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Spin-orbit Splitting of Valence Band in Silicon Whiskers under Strain

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Silicon whiskers with doping concentration of 2×10^{18} cm^{-3} were chosen to investigate magnetoconductance in the range of 0-14 T at cryogenic temperatures under compressive strain up to -2×10^{-3} rel. un. The whiskers were doped with boron during the growth process by chemical vapor deposition method, and the concentration of charge carriers, according to Hall studies, was about 2×10^{18} cm^{-3}. The uniaxial strain of whiskers was carried out by fixing them to the substrates using thermal strain due to the difference between the coefficients of thermal expansion of the crystal and the substrate material. Longitudinal magnetoresistance for unstrained and strained Si whiskers was studied in the temperature range of 4.2 ÷ 70 K. The unstrained whiskers have a quadratic dependence of the magnetoresistance on the magnetic field induction. The strain leads to the appearance of negative magnetoresistance with sufficiently large magnitude (up to 15 %). The possible reasons of the effect were discussed. The most probable reason of negative magnetoresistance appearance is weak localization (WL) of the charge carriers. According to calculations within the WL model, the coherence length L_φ and spin-orbit length L_{so} are proportional to $T^{-0.53}$ and $T^{-0.45}$, respectively. The latter one is closed to $T^{-1/2}$ expected from the theoretical data for a two-dimensional system. This fact is the evidence of the conclusion that conductance in Si whiskers mostly occurs in the subsurface layers of crystals. Strain influence on spin-orbit splitting and the valence band spectrum was studied. As a result, the splitting of light and heavy hole branches was found under compressive strain according to the k-p-method. The spin splitting energy for sub-band of heavy holes Δ_{SO} was found to be 1.8 meV.

Keywords: Si whiskers, Magnetoconductance, Spin-orbit splitting, Strain.

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1. INTRODUCTION

Theoretical and experimental studies of the magnetoresistance of doped semiconductors indicate that the causes of its occurrence are substantially cut off for the metal and dielectric sides of the transition of the metal-dielectric [1].

The theory of quantum corrections [2] works on the metal side of the transition, which operates on three main phenomena:

- interference of electron wave functions on average trajectories that describe the processes of weak localization [3];
- the coherent interaction of electrons in their diffusion, that is, the interaction in the diffusion channel;
- short-term binding of electrons in superconducting pairs, namely, the interaction in the coupling channel.

On the dielectric side, in the case of the transposition of highly localized charge carriers, other mechanisms [4] are used to explain the effect:

- taking into account the scattering of tunneling charge carriers at intermediate centers;
- narrowing of the impurity band in a magnetic field;
- spin effects [5, 6].

Experimental confirmations of the contribution of the phenomena described above to the field dependences of the magnetoresistance were obtained in the investigation of the charge carrier transport in filament-shaped crystals on the basis of silicon with an acceptor impurity concentration corresponding to the proximity to the metal-dielectric transition from both metal and dielectric sides [7, 8].

However, the influence of strain on spin-orbit (SO) splitting in silicon in the vicinity to MIT is insufficiently studied. As shown by Bir and Picus in silicon [9], the influence of the SO interaction on the zone splitting is manifested in significant deviations and nonlinear growth of Δ_{SO} under strain.

Significant SO interaction reduces the symmetry of electron wave functions in the region of hopping conductance. Using strain as a sensitive tool for the influence on the structure of the impurity band, which occurs in the region of cryogenic temperatures, one can obtain important information on the characteristics of the low-temperature charge carrier transport in such crystals.

2. EXPERIMENTAL PROCEDURE

The *p*-type silicon microcrystals were chosen as the object of investigation with boron concentration corresponding to the dielectric side of metal-insulator transition of 2×10^{18} cm^{-3}. Electrical contacts were established by pulse welding using the method described in [7], which provides the necessary ohmic contacts. Conductivity was studied at a temperature of 4.2 K. For these studies, crystals were cooled to liquid helium temperature in the helium cryostat. The temperature was measured by using the Cu-CuFe thermocouple calibrated with CERNOX sensor. The magnetic field effects of the whiskers were studied using the Bitter magnet with the induction to 14 T and the field scan time of 1.75 T/min. Stabilized electric current along the whisker was created by the current source Keithley 224 in the range of 1-100 μA depending on the crystal resistance. CERNOX sensor was used for magnetic measurements, in particular for its thermostabilization. It is weakly sensitive to magnetic field induction. The change of its output signal in the field with induction B = 15 T is about 1 %.

3. EXPERIMENTAL RESULTS

The p-type silicon whiskers with boron concentration of 2×10^{18} cm^{-3} were chosen to investigate magnetoconductance in the range of 0-14 T at 4.2 K under compressive strain up to -2×10^{-3} rel. un. The longitudinal magnetoresistance for unstrained and strained Si whiskers is studied and presented in Fig. 1. As evident from Fig. 1, the unstrained whiskers have a quadratic dependence of the magnetoresistance on the magnetic field induction. The strain leads to the appearance of negative magnetoresistance with sufficiently large magnitude.

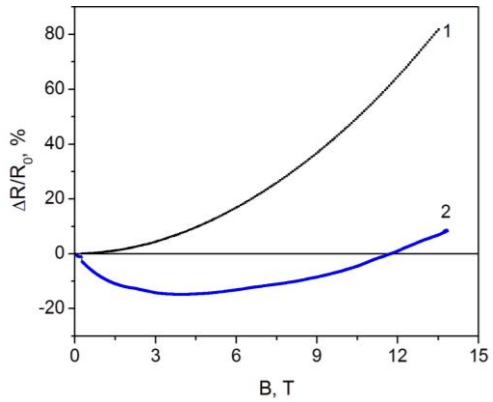

Fig. 1 – Longitudinal magnetoresistance of Si whiskers at a temperature of 4.2 K for samples: 1 – unstrained; 2 – strained

The possible reasons for the effect are a) a strongly defective whisker structure; b) the presence of magnetic impurity; c) size effect; d) week localization (WL). The whiskers have perfect crystalline structure of volume and surface according to their growth conditions by VLS mechanism.

