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Spin-orbit coupling in strained Ge whiskers

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The field dependences of the magnetoresistance for germanium whiskers with gallium doping concentration of $2\cdot10^{17}$cm^{-3} were studied in the magnetic field range 0–14 T at temperature 4.2 K under compressive strain up to 0.2%. The strain influence on a spin-orbit splitting on the valence band spectrum was studied. As a result, the effective mass and the energies of spin-orbit splitting for light and heavy holes were found under the compressive strain according to *kp* method. From an analysis of the Shubnikov–de Haas magnetoresistance oscillations the effective mass of heavy holes $m_c = 0.25\ m_0$ was calculated. The spin-orbit splitting energy of heavy holes $\Delta_{HH} = 1.5$ meV, the Lande factor in direction [111] $g^* = 4.8$ as well as the Rashba cubic parameter of spin-orbit interaction $\beta_{SO} = 1\cdot10^{-28}$ eV·m^3 were found due to the studying of longitudinal magnetoconductance in strained Ge whiskers at low temperatures. The appearance of negative magnetoresistance in the magnetic field range up to 7 T likely results from the effect of charge carrier interaction.

Keywords: germanium whiskers, magnetoresistance oscillations, electron-electron interaction, strain, cryogenic temperatures.

1. Introduction

Nanostructures based on Ge are of great interest due to surprising physical effects such as SdH oscillations [1], weak localization (WL)/weak anti-localization (WAL) crossover [2], extraordinary large Lande factor [3]. The effect of resonance of *g*-factor is likely connected with strong anisotropy resulted from 2 DEG electron conductance on surface layers of the structures [4]. However, the valence band is very important when the external perturbation is applied to the samples. Thus, Rashba spin-orbit interaction is important for heavy-hole–light-hole mixing [5]. The good perturbation tool is the strain [6]. Due to the application of strain to Ge sample, the six-fold degenerated valence band splits into three sub-bands corresponding to light and heavy holes as well as sub-band of SO splitting, which is enough large and amounts to 0.29 eV. Light and heavy hole sub-bands in turns splits due to spin-orbit coupling (SOC) under strain in the **k** direction. The value of the energy splitting Δ_{SO} as well as hole effective mass could be estimated accounting Shubnikov–de Haas (SdH) oscillations or effect of weak localization of charge carriers by use of cubic Rashba parameter β_{SO} [7]. The procedure is widely used for 2DEG holes in Ge nanostructures [1,3,7]. Nevertheless, Ge whiskers have been investigated under strain action showing magnetophonon oscillations and giving the values of effective mass of heavy and light holes [8]. However, SOC in the whiskers have not been studied. Therefore, the purpose of the paper is to study the magnetoresistance of doped germanium whiskers with concentration in the vicinity to MIT under compressive strain and magnetic field up to 14 T to determine the conduction mechanism of such crystals at low temperatures.

2. Experimental procedure

As the object of investigation, the *p*-type germanium microcrystals were chosen with gallium concentration correspondent to dielectric side of metal-insulator transition $2\cdot10^{17}$ cm^{-3}. The germanium whiskers were grown in a closed bromide system by CVD method [9]. Electrical contacts were established by pulse welding, which provides the necessary ohmic contacts. Conductivity was studied at temperature 4.2 K. For these studies, crystals were cooled to liquid helium temperature in the helium cryostat. The temperature was measured by using the thermocouple Cu–CuFe calibrated with the use of the CERNOX sensor. The magnetic field effects of the whiskers were studied using the Bitter magnet with the induction up to 14 T and the time scanning of field 1.75 T/min. Stabilized electric current along the whisker was created by the current source Keithley 224 in the range 1–100 μA depending on the crystal resistance. CERNOX sensor was used for magnetic measurement, 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 longitudinal magnetoresistance of the p-type germanium whiskers with gallium concentration $2\cdot10^{17}$ cm^{-3} was measured in the range 0–14 T at temperatures 4.2–60 K under the compressive strain up to 0.2%. The field dependences of the magnetoresistance for strained and unstrained samples are provided in Fig. 1. As obvious from Fig. 1 the unstrained whiskers have a parabolic dependence of the magnetoresistance on the magnetic field induction. Besides in the range of low magnetic fields, the negative magnetoresistance (NMR) is observed, while at high magnetic fields the magnetoresistance oscillations at 5 and 10 T take place. The strain leads to a decrease in the negative magnetoresistance magnitude as well as an increase of the magnetoresistance oscillations. Besides the range of the NMR is wider (up to 7 T) in strained samples as compared with unstrained ones (up to 2 T) (see inset of Fig. 1). The magnetoresistance oscillation behavior differs in strained and unstrained whiskers. There are two oscillations peaks at 6.5 and 10 T for unstrained whiskers, while oscillations is greater for strained ones. In particular, five magnetoresistance peaks in the range of the magnetic field induction from 5 to 13 T are observed. The field dependences of magnetoresistance for stained samples at various T are shown in Fig. 2. Amplitude of magnetoresistance oscillations substantially drops with the temperature rise. Thus, at temperature 54 K the attenuation of oscillations takes place.

