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Calculation of Electron Mobility for the Strained Germanium Nanofilm

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The values of relative deformation that arises in the germanium nanofilm grown on the $Ge_{(x)}Si_{(1-x)}$ (001) substrate, depending on its component composition, on the basis of the theory of elasticity have been calculated. For such orientation of the substrate, the germanium nanofilm in the crystallographic directions [100], [010] (in the substrate plane) experiences biaxial compression and in the crystallographic direction [001] – uniaxial stretching. It is shown that the internal mechanical strains reach 4 % in the case of a silicon substrate. Calculations of the band structure for a strained germanium nanofilm show that with increasing values of the internal mechanical strains (due to increasing Si content in the substrate), four Δ_1 minima of the conduction band will be descend down, and L_1 minima will ascend up on the energy scale. In doing so, the valence band undergoes splitting into two branches, the upper one of which is the valence band of "heavy" holes. Four Δ_1 minima of the conduction band become the lowest in the energy spectrum of a strained germanium nanofilm when the Ge content in the substrate is less than 60 %. The carried out calculations of electron mobility based on the theory of anisotropic scattering by acoustic phonons show that an increase in the relative content of germanium in the substrate leads to an increase in the electron mobility in the nanofilm. This is explained by the deforming redistribution of electrons between the four L_1 minima with greater mobility and four Δ_1 minima with less mobility. It has been established that for germanium nanofilms of thickness $d > 7$ nm, the electron mobility does not depend on their thickness. The obtained results could be used in modelling the electrical properties of strained germanium nanofilms, on the basis of which various electronic devices of modern nanoelectronics with the projected working characteristics could be created.

Keywords: Uniaxial strain, Germanium nanofilm, Mechanical strains, Anisotropic scattering, Germanium band structure.

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1. INTRODUCTION

Achievements and prospects of further development of micro- and nanolectronics, optics, instrumentation and other branches of new technology are connected with the physics of thin films. Advances in this field became possible by using the controlled epitaxial growth of thin layers of semiconductors, metals and dielectrics in vacuum from various environments [1, 2]. The basis of modern nanoelectronics is heterojunctions and semiconductor superlattices. Of particular interest to researchers is pseudomorphic strained heterostructures, in particular, silicon-germanium structures with a compatible lattice. This is due to the possibility of controlling a wide range of physical properties of the composite layers of the structure by changing the value of strain and the ratio of the thicknesses of the contacting semiconductors [5]. Nanostructures based on the strained germanium attract the attention of technologists and researchers due to the great success of the possibility of creating new prospective devices, which use quantum-size effects [6-10].

Therefore, there is considerable scientific and practical interest in the study of the influence of internal deformation fields on the band structure and electrical properties of nanostructures based on germanium.

2. RESULTS OF CALCULATIONS AND THEIR DISCUSSION

The germanium band structure and electrical properties of the strained germanium nanofilm grown on the $Ge_{(x)}Si_{(1-x)}$ substrate with crystallographic orientation (001) was investigated in this article.

The influence of deformation on the semiconductor is described in the literature in sufficient detail. There are both experimental and theoretical studies [11, 12]. The crystal lattice of most semiconductors (the type of diamond or zinc blende) has cubic symmetry. If the semiconductor is subjected to the action of strain, then, in general, its symmetry decreases and the electron spectrum changes [11].

The discrepancy between the lattice constants of germanium and the $Ge_{(x)}Si_{(1-x)}$ substrate is the cause of occurrence of the internal mechanical strains in the germanium film. We designate the lattice constants in the crystallographic directions [100] and [010] as $a_\parallel$ (the same for the substrate and nanofilm), and in the direction [001] – $a_{\perp i}$ (different for the substrate and nanofilm). We will assume that strains in the nanofilm are homogeneous in thickness. Then the expressions for the lattice constants of the crystalline layers of the substrate and the nanofilm along the contact plane $a_\parallel$ and in the perpendicular direction $a_{\perp i}$ can be written as:

$$a_\parallel = \frac{\sum_{i=1}^{N}\chi_i h_i}{\sum_{i=1}^{N}\frac{\chi_i h_i}{a_i}}, a_{\perp i} = a_i + \frac{2\upsilon_i}{1-\upsilon_i}\left(a_i - \frac{\sum_{i=1}^{N}\chi_i h_i}{\sum_{i=1}^{N}\frac{\chi_i h_i}{a_i}}\right). \quad (1)$$