They have no any magnetic impurities, which was investigated by diamagnetic magnetization like that of bulk silicon. Due to large whisker dimensions (of about 30 μm in diameter), the quantum size effect is hardly responsible for the observed negative magnetoresistance. The main reason for the effect is WL of the charge carriers.

4. DISCUSSION

We proposed to use the WL model to describe the behavior of the whisker magnetoconductance. The magnetoconductance $\Delta\sigma(B)$ normalized by G_0 can be presented in the form [10]:

$$\frac{\Delta\sigma(B)}{G_0} = \frac{\sigma(B)-\sigma(0)}{G_0} = f\left(\frac{B}{H_{so}+H_\varphi}\right) + \\ + \frac{1}{2} f\left(\frac{B}{2H_{so}+H_\varphi}\right) - \frac{1}{2}(1+\beta) f\left(\frac{B}{H_\varphi}\right), \quad (1),$$

where β is the factor of Maki-Thompson correction, B is the magnetic field induction. Therefore,

$$G_0 = e^2 / 2\pi h, \quad (2)$$

where G_0 is the quantum conductivity, $f(x)$ is expressed through the digamma function $\Psi(z)$

$$f(z) = \Psi\left(\frac{1}{2}+\frac{1}{x}\right) + \ln(x). \quad (3)$$

The parameter H_φ is connected with the electron dephase time τ_φ of the electron wave

$$H_\varphi = \frac{\hbar c}{4eD\tau_\varphi}. \quad (4)$$

Accordingly, the parameter H_{so} correlates with the spin-orbit dephase time τ_{so}

$$H_{so} = \frac{\hbar c}{4eD\tau_{so}}, \quad (5)$$

where D is the diffusion coefficient, c is the velocity of light.

The conductivity fluctuation of $\Delta\sigma(B)$ in the magnetic field has been outlined based on experimental dependencies of Si whisker magnetoresistance in a magnetic field using the following equation:

$$\frac{\Delta\sigma(B)}{G_0} = \frac{\sigma(0)}{G_0}\left(\frac{\Delta R(B)}{R(0)} + (\mu H)^2\right), \quad (6)$$

where H is the magnetic field intensity, μ is the Hall mobility.

The obtained magnetic field dependence $\Delta\sigma(B)$ (see Fig. 2) matches the theoretical one.

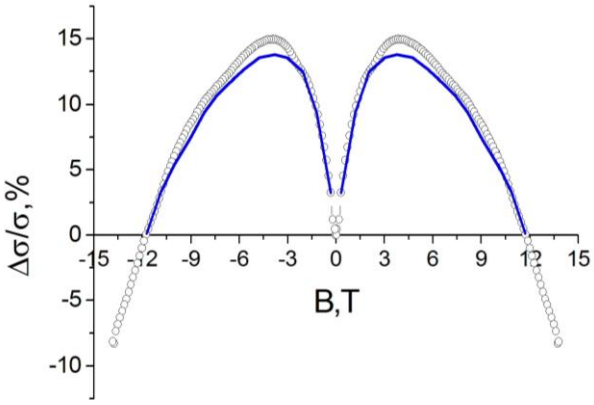

Fig. 2 – Longitudinal magnetoconductance in Si whiskers at a temperature of 4.2 K. Solid line corresponds to the theoretical data, while circles denote experimental ones

As visible from Fig. 2, experimental and theoretical data coincide very well at a temperature of 4.2 K that allows us to determine H_φ and H_{so} parameters. The obtained mentioned parameters allow to calculate the coherence length (L_φ) and spin-orbit length (L_{so}) using the equations

$$L_\varphi^2 = D\tau_\varphi = 4\frac{e}{\hbar c}H_\varphi \\ L_{so}^2 = D\tau_{so} = 4\frac{e}{\hbar c}H_{so} \quad (7)$$

L_φ and L_{so} temperature dependencies in Si whiskers have been calculated from (7). For one- and two-dimensional systems the coherence lengths L_φ are proportional to temperature as $T^{-1/3}$ and $T^{-0.5}$, respectively

[11]. Coherence length L_ϕ and spin-orbit length L_{so} are proportional to $T^{-0.53}$ and $T^{-0.45}$, respectively. The latter one is closed to $T^{-1/2}$ expected from the theoretical data for a two-dimensional system. This fact is the evidence of the conclusion that conductance in Si whiskers mostly occurs in the subsurface layers of crystals.

According to D'yakonov-Perel spin mechanism [12]

$$dL_{so} = \sqrt{12}L_\Omega^2, \tag{8}$$

where d is the diameter of the whisker, L_Ω is the spin processing length, Ω is the spin processing frequency at spin-orbit interaction. Spin processing length has been calculated using the obtained data according to (8) and the value of $L_\Omega = 65$ nm has been defined. Taking into account the equation:

$$L_\Omega = \frac{\hbar}{2m^*\alpha} \tag{9}$$

and the effective mass derived from [13], the Rashba parameter α was found to be $\alpha = 5 \times 10^{-15}$ eV × m, which is in agreement with the literature data in Si quantum wells 4×10^{-15} eV × m [14]. Substituting the magnitude of wave number $k_F = 5 \times 10^8$ m^{-1} [15] and the Rashba parameter α into

$$\Delta_{SO} = 2k_F\alpha, \tag{10}$$

the spin splitting energy Δ_{SO} can be obtained, which, in this case, was found to be equal to $\Delta_{SO} = 1.8$ meV.