One can calculate the magnetoresistance oscillation period as an average difference between the neighboring peaks in the opposite magnetic field. The oscillation period for unstrained samples is 0.52 T^{-1}. The strain is shown to influence slightly on the period of oscillations, while the peak splitting was found to occur. The splitting indicates a strong spin-orbit interaction induced by the strain of the whisker.

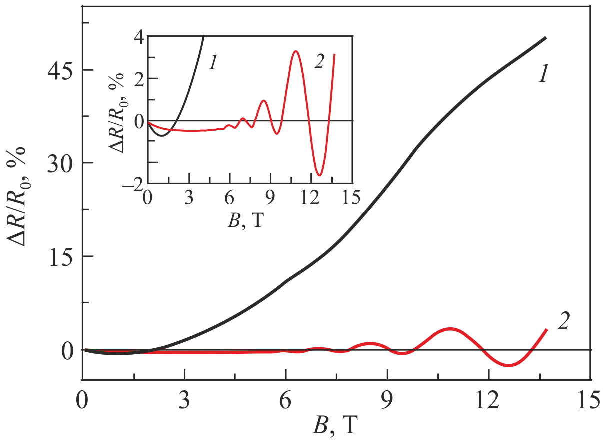

Fig. 1. The field dependences of the longitudinal magnetoresistance for unstrained (*1*) and strained (*2*) germanium samples at temperature 4.2 K. Inset: the field dependences of the negative magnetoresistance.

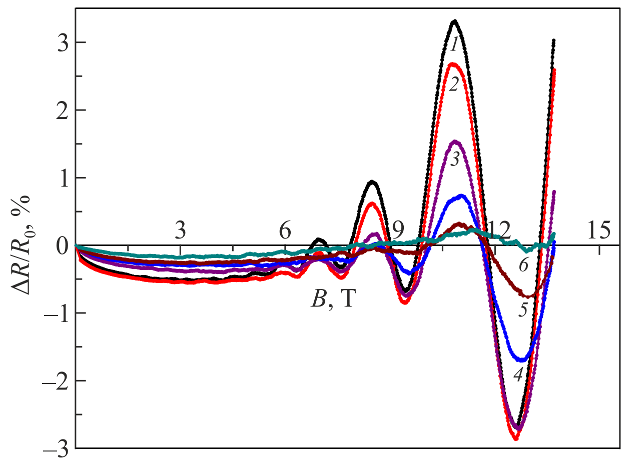

Fig. 2. (Color online) The field dependences of the longitudinal magnetoresistance for germanium whiskers under uniaxial compressive strain at various fixed temperatures: 4.2 (*1*), 6 (*2*), 12 (*3*), 22 (*4*), 35 (*5*), 54 (*6*) K.

4. Discussion

4.1. The mathematical model of perturbation of the strain for the energy spectrum of three subband holes in the valence band of germanium

The strain forces to degenerate energy spectrum of heavy and light holes as described by the perturbation theory, summing up the well-known consideration [10] to arbitrary strains and highlighting the geometric aspects of the theory.

The influence of strain on three subbands of holes $(2\Gamma_8^+, \Gamma_7^+)$ in the valence band of germanium is considered, taking into account their spin-orbit interaction. It is shown that, in accordance with the fourfold degeneracy of the energy spectrum, the effect of finite strain on the heavy ($l = 1$) and light hole ($l = 2$) regions can be written in an invariant tensor form, symmetric with respect to the multiplication $k_i k_j$ accompanying strained system of coordinates of the wave vector and the strain tensor ε:

$$E_l(\mathbf{k},\varepsilon) = Ak^2 + a\,\mathrm{Sp}\,\varepsilon + (-1)^l\Big(\sum B^{ijmn}k_ik_jk_mk_n + 2\Big|\sum D^{ijmn}k_ik_j\varepsilon_{mn}\Big| + \sum d^{ijmn}\varepsilon_{ij}\varepsilon_{mn}\Big)^{1/2}, \quad (1)$$