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The values of relative deformations in each layer are determined by the equations:

$$\begin{aligned}&(\varepsilon_i)_{12}=(\varepsilon_i)_{23}=(\varepsilon_i)_{13}=0,\\&(\varepsilon_i)_{11}=(\varepsilon_i)_{22}=\frac{a_{\parallel}-a_i}{a_i},\\&(\varepsilon_i)_{33}=\frac{a_{\perp i}-a_i}{a_i},\end{aligned}\qquad(2)$$

where the indices 1, 2, 3 determine the crystallographic directions [100], [010], [001], respectively.

Using expressions (1) and (2), one can determine the lattice constants and relative deformations arising in the layers based on semiconductor materials with crystalline lattices of the diamond type or zinc blende.

For the considered case, taking into account that the thickness of the substrate $h_{Ge(x)Si(1-x)}$ is much larger than the thickness of the germanium film h_{Ge}, the expressions (2) (without taking into account deformation in the substrate) can be represented as follows:

$$\begin{aligned}&(\varepsilon_{Ge})_{11}=(\varepsilon_{Ge})_{22}=\frac{a_{\mathrm{Ge(x)Si(1\text{-}x)}}-a_{Ge}}{a_{Ge}},\\&(\varepsilon_{Ge})_{33}=-\frac{2\upsilon_{Ge}}{1-\upsilon_{Ge}}\frac{a_{\mathrm{Ge(x)Si(1\text{-}x)}}-a_{Ge}}{a_{Ge}},\end{aligned}\qquad(3)$$

where $\upsilon_{Ge}=0.26$ [12].

The lattice constant of the $Ge_{(x)}Si_{(1-x)}$ alloy versus the component composition varies according to the law [5]:

$$a_{Ge(x)Si(1-x)}=a_{Si}(1-x)+a_{Ge}x-bx(1-x),\qquad(4)$$

where $b = 1.88\cdot10^{-2}$ Å.

The dependencies of the relative deformations on the component composition of the $Ge_{(x)}Si_{(1-x)}$ substrate can be obtained for the germanium nanofilm, taking into account the expressions (3) and (4), the values of the germanium's a_{Ge} = 5.658 Å and silicon's a_{Si} = 5.431 Å [12] lattice constants (Fig. 1).

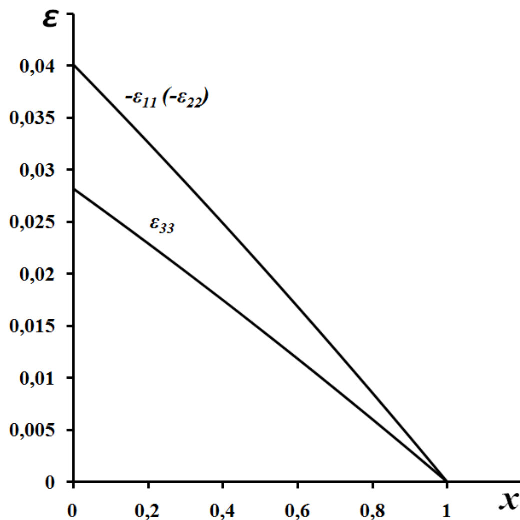

Fig. 1 – Dependencies of the values of relative deformations in the germanium nanofilm on the component composition of the $Ge_{(x)}Si_{(1-x)}$ substrate

As follows from Fig. 1, for the germanium nanofilm in the directions [100], [010] the value of the relative deformation $\varepsilon_{||}$ is negative (the film is compressed) and in the direction [001] the deformation $\varepsilon_{\perp}$ is positive (the film is stretched). The band structure of the strained germanium nanofilm on the $Ge_{(x)}Si_{(1-x)}$ substrate depending on its component composition can be calculated using the data on the components of the deformation tensor.