4.1 Theoretical-group Aspects of Strain Influence on Spin-orbit Splitting on the Valence Band Spectrum

Let us consider the strain removal of the degeneracy of the band spectrum of Si at the point **Γ**, the mutual influence of strain and spin-orbit splitting within the k-p-method of perturbation theory, generalizing the well-known consideration [16] to arbitrary strains, and, distinguishing geometric and theoretical-group aspects of the theory. The concept of strain potential was introduced from the very beginning of the development of the basis of the band theory of solids by Brillouin [9] to describe the electron-phonon interaction. In the case of small strain, its influence is regarded as perturbation. The strain tensor ε is generally defined as the change of the metric space tensor g_{ij} in the associated (object-related) coordinate system:

$$\varepsilon_{ij} = 1/2\ (g_{ij} - \delta_{ij}). \tag{11}$$

We denote by $D(\varepsilon)$ the group-group representation, which transforms the strain tensor. Such a schedule is the basis of the canonical decomposition of the strain tensor itself, as the basis of the group-group representation on a ball (isotropic) part and a deviator (anisotropic non-chip part):

$$\varepsilon_{ij} = 1/3\,\mathrm{Sp}(\boldsymbol{\varepsilon})\,\delta_{ij} + (\varepsilon_{ij} - 1/3\,\mathrm{Sp}(\boldsymbol{\varepsilon})\,\delta_{ij}), \tag{12}$$

where $\mathrm{Sp}(\boldsymbol{\varepsilon}) = \sum_i \varepsilon_{ij}$ is the strain tensor shaft. In unstrained Si crystals, due to the point symmetry $\boldsymbol{O_h}$ of their crystalline lattice, without spin-orbit interaction and spin, the energy spectrum of the valence band has a triple degenerate maximum in the center of the Brillouin zone-point **Γ**. The wave functions of an arbitrary quasiparticle at this point, with this approximation, must have the symmetry of the irreducible representation of $\boldsymbol{\Gamma_{25}'}$. Given the spin, this symmetry corresponds to a six-degenerate energy state. As is well known [16], significant spin-orbit interaction reduces the symmetry of wave functions of a quasiparticle. The representation $\boldsymbol{\Gamma_{25}'}$ becomes a condensation, which leads to a partial degeneration at this point: the band spectrum has a quadruple degenerate maximum, taking into account the spin. The group of wave vectors is the sum of irreducible representations of $\boldsymbol{\Gamma_7^+ + \Gamma_8^+}$. In the group-theoretical group, the perturbation of the symmetry of a crystal can be represented as the result of a direct product of the initial representation and representation, according to which perturbation is converted:

$$\boldsymbol{\Gamma_{25}' \times D^{(1/2)} = \Gamma_7^+ + \Gamma_8^+}, \tag{13}$$

where $\boldsymbol{D^{(1/2)}}$ is the perturbation due to spin-orbit interaction (taking into account spin irreducible representation), $\boldsymbol{\Gamma_8^+}$ is the quadruple degenerate level; $\boldsymbol{\Gamma_7^+}$ is a two-dimensional (by spin) level that is spin-orbit splitted into the energy gap Δ_{so}; × is the direct multiplication of the corresponding composite and irreducible representations.

From the group-theoretical point of view, strain disturbance can be included in two ways. The first method takes into account first the spin-orbit interaction, that is, accounts the strain which is already in the partially withdrawn degenerate state $\boldsymbol{\Gamma_7^+ + \Gamma_8^+}$

$$\boldsymbol{(\Gamma_{25}' \times D^{(1/2)}) \times D(\varepsilon) = (\Gamma_8^+ + \Gamma_7^+) \times D(\varepsilon) =}$$
$$\boldsymbol{= (\Gamma_8^+ \times D(\varepsilon)) + \Gamma_7^+}. \tag{14}$$

Under the influence of general strain (second rank symmetric tensor), only the central symmetry and spin degeneracy will remain in the point group of the crystal, and, accordingly, all irreducible representations will be connected and all degenerations (except for two-dimensional spin) will be removed. In particular, the $\boldsymbol{\Gamma_7^+}$ strain of the crystal is not able to influence the spin degeneracy of two-dimensional states. In fact, in this method, strain removal of degeneration is investigated only twice (without spin) of the degenerate level of $\boldsymbol{\Gamma_8^+}$: the splitting of the branches of the light and heavy holes. The influence of strain and spin-orbit splitting cannot be studied in this way. The spin-orbit split zone of the $\boldsymbol{\Gamma_7^+}$ shifts as a whole only with the general change in the bandgap width. Thus, this corresponds to a two-zone approximation in the *k-p*-method of perturbation theory.

The strain genesis of the valence band in this way is shown in Fig. 3.

This is marked by δE strain splitting of the branches of the light and heavy holes.