where B^{ijmn}, D^{ijmn}, d^{ijmn} are generalized contravariant tensors of the band parameters and strain constants. To represent Γ_8^+ these tensors have the following components:

$$B^{iiii} = B^2,\ B^{iimm} = -B^2/2,\ B^{ijmn} = D^2/4,$$
$$D^{iiii} = Bb,\ D^{iimm} = -Bb/2,\ D^{ijmn} = Dd/4,$$
$$d^{iiii} = b^2,\ d^{iimm} = -b^2/2,\ d^{ijmn} = d^2/4,\ i \ne j,\ m \ne n, \quad (2)$$

where A, B, D are band parameters, a, b, d are the strain constants of the valence band.

The splitting of the zones of heavy and light holes in the center of the Brillouin zone is equal

$$\delta E = 2\left(\sum d^{ijmn}\varepsilon_{ij}\varepsilon_{mn}\right)^{1/2}. \quad (3)$$

On a one-parameter subgroup, the strain of the splitting $\delta E \sim |\varepsilon|$ is not an analytic function of strain in the vicinity $\varepsilon \to 0$. In the multiparameter case $\delta E \sim \varepsilon_{ij}^2$ with $\varepsilon \to 0$. Figure 3 shows the energy spectrum of the valence band of Ge under the uniaxial compressive strain along the crystallographic direction [111] (E = 180 meV).

To account for the spin-orbit-deflated so-zone ($l = 3$) having the representation symmetry Γ_7^+, we accept the known nonlinear strain of the approximation of the energy spectrum in the vicinity $\mathbf{k} \approx 0$ obtained by the invariant method. In Ge, the influence of the so-zone is felt only with significant compressive and tensile strain $|\varepsilon| > 0.6\%$.

A convenient calculation formula was proposed for determining the density of states $g_l(E, \varepsilon)$ of the lth carrier type in a strained semiconductor: a measure that occurs when the volume element dk^3 is averaged over the isoelectric surface of the S_E:

$$g_l(E,\varepsilon)dE = \left\langle \left(dk^3\right)\right\rangle = \left\langle \left|\mathbf{J}_l^{-1}\right|\right\rangle dE = \frac{dE}{4\pi}\int_{S_E} \mathrm{Det}\left(\mathbf{J}_l^{-1}\right) dS_E, \quad (4)$$

where $dS_E = d\zeta_1 d\zeta_2$ is the element of the surface in arbitrary coordinates (ζ_1, ζ_2) of the isoenergy surface; $\mathbf{J}_l$ is Jacobi matrix of coordinate change $(E, \zeta_1, \zeta_2) \to (k_1, k_2, k_3)$.

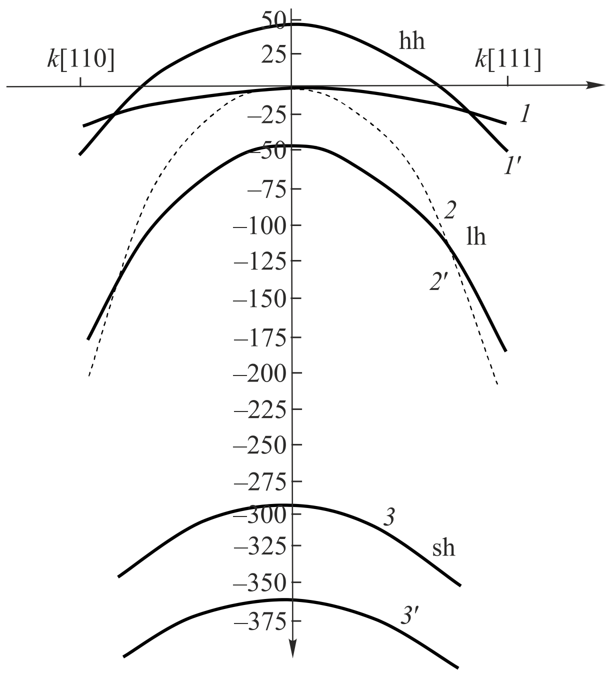

Fig. 3. The energy spectrum of the valence band of Ge under the uniaxial compression along the crystallographic direction [111]: *1*, *1′* — hh (heavy hole), *2*, *2′* — lh (light hole), *3*, *3′* — sh; *1*, *2*, *3* — ε = 0; *1′*, *2′*, *3′* — ε = 0.4%.