A simple compression or stretching (without shear deformations) along the crystallographic directions [100], [010] and [001] lead to the same shift of the four L_1 minima of the germanium conduction band [11]

$$\Delta E_i=\left(\Xi_d^{L_1}+\frac{1}{3}\Xi_u^{L_1}\right)\Delta,\qquad(5)$$

where $\Delta=\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}$ is a change in volume at deformation.

For germanium, the constants of the deformation potential are $\Xi_d^{L_1}$ = – 6.4 eV and $\Xi_u^{L_1}$ = 16.4 eV [12].

Shift of the energy minima of type Δ_1 of the germanium conduction band, which are located in the directions [100], [010] and [001], under the influence of deformation is determined by the equations [11]:

$$\begin{aligned}&\Delta E_1[100]=\Xi_d^{\Delta_1}\Delta+\Xi_u^{\Delta_1}\varepsilon_{11};\\&\Delta E_2[010]=\Xi_d^{\Delta_1}\Delta+\Xi_u^{\Delta_1}\varepsilon_{22};\\&\Delta E_3[001]=\Xi_d^{\Delta_1}\Delta+\Xi_u^{\Delta_1}\varepsilon_{33}.\end{aligned}\qquad(6)$$

The values of the constants of the deformation potential $\Xi_u^{\Delta_1}=11{,}82$ eV and $\Xi_d^{\Delta_1}=-1{,}29$ eV for Δ_1 minimum have been found in work [14].

Shift of the Γ_2 minimum, which is located in the center of the Brillouin zone, is described by the expression [11]:

$$\Delta E[000]=\Xi^{\Gamma_2}\Delta,\qquad(7)$$

Ξ^{Γ_2} = – 6.8 eV [12].

Change in the valence band under the action of deformation has a complex character. For homogeneous deformations, the expression for splitting of the valence band can be represented as [11]:

$$\Delta E_{\upsilon}=a_{\upsilon}\Delta\pm b_{\upsilon}\left|(\varepsilon_{11}-\varepsilon_{33})\right|,\qquad(8)$$

where a_{υ} and b_{υ} are the constants of the deformation potential of the valence band. For germanium, a_{υ}(Ge) = 1.24 eV, b_{υ}(Ge) = – 2.86 eV at T = 300 K [15], the sign «+» corresponds to "light" holes and the sign «–» – to "heavy" holes. The action of deformations in Ge leads to the lifting of degeneration of the valence zones of the "light" and "heavy" holes at the point Γ_{25} and their splitting.

On the basis of expressions (5)-(8), taking into account the values of the constants of the deformation potential of the germanium conduction and valence bands, the calculations of the band structure of the strained germanium nanofilm depending on the component composition of the $Ge_{(x)}Si_{(1-x)}$ substrate have

been conducted. In Fig. 2, we illustrate the results of the calculations. As seen from Fig. 2, for the case of a silicon substrate ($x = 0$), the four Δ_1 minima of the conduction band of the germanium nanofilms will be the lowest on the energy scale, and the valence band of the "heavy" holes will be on the top. The growth of the germanium content in the substrate leads to an increase in the band gap width and decrease in the band splitting of the "light" and "heavy" holes of the nanofilm. In the case, when the germanium content in the substrate is $x > 0.6$, the L_1 minima become dominant in the energy spectrum of the germanium nanofilm. It is also obvious that the deformation leads to both quantitative and qualitative changes of the band structure of deformed semiconductors; this, in turn, will lead to a significant change in the electrical properties of the strained Si/Ge heterojunction.

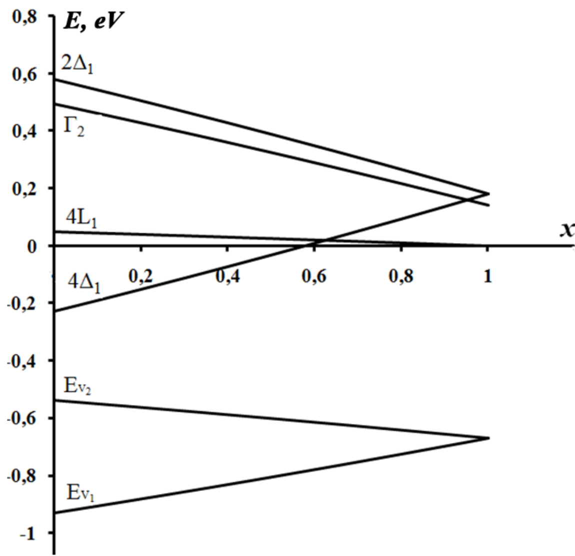

Fig. 2 – The band structure of the strained germanium nanofilm grown on the $Ge_{(x)}\,Si_{(1-x)}$ (001) substrate