According to the second method of strain inhibition and spin, the orbit interaction is taken into account simultaneously in the initially non degenerate state of $\boldsymbol{\Gamma_{25}^+}$:

$$\boldsymbol{(\Gamma_{25}' \times D^{(1/2)}) \times D(\varepsilon) = (\Gamma_8^+ + \Gamma_7^+) \times D(\varepsilon)}$$
$$\boldsymbol{(\Gamma_{25}' \times D^{(1/2)}) \times D(\varepsilon) = (\Gamma_8^+ \times D(\varepsilon)) + \Gamma_7^+}. \tag{15}$$

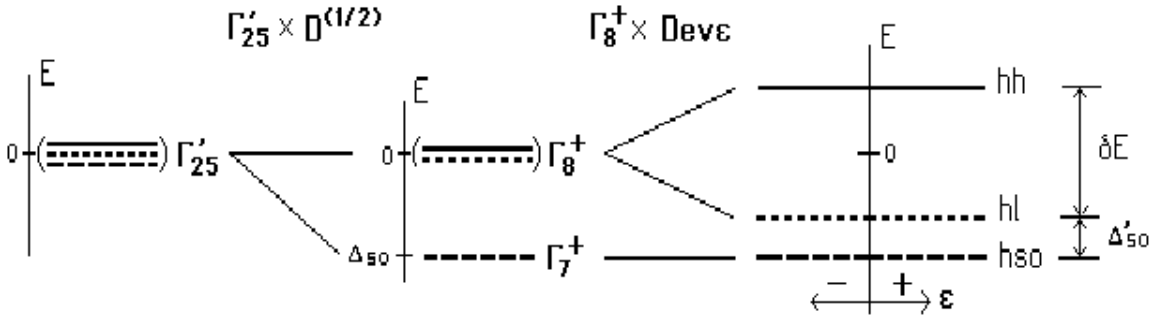

Fig. 3 – The strain genesis of the valence band in a two-zone approximation

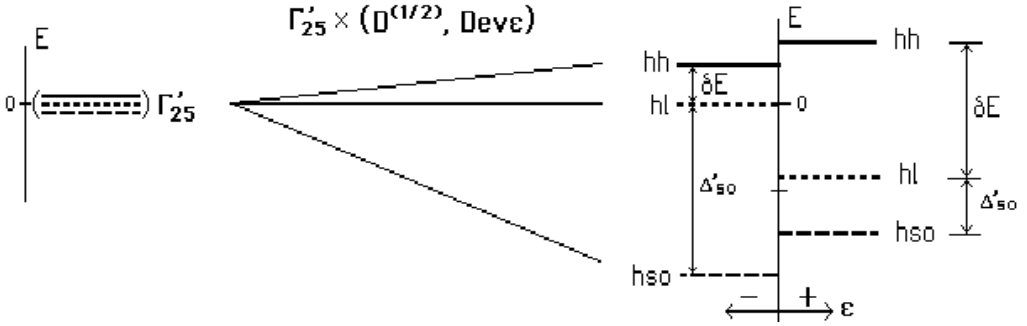

Fig. 4 – The strain genesis of the valence band in a three-zone approximation

This method allows to simultaneously investigate the influence of strain and spin-orbit interaction. It corresponds to a three-zone approximation and is more complex from the design point of view. The strain genesis of the valence band in this way is shown in Fig. 4.

$$\mathbf{H}(\boldsymbol{\varepsilon}) = \frac{\mathbf{p}'(\boldsymbol{\varepsilon})^2}{2m} + \mathrm{V}(\boldsymbol{\varepsilon},\mathbf{x}') + \frac{\hbar^2}{4m^2c^2}\nabla\mathrm{V}(\boldsymbol{\varepsilon},\mathbf{x}')\left[\mathbf{p}'(\boldsymbol{\varepsilon})\boldsymbol{\sigma}\right], \qquad (16)$$

where $\mathbf{p} = -i\hbar\nabla$ is the momentum operator, $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$ is the Pauli matrix, V(***ε***, ***x***') is a self-consistent periodic potential in the new strained (accompanying) axes of the coordinate x' of the strained crystal. The operator $H(\varepsilon)$ differs from the Hamiltonian of the unstrained crystal by the substitution of the operator p with p'(ε) and the potential $V(x)$ with V(**ε**, **x**'). The Pauli matrices do not change with strain, since they are the basis of the spinor representation of the $SU(2)$ group, which obviously does not depend on the strain of the crystal. At first glance, the main perturbation is to change the potential $V(\varepsilon, x')$ for strain, but it is not true in the case of degenerate zones. Consider the perturbation within the linear theory of infinitesimal strains. An infinitesimal strain does not affect the basic coordinate system $x = x'$ and the conditions for preserving the periodicity of the crystal lattice are trivial. In the non-relativistic approximation in this case, the matrix elements of perturbations include only the following additional members associated with the strain:

$$H^{\varepsilon}_{m'm} = \sum_{ij} V^{ij}_{m'm}\,\varepsilon_{ij} = \sum_{ij} D^{ij}_{m'm}\,\varepsilon_{ij}, \qquad (17)$$

where $D^{ij}_{m'm}$ is the strain potential.

In the cubic crystals in the center of the Brillouin zone in accordance with the rules of selection, this relation becomes dependent only on the scalar part of the strain

$$H^{\varepsilon}_{m'm} = D_{m'm}\,\mathrm{Sp}(\varepsilon), \qquad (18)$$

and since the perturbation matrix is actually a scalar, the result of the strain effect on the energy spectrum in the vicinity of the extremum can be only the general displacement of the degenerate zone. Thus, the degeneration of degenerate zones is possible only within the theory of finite strains, which change the basic coordinate system. Let's also consider the well-known methods, which are based on the decomposition of strained disturbances of eigenfunctions to the first-order elements of the strain tensor in the form: (3.2)

$$\varphi'_n(\mathbf{x}') = \varphi_n(\mathbf{x}) + \sum_{ij}\varepsilon_{ij}\sum_m \frac{\varphi_m(\mathbf{x})\left\langle m\left|V_{ij}\right|n\right\rangle}{E_n - E_m}, \qquad (19)$$

where the sum is taken for all states m at $E_m \neq E_n$.