The effective density masses of the states of the m_{dl} holes in the strained Ge were determined by comparing the densities of the first-degree holes in the strained semiconductor with the corresponding expression for the standard (isotropic and parabolic) zone, calculated numerically from expression (4)

$$\frac{\left(2m_{dl}\left(E,\varepsilon\right)\right)^{3/2} E^{1/2}}{2\pi^2\hbar^3} = \left\langle\left|\mathbf{J}_l^{-1}\right|\right\rangle. \quad (5)$$

Calculated in this way, the charge carrier effective masses of density states vs energy E_1 for the heavy and light holes in Ge is shown in Fig. 4.

Depending on the energy and strain, these masses change in several times, and at low energies the intervals of their values intersect. Attracts the attention the jump-like behavior of effective masses in the vicinity of $E \to 0$, $\varepsilon \to 0$:

$$\lim_{E\to 0,\varepsilon\to 0} m_{dl} = \left(m_{dl}\right)_{\mathrm{el}} \neq \lim_{E\to 0,\varepsilon\to 0} m_{dl} = m_{dl}\left(\varepsilon = 0\right) \quad (6)$$

which is a consequence of the nonanalyticity of the band spectrum on one-parameter subgroups of strain in the vicinity $\mathbf{k} \to 0$, $\varepsilon \to 0$. The values of the chemical potential were calculated numerically, accounting for the level of boron doping and the conditions of constant concentration of holes at anisotropic strain. The chemical potential increases both in compression and in tensile, that is, with the strain the degeneration of the hole gas increases.

4.2. Analysis of SdH oscillations in strained Ge *whiskers*

The magnetoresistance oscillation period P in the opposite field for quadratic dispersion law is described as

$$P = \Delta\left(\frac{1}{H}\right) = \frac{\hbar|e|}{E_F m_c c}, \quad (7)$$

where e is the elementary charge; h is the Planck constant; E_F is the Fermi energy; m_c is the effective mass of holes.

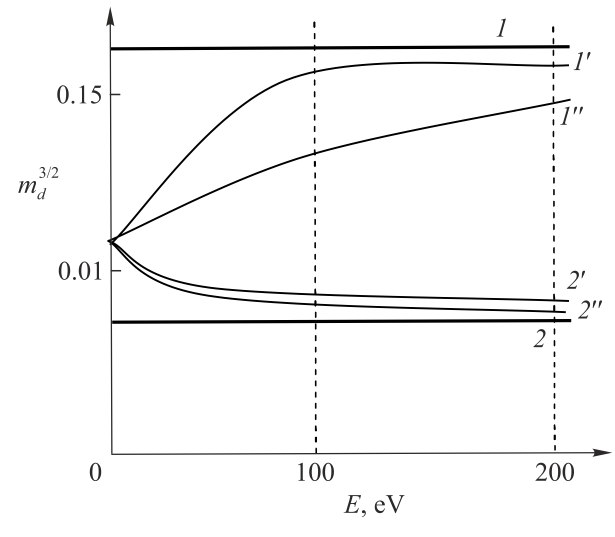

Fig. 4. Effective masses of the density states of hole in uniaxial compressed germanium: *1*, *1′*, *1″* — hh (heavy hole), *2*, *2′*, *2″* — lh (light hole), at strain: *1*, *2* — ε = 0; *1′*, *2′* — ε = 0.4%; *1″*, *2″* — ε = 1.2%.

The effective cyclotron mass was determined according to the relative change in the amplitude of oscillations at two different temperatures [11]:

$$m_c = \frac{|e|\hbar H}{2\pi^2 k T_1 c} \operatorname{arccosh} \frac{A(T_1,H)}{A(T_2,H)}, \tag{8}$$

where k_B is the Boltzmann constant.

This expression applies in the semiclassical region of fields assuming that it does not change with temperature and magnetic field. For small magnetic fields, $m_c = 0.25\, m_0$, which is consistent with literature data for heavy holes for strained Ge crystals [12,13]. Substituting the value of effective mass in the Eq. (7) one can obtain the Fermi energy $E_F = 180$ meV. According to Fig. 2 at such hole energy, the value of effective mass corresponds to 0.25 m_e. Thus, the value of effective mass for heavy holes calculated by the use of *kp* method and SdH oscillations almost coincides confirming the adequate approach.