Specific electrical conductivity of the strained germanium nanofilm in the considered case can be written as

$$\sigma = qn\mu = q(n_{L_1}\mu_{L_1} + n_{\Delta_1}\mu_{\Delta_1}), \qquad (9)$$

where n_{L_1}, n_{Δ_1}, $\mu_{L_1}, \mu_{\Delta_1}$ are the electron concentrations and mobilities for L_1 and Δ_1 minima, respectively, μ is the effective electron mobility, n is the electron concentration in the conduction band (equal to the sum of electron concentrations in L_1 and Δ_1 minima), q is the module of electron charge.

The total energy of the current carrier of the nanofilm has a discrete-continuous spectrum. It represents the sum of the discrete levels of energy associated with motion in the direction of quantization and a continuous component that describes the motion in the nanofilm plane [16]. Let the nanofilm is located in the XOY plane, where its dimensions are macroscopic and its thickness d (which has a nanosize) is counted along the Z coordinate. Under these conditions, the motion of the current carrier along the Z-axis is equivalent to the motion in a rectangular potential well of width d.

The electron concentration in the nanofilm in the case of the non-degenerate electron gas [17]:

$$n = \left(\frac{2}{d}\sum_{n=1}^{\infty} e^{-\frac{h^2 n^2}{8m_{\parallel} kTd^2}}\right)\frac{2\pi m_{\perp} kT}{h^2}\cdot e^{\frac{E_F - E_C}{kT}}, \qquad (10)$$

where E_F is the Fermi energy, E_C is the energy position of the bottom of the conduction band, $m_{\parallel}$ and $m_{\perp}$ are the components of the effective mass tensor of an electron.

Then, according to (9), the relative change of the effective electron mobility

$$\frac{\mu}{\mu_{L_1}} = \frac{A + \frac{\mu_{\Delta_1}}{\mu_{L_1}}}{A+1}. \qquad (11)$$

In this expression, A is the ratio of the electron concentrations in the L_1 and Δ_1 minima, which according to (10) is equal:

$$A = \frac{n_{L_1}}{n_{\Delta_1}} = \frac{\sum_{n=1}^{\infty} e^{-\frac{h^2 n^2}{8m_{\parallel}^{L_1} kTd^2}}}{\sum_{n=1}^{\infty} e^{-\frac{h^2 n^2}{8m_{\parallel}^{\Delta_1} kTd^2}}}\left(\frac{m_{\perp}^{L_1}}{m_{\perp}^{\Delta_1}}\right)\cdot e^{\frac{E_{\Delta_1} - E_{L_1}}{kT}} = f(d)\cdot e^{\frac{E_{\Delta_1} - E_{L_1}}{kT}}, \qquad (12)$$

where E_{L_1}, E_{Δ_1} are the energy positions of the L_1 and Δ_1 minima of the conduction band of the strained germanium nanofilm.

The growth of the electron mobility for the strained germanium nanostructure in the case of isotropic electron scattering by the acoustic deformation potential was estimated in [18]. The calculations of the authors of this work showed that with such values of internal mechanical strains, when germanium becomes a direct-gap semiconductor material, the electron mobility increases hundreds of times. For a more accurate estimation, it is also necessary to take into account the influence of electron mobility anisotropy.

Constant-energy surfaces for both L_1 and Δ_1 minima are the ellipsoids of rotation. Then, the charge carrier mobility in an arbitrary direction can be determined from the relation [11]:

$$\mu = \mu_{\perp}\sin^2\theta + \mu_{\parallel}\cos^2\theta, \qquad (13)$$

where θ is the angle between the considered direction and the principal axis of the ellipsoid; $\mu_{\perp}$ and $m_{\parallel}$ are the mobilities of charge carriers across and along the ellipsoid axis, respectively.