The average position for the i-th particle in a strained state is determined by the following expression:

$$\left\langle \mathbf{y}^i \right\rangle = \int |\varphi'_n(\mathbf{y})|^2\, \mathbf{y}^i\, \mathrm{d}\,\mathbf{y} \qquad (20)$$

or, after integration,

$$\left\langle \mathbf{y}^i \right\rangle = \left\langle \mathbf{x}^i \right\rangle_0 + \\ + \sum_{kj}\left(\varepsilon_{kj}\left\langle \mathbf{x}^i \right\rangle_0 + \varepsilon_{kj}\sum_{mn}\frac{\left\langle n \mid \mathbf{x}^i \mid m\right\rangle\left\langle m \mid V_{kj} \mid n\right\rangle}{E_n - E_m}\right). \qquad (21)$$

In accordance with the selection rules for anisotropic part of the strain, all matrix elements in the center of the Brillouin zone are zero.

4.2 Calculation of the Energy Spectrum of the Valence Band in a Two-Zone Approximation

In the general case of degeneration at the extremum point, the energy spectrum is determined by the solu-

tion of the secular equation for a strainably perturbed Hamiltonian

$$\mathrm{Det}\left\| H_{ij}(\mathbf{k},\boldsymbol{\varepsilon}) - E(\mathbf{k},\boldsymbol{\varepsilon})\delta_{ij} \right\| = 0, \qquad (22)$$

the degree of which is determined by the symmetry (irreducible representation) of the investigated level relative to the group of the wave vector and depends on the multiplicity of degeneration of this level in the extreme point of Hamiltonian

$$\mathbf{H}(\mathbf{k},\boldsymbol{\varepsilon}) = \sum_l a_l \sum_i f_i^l(\mathbf{k},\boldsymbol{\varepsilon})\mathbf{X}_i^l, \qquad (23)$$

where constants a_l provide the Hermitian H(k, ε). In accordance with the scheme of the strain genesis of the valence band at point **Γ** (see Fig. 3), strain disturbance is included in the already considered spin-orbit interaction in the Hamiltonian (two-zone approximation) representation

$$\mathbf{H}(\mathbf{k},\boldsymbol{\varepsilon}) = (A - 5/4B)\,\mathbf{k}^2\mathbf{I} + (a - 5/4b)\,\mathrm{Sp}(\boldsymbol{\varepsilon})\,\mathbf{I} + \sum_i (B^2k_i^2 + b\varepsilon_{ii})\mathbf{J}_i^2 + 1/\sqrt{3}\sum_i (D^2k_ik_j + d\varepsilon_{ij})\left[\mathbf{J}_i\mathbf{J}_j\right], \qquad i \neq j, \qquad (24)$$

where A, B, D are the standard zone parameters, a, b, d are the constants of the strain potential, $\mathbf{J}_i$ is the angular momentum matrix, **I** is a unit matrix, [×] is the vector multiplication.

The angular moments on this basis have the form

$$\mathbf{J}_1 = \begin{Vmatrix} 0 & i\sqrt{3/2} & 0 & 0 \\ -i\sqrt{3/2} & 0 & i & 0 \\ 0 & -i & 0 & i\sqrt{3/2} \\ 0 & 0 & i\sqrt{3/2} & 0 \end{Vmatrix}.$$

$$\mathbf{J}_2 = \begin{Vmatrix} 0 & \sqrt{3/2} & 0 & 0 \\ -\sqrt{3/2} & 0 & 1 & 0 \\ 0 & -1 & 0 & \sqrt{3/2} \\ 0 & 0 & \sqrt{3/2} & 0 \end{Vmatrix}, \qquad (25)$$

$$\mathbf{J}_3 = \begin{Vmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{Vmatrix}.$$

The proper values of the Hamiltonian remain twice degenerate in spin, and therefore the secular equation in this case has at most two different solutions. For the solution of the secular equation, we use the method of the characteristic polynomial

$$\mathbf{H} = H_s + \mathbf{H}_a\,\mathbf{I}, \qquad H_s = \mathrm{Sp}\mathbf{H}_a = 0,$$

$$H_s = E_s = Ak^2 + a\mathrm{Sp}(\boldsymbol{\varepsilon}). \qquad (26)$$

From such a schedule, the sufficiency of finding only the eigenvalues of the non-observable part of $\mathbf{H}_a$ follows.

Since $\mathrm{Sp}\mathbf{H}_a = 0$, then characteristic polynomial has a form:

$$E^2 + \varphi_2(\mathbf{H}_a) = 0, \qquad (27)$$

where

$$\mathrm{Sp}(\mathbf{H}_a^2) = -4\varphi_2(\mathbf{H}_a). \qquad (28)$$

Let us denote

$$\mathbf{H}_a(\mathbf{k},\,\boldsymbol{\varepsilon}) = \mathbf{R} + 1/\sqrt{3}\,\mathbf{S}, \qquad (29)$$

where

$$\mathbf{R} = \sum_i (B^2k_i^2 + b\varepsilon_{ii})\,\mathbf{J}_i^2, \qquad (30)$$

$$\mathbf{S} = \sum_i (D^2k_ik_j + d\varepsilon_{ij})\left[\mathbf{J}_i\mathbf{J}_j\right], \qquad i \neq j.$$

Then

$$\mathrm{Sp}(\mathbf{H}_a^2) = \mathbf{R}^2 + 1/3\,\mathbf{S}^2 \qquad (31)$$

and after the transformations we obtain:

$$E_a^2 = 1/4\,\mathrm{Sp}(\mathbf{H}_a^2) = B^2\left(\sum_i k_i^2\right)^2 + 1/2C^2\sum_{i,j} k_i^2k_j^2 + \left|Bb\left(3\sum_i k_i^2\varepsilon_{ii} - k^2\,\mathrm{Sp}(\boldsymbol{\varepsilon})\right)\right| +$$

$$+ \left|Dd\sum_{i,j} k_ik_j\right| + 1/2\left|b^2\left(3\sum_i \varepsilon_{ii}^2 - \left(Sp(\boldsymbol{\varepsilon})\right)^2\right) + d^2\sum_{i,j}\varepsilon_{ij}\varepsilon_{ij}\right|, \quad i \neq j. \qquad (32)$$

In this relation, in addition to the known spectrum (4), the necessity of a positive definiteness of the right-hand side in arbitrary strains is taken into account.