The Shubnikov–de Haas oscillations splitting of the Rashba spin-splitting holes may be described by the following equation [14]:

$$\frac{\Delta\rho_{xx}(B)}{\rho_{xx}(0)} = 4\cos\left(\frac{2\pi m^*\left(E_F \pm \beta_{SO} k_F^3\right)}{\hbar e B}\right) \times \exp\left(-\frac{\pi m^* \alpha_D}{e B \tau_t}\right)\frac{\psi}{\sinh\psi}, \tag{9}$$

where E_F is the Fermi energy, $\alpha_D = \tau_t/\tau_q$ is the Dingle ratio, where τ_t is the transport scattering time and τ_q is the quantum scattering time, β_{SO} is the cubic Rashba spin-orbit parameter and

$$\psi = \frac{2\pi^2 k_B T m^*}{\hbar e B}. \tag{10}$$

Equation (9) may be solved iteratively to determine the two unknown parameters, the cubic Rashba coefficient β_{SO} and the Dingle ratio α_D [7,15]. The two curves of Fig. 2 at various temperatures were involved in this iterative process giving cubic Rashba coefficient $\beta_{SO} = 1.5\cdot10^{-28}$ eV·m^3 and a Dingle ratio $\alpha_D = 17$. The obtained Rashba parameter β_{SO} is in agreement with the literature data in Ge quantum wells $1\cdot10^{-28}$ eV·m^3 [15]. Nevertheless, it should be noted that the estimation of a Dingle ratio over a wide range of magnetic fields gives rather different results changing from 19.7 to 10.6 with a magnetic field induction increase for SiGe/Ge/SiGe heterostructures [16]. Therefore, our estimations in the range of magnetic field 8.5–11 T, where the most pronounced maxima were observed, have only approximate character.

Substituting the magnitude of wave number $k_F = 2\cdot10^8$ m^{-1} [17] in

$$\Delta_{HH} = 2k_F^3 \beta_{SO} \tag{11}$$

spin splitting energy Δ_{HH} can be obtained, which, in this case, was found to be $\Delta_{HH} = 1.5$ meV.

The magnetoresistance oscillation splitting allows us to find the *g*-factor. The spin-orbit splitting peaks of magnetoresistance oscillations at the magnetic field B_2 $g^*\mu_B B$ coincides with the Landau level splitting $\Gamma = \hbar e B_1 / m_c^*$, that can be written as $\Gamma = \hbar e B_1 / m_c = g^* \mu_B B_2$. Since the Bohr magneton $\mu_B = e\hbar / 2m_0$, then we obtained [18,19]

$$g^* = 2\left(B_1 m_0 / B_2 m_c^*\right). \tag{12}$$

The estimated value of the *g*-factor for strained Ge whiskers with a direction [111] $g = 4.8$. The value is in good agreement with the literature data, in particular, 4.3 [3] and 7 [20] for Ge quantum wells. However, the *g*-factor in *p*-Ge quantum wells is very anisotropic and depending on the strain direction it could changes in the wide range, i.e., from 1.3 to 28 [21].

The possible reasons for the NMR effect in the magnetic field induction range 0–7 T are: a) strongly defective whisker structure; b) presence of magnetic impurity; c) size effect; d) week localization (WL); e) electron-electron interaction (EEI).

The whiskers have perfect volume and surface crystalline structure according to their growth conditions by VLS mechanism. They have no magnetic impurities, which was investigated by the diamagnetic magnetization like that of bulk germanium. Due to large whisker dimensions (of about 30 μm in diameter) the quantum size effect is hardly responsible for the observed negative magnetoresistance similar to Si whiskers [22]. As has been shown in [23], a diffusive regime of charge carrier transport in Ge crystals, where approximation of weak localization is fair, occurs at weak magnetic fields (up to 0.2 T). Thus, NMR observing in the range of magnetic field induction 0.2–9 T (Fig. 2) could not be connected with weak localization. Transport of charge carriers in the investigated magnetic fields takes place in intermediate and ballistic regime [23]. Then NMR can be explained by charge carrier interaction (EEI). The authors of [24] have observed the negative quadratic magnetoresistance in SiGe/Ge/SiGe heterostructures in a wide interval of magnetic fields with the onset of SdH oscillations as monotonic line which combines the geometric locus of midpoints between adjacent maxima and minima. Taking into account the interference of electron wave in the short-range scattering on impurity potential the interaction correction gives negative magnetoresistance in a wide range of the inequality $k_B T\tau/h > 1$ [25]. Therefore, we can explain qualitatively the NMR by charge carrier interaction. For quantitative evaluations, additional research of Hall magnetoresistance of the whiskers is needed, which will be the next stage of the consideration.