According to (13), for the L_1 minimum

$$\mu^{L_1} = \frac{1}{3}\mu_{\parallel}^{L_1} + \frac{2}{3}\mu_{\perp}^{L_1} \qquad (14)$$

and for the case of four-ellipsoidal Δ_1 model of the conduction band of the strained germanium nanofilm (see Fig. 2)

$$\mu^{\Delta_1} = \frac{1}{2}\mu_{\parallel}^{\Delta_1} + \frac{1}{2}\mu_{\perp}^{\Delta_1} . \quad (15)$$

The components of the mobility tensor $\mu_{\perp}$ and $\mu_{\parallel}$ for the L_1 and Δ_1 minima are equal to

$$\mu_{\parallel}^{L_1,\Delta_1} = \frac{q}{m_{\parallel}^{L_1,\Delta_1}} < \tau_{\parallel}^{L_1,\Delta_1} >; \quad \mu_{\perp}^{L_1,\Delta_1} = \frac{q}{m_{\perp}^{L_1,\Delta_1}} < \tau_{\perp}^{L_1,\Delta_1} > . \quad (16)$$

Based on the theory of anisotropic scattering, we write the expressions for $\tau_{\parallel}^{L_1,\Delta_1}$ and $\tau_{\perp}^{L_1,\Delta_1}$ under the conditions of electron scattering by impurity ions and acoustic phonons [11]:

$$\tau_{\parallel}^{L_1,\Delta_1} = \frac{a_{\parallel}^{L_1,\Delta_1}}{\sqrt{k}T^{\frac{3}{2}}} \cdot \frac{1}{\sqrt{x}} , \quad \tau_{\perp}^{L_1,\Delta_1} = \frac{a_{\perp}^{L_1,\Delta_1}}{\sqrt{k}T^{\frac{3}{2}}} \cdot \frac{1}{\sqrt{x}} . \quad (17)$$

(The necessary designations in expressions (17) are presented in the Appendix).

In order to calculate the effective electron mobility in the strained germanium film, it is necessary to have the acoustic deformation potential constants and components of the effective mass tensor for the L_1 and Δ_1 minima. The values of the of the acoustic deformation potential constants $\Xi_u = 11,82$ eV and $\Xi_d = -1,29$ eV, the components of the effective mass tensor $m_{\parallel} = 1,65 m_0$ and $m_{\perp} = 0,32 m_0$ for the Δ_1 minima of the germanium conduction band have been found earlier on the basis of measurements of the tensoresistance at high uniaxial pressures [14, 19]. The appropriate parameters $\Xi_u = 16,4$ eV, $\Xi_d = -6,4$ eV, $m_{\parallel} = 1,58 m_0$, $m_{\perp} = 0,082 m_0$ for the L_1 minima are also known [12]. Taking into account the values of these parameters for the L_1 and Δ_1 minima of the germanium conduction band and the energy position of these minima in the band diagram of the strained germanium nanofilm (Fig. 2), on the basis of expression (11), the dependencies of the relative change of the effective electron mobility in the nanofilm on the component composition of the substrate were obtained. The calculations are represented in the Fig. 3 and Fig. 4. As follows from the given figures, an increase in the germanium content in the substrate leads to a growth of effective electron mobility in the nanofilm. This is due to the deforming redistribution of electrons between the four L_1 minima with greater mobility, which descend down, and the four Δ_1 minima of less mobility, which ascend up on the energy scale.

In expression (12), the function $f(d)$ takes into account the influence of the nanofilm thickness d on the effective electron mobility. As the calculations show, this function does not depend on the nanofilm thickness and temperature for $d > 7$ nm. According to the expressions

