Therefore, the profile of both valence bands of silicon in the vicinity of the ($\mathbf{k} = 0$)-point is described by the expression

$$\varepsilon(k) = \frac{\hbar^2}{2m_0}\times$$

$$\times\left\{Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2}\right\}, \quad (1)$$

where A, B, and C are dimensionless constants equal to 4 ± 0.1, 1.1 ± 0.4, and 4.1 ± 0.4, respectively. The positive and negative signs before the root in Eq. (1) correspond to the light- and heavy-hole bands, respectively. The isoenergetic surfaces of heavy holes have concave sections, where negative transverse effective masses are realized (Fig. 1).

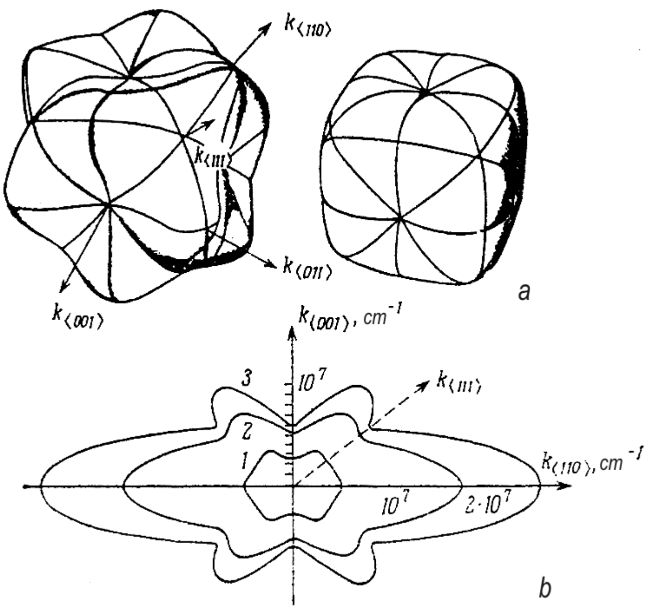

Fig. 1. *a* – Isoenergetic surfaces near the top of the heavy-hole valence band in silicon in the **k**-space (for the low energy on the right, and for the high energy on the left). *b* – Cross-sections of isoenergetic surfaces in the plane [011]

As follows from Eq. (1), the term with the multiplier C^2 is responsible for the deviation of the shape of isoenergetic surfaces from the spherical one and, hence, for the appearance of negative effective masses. If $C^2 < 0$, there are no negative effective masses in the heavy-hole band, but they can be in the light-hole one. If $C^2 > 0$, the splitting between two energy bands is maximal in the [111]-direction and minimal in the [001]-one.

Rigorous calculations of the geometry of negative-effective-mass regions on the basis of Eq. (1) give rise to the equations, whose orders are higher than that of Eq. (1), so that they cannot be solved analytically. However, if one takes into account that the regions of negative effective masses are located in the vicinity of axes of the [001]-type, where the term with the multiplier C^2 is small, a rather good approximation to the solution can be found. By expanding the root in Eq. (1) into a series, we obtain

$$\varepsilon(k) = \frac{\hbar^2}{2m_0}\left(\alpha_0k^2 - \beta_0\frac{k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2}{k^2}\right), \quad (2)$$

where $\alpha_0 = A - B$ and $\beta_0 = C^2/(2B)$. As follows from expression (2), the quantity β_0 is a measure for the deviation of an isoenergetic surface from the spherical shape. In particular, for silicon, $\alpha_0 = 3.53$ and $\beta_0 = 18.4$.