5. Conclusion

The *p*-type germanium whiskers with boron concentration $2\cdot10^{17}$ cm^{-3} in the vicinity to the MIT were chosen to investigate the longitudinal magnetoconductance in the range 0–14 T at 4.2 K under the compressive strain up to 0.2%. The studies have shown that unstrained whiskers have a parabolic dependence of the magnetoresistance on the magnetic field induction. The strain leads to the appearance of the negative magnetoresistance with a sufficiently large magnitude (up to 15%). The results of the studies have confirmed that the conductance mostly occurs in the subsurface layers of Ge whiskers. According to the two-zone approximation of the *kp*-method, the strain removal twice degenerate level Γ_8^+ that leads to the splitting of light and heavy hole branches. From the SdH magnetoresistance oscillations, the calculated effective mass of heavy holes $m_c = 0.25m_0$ corresponds to decreased value due to the compressive strain. The spin splitting energy for heavy holes $\Delta_{HH} = 1.5$ meV was also obtained due to the obtained Rashba parameter $\beta_{SO} = 1\cdot10^{-28}$ eV·m^3. The splitting of magnetoresistance oscillations under the strain in the direction [111] allows us to determine the *g*-factor in Ge whiskers which is equal to 4.8 and is in good agreement with the literature data for Ge quantum wells. Negative magnetoresistance observed in the range of magnetic field induction up to 7 T could be explained by charge carrier interaction due to their interference in the short-range scattering on impurities.

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Спін-орбітальна взаємодія у деформованих ниткоподібних кристалах Ge

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Вивчено польові залежності магнітоопору ниткоподібних кристалів германію з концентрацією легувальної домішки галію $2\cdot10^{17}$ см$^{-3}$ в діапазоні магнітних полів 0–14 Тл за температури 4,2 К під дією деформації стиску 0,2%. Проведені розрахунки впливу одновісної деформації на спектр валентної зони германію за *kp*-методом дозволили оцінити енергії спін-орбітального розщеплення та ефективні маси легких та важких дірок. На основі аналізу осциляцій магнітоопору Шубнікова–де Гааза одержано значення ефективної маси важких дірок $m_c = 0{,}25m_0$, енергії спін-орбітального розщеплення $\Delta_{HH} = 1{,}5$ меВ, *g*-фактора Ланде в напрямі [111] $g^* = 4{,}8$ та кубічного параметра Рашби спін-орбітальної взаємодії $\beta_{SO} = 1\cdot10^{-28}$ еВ·м^3. Згідно теорії слабкої локалізації, для поздовжньої магнітопровідності деформованих ниткоподібних кристалів Ge за низьких температур визначено довжини фазової та спін-орбітальної когерентності носіїв заряду.

Ключові слова: ниткоподібні кристали германію, осциляції магнітоопору, слабка локалізація, деформація, кріогенні температури.

Спин-орбитальное взаимодействие в деформированных нитевидных кристаллах Ge

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Изучены полевые зависимости магнитосопротивления нитевидных кристаллов германия с концентрацией легирующей примеси галлия $2\cdot10^{17}$ см$^{-3}$ в диапазоне магнитных полей 0–14 Тл при температуре 4,2 К под действием деформации сжатия 0,2%. Проведенные расчеты влияния одноосной деформации на спектр валентной зоны германия по *kp*-методу позволили оценить энергии спин-орбитального расщепления и эффективные массы легких и тяжелых дырок. На основе анализа осцилляций магнитосопротивления Шубникова–де Гааза получены значения эффективной массы тяжелых дырок $m_c = 0{,}25m_0$, энергии их спин-орбитального расщепления $\Delta_{HH} = 1{,}5$ мэВ, *g*-фактора Ланде в направлении [111] $g^* = 4{,}8$ и кубического параметра Рашбы спин-орбитального взаимодействия $\beta_{SO} = 1\cdot10^{-28}$ эВ·м^3. Согласно теории слабой локализации, для продольной магнитопроводимости деформированных нитевидных кристаллов Ge при низких температурах определены длины фазовой и спин-орбитальной когерентности носителей заряда.

Ключевые слова: нитевидные кристаллы германия, осцилляции магнитосопротивления, слабая локализация, деформация, криогенные температуры.