Thus, the full range of holes in strained Si by the first method (two-zone approximation) is equal to:

$$E_l(\mathbf{k},\boldsymbol{\varepsilon}) = Ak^2 + a\,\mathrm{Sp}(\boldsymbol{\varepsilon}) - (-1)^l\sqrt{\Xi_k + |\,\Xi_{\varepsilon k}\,| + \Xi_\varepsilon},\ l = 1,2;\ E_3 = E_{so} = -\Delta_{so} + Ak^2, \qquad (33)$$

where $\Xi_{ek} = B^2\mathbf{k}^4 + C^2(k_1^2k_2^2 + k_1^2k_3^2 + k_2^2k_3^2)$,

$$\Xi_k = Bb\left(3(k_1^2\varepsilon_{11} + k_2^2\varepsilon_{22} + k_3^2\varepsilon_{33}) - \mathbf{k}^2\,\mathrm{Sp}(\boldsymbol{\varepsilon})\right) + 2Dd\left(k_1k_2\varepsilon_{12} + k_1k_3\varepsilon_{13} + k_2k_3\varepsilon_{23}\right),$$

$$\Xi_e = b^2/2)\left((\varepsilon_{11} - \varepsilon_{22})^2 + (\varepsilon_{22} - \varepsilon_{33})^2 + (\varepsilon_{33} - \varepsilon_{11})^2\right) + d^2\left(\varepsilon_{12}^2 + \varepsilon_{13}^2 + \varepsilon_{23}^2\right), \quad C^2 = D^2 - 3B^2.$$

In formula (24), the term $Sp(\varepsilon)$ defines a displacement of the valence band as a whole under the influence of a hydrostatic pressure and changes only the band gap width, and the term $\Xi\varepsilon$ defines the splitting of the zone at the point $k = 0$ by the value

$$\delta E = 2\sqrt{\Xi_\varepsilon}\,. \tag{34}$$

The values of the band parameters A, B, C in units of $\hbar^2/2m$ and spin-orbit splitting are equal to 4.27, – 0.63, 5.03 and 1.8 meV, respectively.

It is known [17] that in practically significant cases of mechanical value sensors, filamentous crystals are usually in a uniaxially stressed state along the direction [111] (uniaxial stress ε | | [111]) and the strain tensor for this case in the coordinate system of the strained whiskers has the form:

$$\varepsilon'_{ik} = \varepsilon \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\nu_{111} & 0 \\ 0 & 0 & -\nu_{111} \end{bmatrix}. \tag{35}$$

where ε is the magnitude of the longitudinal strain of the whiskers, that is, the strain transmitted to the crystal in the sensors, ν_{111} is the corresponding Poisson coefficient, which is the same for all directions perpendicular to [111]

$$\mathrm{v} = \nu_{111} = \frac{1/2(c_{11}+2c_{12})-c_{44}}{c_{11}+2c_{12}+c_{44}}\,, \tag{36}$$

where c_{11}, c_{12}, c_{44} are the elastic constants, for silicon $\mathrm{v} \approx 0.1838$.

In the relations describing the energy spectrum in strained crystals, the strain tensor is tied to the crystallographic coordinate system. Using the transformations, we obtain the form of ε | | [111] in these axes:

$$\varepsilon_{ik} = \varepsilon \begin{bmatrix} \gamma_1 & \gamma & \gamma \\ \gamma & \gamma_1 & \gamma \\ \gamma & \gamma & \gamma_1 \end{bmatrix}. \tag{37}$$

The numerical values of γ and γ_1 coefficients are 0.394 and 0.211, respectively.

For such a form of strain, expressions describing the energy spectrum are somewhat simplified:

$$\begin{aligned} E_l(\mathbf{k}, \boldsymbol{\varepsilon}) &= Ak^2 + a\gamma_1\varepsilon - (-1)^l \times \\ &\times \sqrt{\Xi_k + |\gamma D^2 d^2 \varepsilon^2 \textstyle\sum_{ij}(k_i k_j)| + 3\gamma d^2\varepsilon^2} \\ E_3 &= E_{so} = -\Delta_{so} + Ak^2. \end{aligned} \tag{38}$$

As can be seen from relation (38), in the two-zone approximation, strain splitting of zones of heavy and light holes does not depend on the sign of strain in ε:

$$\delta E = 2\gamma |d\varepsilon|\,. \tag{39}$$

At $E \to 0$, $\varepsilon \neq 0$ we have the asymptotic expression:

$$\begin{aligned} E_{El}(k, \varepsilon) &= Ak^2 + a\gamma_1\varepsilon - (-1)^l \times \\ &\times \left(\gamma |d\varepsilon| - \mathrm{signum}(\varepsilon) D \textstyle\sum_{ij} k_i k_j / 1\sqrt{3}\right) \end{aligned} \tag{40}$$

In accordance with the relation (40), the isoenergy surfaces look like ellipsoids only when $E << \delta E$, that is, at low temperatures and significant strains. None of these cases in the overwhelming majority of semiconductor sensitive elements of mechanical sensors is not realized.

4.3 Peculiarities of the Influence of Strain on Spin-Orbit Splitting in Silicon

In order to take into account the spin-orbit splitting zone ($l = 3$) having the symmetry of the representation of $\mathbf{\Gamma_7^+}$, a known nonlinear strain of the energy spectrum approximation in the vicinity of $k \sim 0$ was obtained by the method of invariant theory and corresponds to simultaneous perturbation of the 6-fold degenerate spectrum with symmetry $\mathbf{\Gamma_{25}}$ '(three-zone approximation).