The equation for the effective mass in the [100] direction can be written down in the form

$$\frac{1}{m_{100}} = \frac{1}{\hbar^2}\frac{\partial^2\varepsilon}{\partial k_x^2}. \tag{3}$$

Then, from the law of heavy hole dispersion (2), we find

$$\frac{\partial^2\varepsilon}{\partial k_x^2} = \frac{\hbar^2}{m_0}\times$$

$$\times\left\{\alpha_0 - \frac{\beta_0}{k^6}\left(k_y^4 + k_y^2k_z^2 + k_z^4\right)\left(-3k_x^2 + k_y^2 + k_z^2\right)\right\}. \tag{4}$$

From Eqs. (3) and (4), one can derive the equation for the effective mass in the [100] direction as

$$\frac{1}{m_{100}} = \frac{1}{m_0}\times$$

$$\times\left\{\alpha_0 - \frac{\beta_0}{k^6}\left(k_y^4 + k_y^2k_z^2 + k_z^4\right)\left(-3k_x^2 + k_y^2 + k_z^2\right)\right\}. \tag{5}$$

It is evident that the effective mass m_{100} is negative at the axes [010] and [001], as well as in some region around them, if $\beta_0 > \alpha_0$ or, equivalently,

$$\beta_0 > \alpha_0 \quad \text{или} \quad C^2/2B > A - B. \tag{6}$$

This condition is valid for silicon. The transverse effective mass at the axes [010] and [001] satisfies the equality

$$\frac{1}{m_{100}} = \frac{1}{m_0}(\alpha_0 - \beta_0). \tag{7}$$

While moving away from the directions [010] and [001], the absolute value of m_{100}^{-1} first diminishes down to zero, and then the quantity m_{100}^{-1} itself becomes positive. The value of m_{100} for silicon differs from that calculated by formula (7) by approximately a factor of 6.5. This circumstance testifies that approximation (1) is not good as the law of heavy hole dispersion; it is especially true for silicon, where the parameter $\beta_0 = 18.4$ [2].

In this work, we study the longitudinal magnetoresistance of pure p-Si in quantizing magnetic fields, making use of a strong uniaxial elastic compressive strain.

2. Experimental Results and Their Discussion

One of the most important methods for studying the features of the band structure and the mechanisms of current carrier scattering in semiconductors is a research of galvano-magnetic effects. It is the study of galvano-magnetic phenomena that allowed one to first obtain the correct information concerning the shape of isoenergetic surfaces of germanium and silicon and their arrangement in the **k**-space. However, the study of those effects is more interesting in the range of strong magnetic fields and low temperatures, when the motion of current carriers becomes quantized.

Strong magnetic fields extended the scope of researches of galvano-magnetic effects. Owing to their application, it became possible to carry out measurements under such conditions, when quantum-mechanical effects play a key role, i.e. when

$$\omega_c\tau \gg 1, \quad \hbar\omega_c \gg k_B T, \tag{8}$$

where ω_c is the cyclotron frequency, τ is the relaxation time, $\hbar$ is Planck's constant divided by 2π, k_B is the Boltzmann constant, and T is the absolute temperature.

According to the classical theory, magnetoresistance becomes saturated in a strong magnetic field. Really, such a complete saturation of the longitudinal magnetoresistance in silicon of the p-type was observed for the first time in work [3]. However, the theory of longitudinal magnetoresistance, which would take into account the structure of the silicon valence band in either the classical case of strong magnetic fields or the case of quantizing magnetic fields, has not been developed yet. This circumstance does not allow one to make a quantitative comparison of experimental results with theoretical ones. In addition, the saturation of magnetoresistance has not been observed in all previous experimental works because of a narrow range of achieved magnetic fields. By having expanded the range of magnetic fields substantially (due to the use of pulse magnetic fields [3]), we managed to establish that if $\omega_c\tau \geq 4$, the magnetoresistance saturation is observed irrespective of crystallographic directions, concentration, and temperature.