For this purpose we choose a simplified Hamiltonian, respectively, in the direct product of bases $Y_m^1 \times \sigma_i$

$$\begin{aligned} \mathbf{H}(\mathbf{k}, \boldsymbol{\varepsilon}) &= Ak^2\,\mathbf{I} + a\mathrm{Sp}(\boldsymbol{\varepsilon})\,\mathbf{I} + 3\textstyle\sum_{i,j}(Bk_i^2 + b\varepsilon_{ij})\left(\mathbf{J}_i^2 - 1/3\mathbf{J}^2\right) + \\ &+ 1/\sqrt{3}\textstyle\sum_{i,j}\left(Dk_i k_j + d\varepsilon_{ij}\right)\left[\mathbf{J}_i\mathbf{J}_j\right] + \Delta/3\textstyle\sum_i \mathbf{J}_i\sigma_i, \quad i \neq j, \quad \Delta = \Delta_{so}\,. \end{aligned} \tag{41}$$

Here, the matrixes of the angular moments have a standard form

$$\mathbf{J}_1 = \begin{Vmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{Vmatrix}, \quad \mathbf{J}_2 = \begin{Vmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{Vmatrix}, \quad \mathbf{J}_3 = \begin{Vmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{Vmatrix}. \tag{42}$$

In the center of the Brillouin zone we have

$$\mathbf{H}(0, \boldsymbol{\varepsilon}) = a\,\mathrm{Sp}(\boldsymbol{\varepsilon})\,\mathbf{I} + 3\,3\textstyle\sum_{i,j} b\varepsilon_{ij}(\mathbf{J}_i^2 - 2/3\mathbf{I}^2) + 1/\sqrt{3}\textstyle\sum_{i,j} d\varepsilon_{ij}\left[\mathbf{J}_i\mathbf{J}_j\right] + \Delta/3\textstyle\sum_i \mathbf{J}_i\sigma_i\,, \quad i \neq j. \tag{43}$$

The characteristic polynomial in such an approximation of the interaction has the form:

$$E_a^3 + \varphi_2(\mathbf{H}_a)E_a - \varphi_3(\mathbf{H}_a) = 0, \tag{44}$$

where the scalar function $\varphi_3(\mathbf{H}_a)$ is determined by the following invariant of the Hamiltonian matrix:

$$\varphi_3(\mathbf{H}_a) = \mathrm{Sp}(\mathbf{H}_a^3). \tag{45}$$

We denote the independent part of this Hamiltonian as follows:

$$\mathbf{H}_a(\boldsymbol{\varepsilon}) = \mathbf{P} + 1/\sqrt{3}\,\mathbf{Q} + \Delta/3 \sum_i \mathbf{J}_i \sigma_i ,$$

where

$$\mathbf{P} = \sum_i \alpha_{ii} \left(\mathbf{J}_i^2 - 2/3\mathbf{I} \right),$$

$$\mathbf{Q} = \sum_i \alpha_{ii} \left[\mathbf{J}_i \mathbf{J}_j \right], \qquad i \neq j,$$

$$a_{ii} = 3b\varepsilon_{ii} , \qquad a_{ij} = 3d\varepsilon_{ij}.$$

By analogy to expression (31) we have

$$\mathrm{Sp}(\mathbf{H}_a^2) = -4\varphi_2(\mathbf{H}_a) = \mathrm{Sp}(\mathbf{P}^2) + 1/3\mathbf{Q}^2, \quad (46)$$

where the following notation is introduced:

$$\mathrm{Sp}(\mathbf{P}^2) = \frac{2}{3}\left((\alpha_{11} - \alpha_{22})^2 + (\alpha_{22} - \alpha_{33})^2 + (\alpha_{33} - \alpha_{11})^2 \right),$$

$$\mathrm{Sp}(\mathbf{Q})^2 = 4\left(\alpha_{12}^{\ 2} + \alpha_{23}^{\ 2} + \alpha_{13}^{\ 2} \right),$$

$$\mathrm{Sp}(\mathbf{H}_a^3) = 6\varphi_3(\mathbf{H}_a) = \mathrm{Sp}(\mathbf{P}^3) + \frac{1}{3\sqrt{3}} \mathrm{Sp}(\mathbf{Q}^3) + \left(\Delta/3\right)^3 \mathrm{Sp}\left(\mathbf{J}_i \sigma_i\right)^3 + 4\,\mathrm{Sp}\left(\mathbf{P}\mathbf{Q}^2\right).$$

After the transformation we get

$$\varphi_2(\mathbf{H}_a) = -\frac{1}{3}\Delta^2 - \frac{1}{6}\left((\alpha_{11} - \alpha_{22})^2 + (\alpha_{22} - \alpha_{33})^2 + (\alpha_{33} - \alpha_{11})^2 \right) - 1/3\left(\alpha_{12}^{\ 2} + \alpha_{23}^{\ 2} + \alpha_{13}^{\ 2} \right),$$

$$\varphi_3(\mathbf{H}_a) = -\frac{2}{3}(\Delta/3)^3 - \frac{1}{9}\left(\alpha_{11}^{\ 2} + \alpha_{22}^{\ 2} + \alpha_{33}^{\ 2} \right) + \frac{1}{27}(\alpha_{11} + \alpha_{22} + \alpha_{33})^3 - \frac{2}{3}\alpha_{11}\alpha_{22}\alpha_{33} - 2/(3\sqrt{3})\,\alpha_{12}\alpha_{23}\alpha_{31}$$

$$+ \frac{1}{9}\left(\alpha_{23}^{\ 2}(2\alpha_{11} - \alpha_{22} - \alpha_{33}) + \alpha_{31}^{\ 2}(2\alpha_{22} - \alpha_{11} - \alpha_{33}) + \alpha_{12}^{\ 2}(2\alpha_{22} - \alpha_{11} - \alpha_{22}) \right).$$