In Fig. 2, the experimental data obtained for high-resistance crystals of p-silicon ($\rho_{300\text{ K}} = 2700\ \Omega \times \text{cm}$) at $T = 77.4$ K and $B = 45$ T are presented. One can see that, in the case $\mathbf{J}\|\mathbf{B}\|[001]$, a complete saturation of magnetoresistance is observed until the current carriers become quantized (curve *1*). Nevertheless, the negative component of the magnetoresistance, resulted from the nonparabolicity of the valence band, does not manifest itself. It may be probably related to the fact that $C^2 < 0$. The coefficient C^2 is responsible for the deviation of the shape of isoenergetic surfaces from the spherical one and,

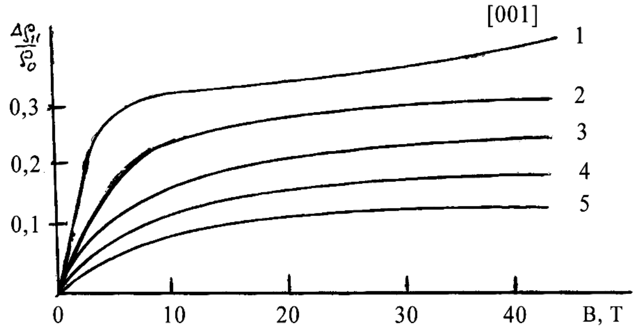

Fig. 2. Dependences of longitudinal magnetoresistance of p-silicon ($\rho_{300\text{ K}} = 2700\ \Omega \times \text{cm}$) on the magnetic field directed along the crystallographic direction [001] at the temperature $T = 77.4$ K for various values of pressure: 0 (*1*), 2×10^3 (*2*), 4×10^3 (*3*), 6×10^3 (*4*), and 7×10^3 kg/cm^2 (*5*)

therefore, for the manifestation of negative effective masses [4–6]. Moreover, the experimental temperature, which the current carrier scattering depends on, was high enough.

The character of valence-band spectrum variation under a uniaxial elastic deformation opens new opportunities for studying the processes of current carrier scattering and band reconstruction. In this connection, it is of interest to study the influence of the uniaxial elastic deformation on the valence band and, hence, on the magnetoresistance. The effect can be observed, because the deformation removes degeneration and changes the valence band structure so that, provided that the gap between valence subbands of heavy and light holes is large enough, the energy splitting becomes so large that all current carriers should transit into the lower – by energy – subband of heavy holes. In this case, it becomes possible to study the magnetoresistance only in the heavy-hole band, if measurements are carried out at weak electric fields.

Hence, in the case of high uniaxial pressure, we actually deal with the heavy-hole band only (in this case, two ellipsoids – one prolate and another oblate along the deformation axis – are formed in the bands $M_j = \pm 1/2$ and $M_j = \pm 3/2$, respectively [7]).

In effect, the uniaxial elastic deformation substantially influences the magnitude of magnetoresistance, which can be seen from Fig. 2 (curves *2* to *5*). The uniaxial elastic deformation makes the magnetoresistance value approximately three times lower. This phenomenon originates from the fact that if the crystal is subjected to a uniaxial elastic compressive strain, there occurs, besides the transition of light holes into the heavy-hole band, a reconstruction of the band spectrum; the result of this reconstruction is that heavy holes become lighter as the pressure increases, and their mobility grows; hence, the magnitude of magnetoresistance decreases.

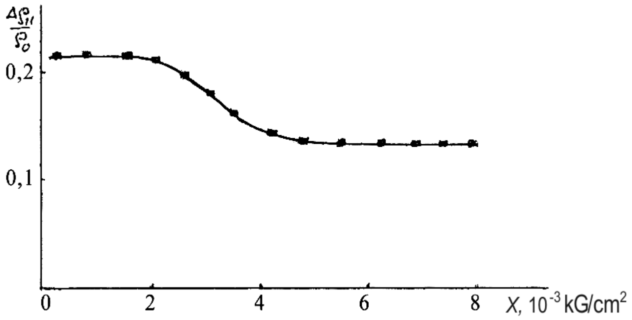

Fig. 3. Dependence of the p-silicon magnetoresistance on the uniaxial pressure at the temperature $T = 77.4$ K

In Fig. 3, the dependence of longitudinal magnetoresistance at saturation ($B_{\text{const}} = 12$ T) on the pressure is depicted. As the pressure grows, the magnetoresistance starts to gradually decrease and, when the pressure achieves the value of 4.5×10^3 kg/cm^2, becomes independent of it. It can be explained by the fact that, at large compressive strains, the magnetoresistance is governed by current carriers from the band $M_j = \pm 1/2$ only, the isoenergetic surface of which is ellipsoidal.