The roots of the characteristic polynomial are:

$$E_1' = 2(\varphi_2/3)^{1/2}\cos(\Theta/3),$$

$$E_2' = 2(\varphi_2/3)^{1/2}\cos(\Theta/3 - 2/3\pi), \quad (47)$$

$$E_3' = 2(\varphi_2/3)^{1/2}\cos(\Theta/3 + 2/3\pi),$$

where

$$\Theta = \arccos(2\varphi_3(-\varphi_2/3)^{-3/2}). \quad (48)$$

When starting energy from the zone of heavy holes, the total displacements of all three zones under strain, respectively, have the form:

$$E_1(0, \varepsilon) = E_1' - \Delta/3. \quad (49)$$

In the case of whiskers with $\varepsilon \,||\, [111]$, the splitting between heavy and light and heavy holes zones equals:

$$\delta E = 2\sqrt{\Xi_\varepsilon + (\Delta_{so}/3)^2 \left(\cos(\Theta/3) - \cos(\Theta/3 + 4/3\pi) \right)} \quad (50)$$

$$\Theta = \arccos\left(\frac{-3^{3/2}(\Delta_{so}/3)^3 \,|\, d\gamma\varepsilon \,|^3}{\left((\Delta_{so}/3)^2 + \Xi_\varepsilon \right)^{3/2}} \right).$$

Strain dependences of displacements and strain splits of all three zones are calculated for $\varepsilon \,||\, [111]$. Initial shifts of the branches of the zones are also conditionally reflected in the strain genesis of the valence band, which was shown in Fig. 4. Significant increase of spin-orbit splitting and fast saturation of δE, as well as insignificant dependence of shift of the light hole zone under the action of compression strain in Si whiskers, was revealed. The influence of a SO-zone in Si whiskers leads to increase of conduction of holes on twice localized impurities that is observed in negative magnetoresistance.

5. CONCLUSIONS

The p-type silicon whiskers with boron concentration of 2×10^{18} cm^{-3} in the vicinity of MIT were chosen to investigate the longitudinal magnetoconductance in the range of 0-14 T at 4.2 K under compressive strain up to -2×10^{-3} rel. un. The studies have shown that the unstrained whiskers have a quadratic dependence of the magnetoresistance on the magnetic field induction. The strain leads to the appearance of negative magnetoresistance with sufficiently large magnitude (up to 15 %). We proposed to use the WL model to describe the behavior of the whisker magnetoconductance. That allows us to estimate the coherence length L_φ and the spin-orbit length L_{so} corresponding to $T^{-0.53}$ and $T^{-0.45}$, respectively, in a two-dimensional system. Results of studies have confirmed that the conductance mostly occurs in the subsurface layers of Si whiskers. Spin splitting energy $\Delta_{SO} = 1.8$ meV was also obtained due to the known Rashba parameter $a = 5 \times 10^{-15}$ eV·m. According to the two-zone approximation of the *k-p*-method, the strain removal twice degenerate level Γ_8^+ that leads to splitting of light and heavy hole branches, while according to the three-zone model spin-orbit interaction leads to conduction of doubly-occupied states of holes on impurities that is observed in negative magnetoresistance.

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Спін-орбітальне розщеплення валентної зони в кремнієвих ниткоподібних кристалах під дією деформації

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Магнітопровідність ниткоподібних кристалів Si з концентрацією легуючої домішки 2×10^{18} см$^{-3}$ досліджували в інтервалі магнітних полів 0-14 Тл при кріогенних температурах за деформації стиску до -2×10^{-3} відн. од. Легування кристалів бором здійснювали у процесі росту методом хімічного парофазного осадження і концентрація носіїв заряду, згідно холлівських вимірювань, становила порядку 2×10^{18} см$^{-3}$. Одновісну деформацію ниткоподібних кристалів здійснювали шляхом їх закріплення на підкладках з використанням термічної деформації за рахунок різниці коефіцієнтів термічного розширення кристала і матеріалу підкладки. Досліджено поздовжній магнітоопір для недеформованих і деформованих зразків Si в інтервалі температур $4.2 \div 70$ К. Недеформовані зразки мають квадратичну залежність магнітоопору від індукції магнітного поля. Деформація приводить до появи великого від'ємного магнітоопору з максимальною величиною до 15 %. Обговорюються можливі причини цього ефекту. Найбільш вірогідною причиною виникнення від'ємного магнітоопору є слабка локалізація носіїв заряду. Згідно з розрахунками у моделі слабкої локалізації носіїв заряду показано, що довжина когерентності L_φ і довжина спін-орбітальної взаємодії L_{so} пропорційна $T^{-0.53}$ і $T^{-0.45}$, відповідно, що відповідає теоретичним даним $T^{-1/2}$ для двовимірної системи. Це свідчить про те, що основний внесок у провідність ниткоподібних кристалів Si вносить транспорт носіїв заряду у приповерхневих шарах кристалів. Досліджено вплив деформації на спін-орбітальне розщеплення та спектр валентної зони ниткоподібних кристалів. В результаті розрахунків згідно k-p-методу виявлено значне розщеплення гілок легких і важких дірок під дією деформації стиску. Отримано енергію спін-орбітального розщеплення підзони важких дірок Δ_{SO}, яка становить 1.8 меВ.

Ключові слова: Ниткоподібні кристали Si, Магнітопровідність, Спін-орбітальне розщеплення, Деформація.