The experiments dealing with the cyclotron resonance in uniaxially deformed p-silicon crystals [8, 9] demonstrated that the resonance lines of both light and heavy holes disappear as the deformation increases; instead, there appears a new line which corresponds to holes belonging to the upper (from the split ones) valence band. By their effective mass, these holes are in-between light and heavy ones.

It is worth noting that there is no information, except for our one, in the literature concerning the experiments dealing with the magnetoresistance in uniaxially deformed p-silicon crystals. Researches similar to ours, but for p-germanium, were carried out in work [10].

3. Conclusions

We would like to note that, in 1958, Krömer [1] proposed a device – Negative Effective Mass Amplifier and Generator (NEMAG), – where the features of the motion of current carriers with negative effective masses were used. A wide range of operating frequencies (from 0 to 10^{12} Hz) was obtained owing to the nonresonance mechanism of functioning, so that the device attracted the keen interest. A lot of authors attempted to reveal this effect in germanium; however, all attempts to construct a germanium-based NEMAG failed, because the nonparabolicity of valence bands in germanium is lower than that in silicon. In our opinion, the most suitable element for this purpose is silicon, because the corresponding magnitude of spin-orbit splitting between the third band and the band of light and heavy holes amounts to only 0.04 eV; this fact is favorable to the formation of current carriers with negative effective masses in the heavy-hole band and, hence, to the emergence of negative resistance.

It has been found that, in the case of p-Si, the saturation of longitudinal magnetoresistance takes place irrespective of crystallographic orientation, the concentration of current carriers, and the temperature, provided that $\omega_c\tau \geq 4$. The mechanism of a considerable reduction of magnetoresistance, which accompanies a strong uniaxial elastic deformation of the crystal, has been elucidated.

1. H. Krömer, Phys. Rev. **109**, 1856 (1958); Proc. IRE **47**, 407 (1959).
2. I.M. Tsidilkovskii, *Electrons and Holes in Semiconductors* (Nauka, Moscow, 1972) (in Russian).
3. B. Orazgulyev, Fiz. Tverd. Tela **8**, 2780 (1966).
4. G. Dousmanis, R. Duncan, J. Thomas, and F. Williams. Phys. Rev. Lett. **1**, 404 (1958).
5. Yu.M. Kagan, Zh. Eksp. Teor. Fiz. **38**, 1854 (1960).
6. F. Williams and F. Herman, in *Proceedings of the International Conference on Semiconductor Physics* (Prague, 1960), p. 599.
7. B. Orazgulyev, Ukr. Fiz. Zh. **33**, 1691 (1988).
8. J.C. Hensel and G. Feher, Phys. Rev. **129**, 1041 (1963).
9. J.C. Hensel, H. Hasegawa, and M. Nakayama, Phys. Rev. **138**, A225 (1965).
10. P.I. Baranskii, V.Ya. Duchal, V.V.Kolomoets, and V.V. Chernysh, Fiz. Tekh. Poluprovodn. **20**, 2112 (1986).

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ПОЗДОВЖНІЙ МАГНЕТООПІР ОДНОВІСНО ДЕФОРМОВАНОГО КРЕМНІЮ p-ТИПУ ПРИ $\mathbf{J}\|\mathbf{B}\|[001]$

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Резюме

Досліджено вплив одновісного тиску на поздовжній магнетоопір чистих кристалів p-Si при температурі $T = 77,4$ K в магнітному полі $B = 45$ Т. Результати обговорюються з врахуванням впливу негативної маси дірок. Зменшення магнетоопору зі збільшенням тиску пов'язано зі зменшенням ефективної маси дірок.