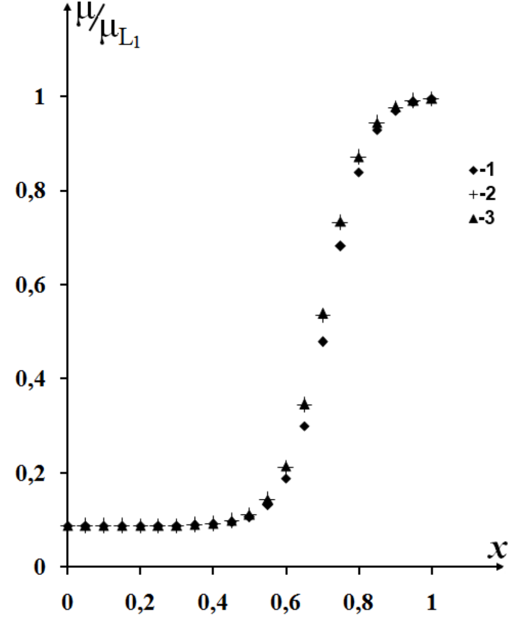

Fig. 3 – Dependencies of the effective electron mobility on the component composition of the $Ge_{(x)}Si_{(1-x)}$ substrate at $T = 300$ K for different thicknesses of the strained germanium nanofilm d, nm: 1 – 2, 2 – 7, 3 – 10

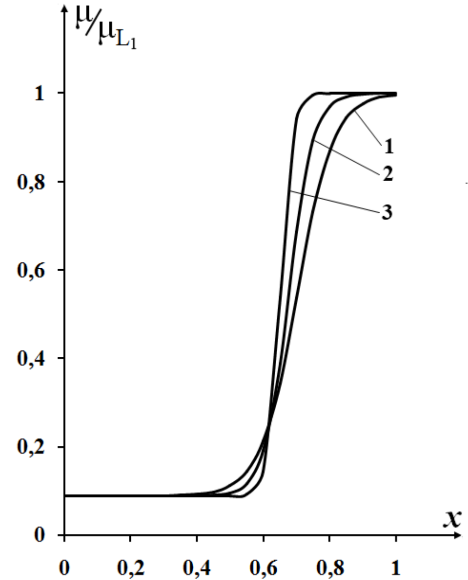

Fig. 4 – Dependencies of the effective electron mobility on the component composition of the $Ge_{(x)}Si_{(1-x)}$ substrate for the strained germanium nanofilm of thickness $d = 7$ nm at different temperatures T, K: 1 – 300, 2 – 200, 3 – 100

(11) and (12), the effective electron mobility will also be the same for different nanofilms whose thickness satisfies this condition. This fact explains the obtained dependencies of the effective electron mobility on the different thicknesses of the strained germanium nanofilm (see Fig. 3).

3. CONCLUSIONS

Thus, the arising internal mechanical strains in the strained germanium nanofilm lead to noticeable changes in its band structure and the effective electron mobility.

Change in the component composition of the substrate on the basis of the $Ge_{(x)}Si_{(1-x)}$ alloy allows to preliminarily control the parameters of the band structure, and hence the electrical properties of such films. The impact of the nanofilm thickness on the effective electron mobility becomes noticeable when $d < 7$ nm. The presented calculations of the magnitude of internal deformation fields, band structure and effective electron mobility for the strained germanium nanofilm can be useful in the modelling of electrical characteristics of devices made on the basis of the strained semiconductor nanostructures with heterojunctions.

APPENDIX A

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

$$\Phi_{0a} = 1 + \frac{2(1+\beta^2)}{\beta^2}\left(1 - \frac{3}{\beta^2} + \frac{3}{\beta^3}\alpha\right)\frac{\Xi_u}{\Xi_d} + \frac{(1+\beta^2)}{\beta^4}\frac{\Xi_u^2}{\Xi_d^2}\left((1+\beta^2)\left(1 - \frac{6}{\beta^2} - \frac{3}{2\beta^2(1+\beta^2)} + \frac{15\alpha}{2\beta^3}\right) + \frac{C_{11}}{C_{44}}\left(2 + \frac{15}{2\beta^2} - \frac{3}{2\beta^3}(5+3\beta^2)\alpha\right)\right) \tag{2}$$

$$\Phi_{1a} = 1 + \frac{1+\beta^2}{\beta^2}\left(2 + \frac{3}{\beta^2} - \frac{3(1+\beta^2)}{\beta^3}\alpha\right)\frac{\Xi_u}{\Xi_d} + \frac{(1+\beta^2)}{\beta^4}\frac{\Xi_u^2}{\Xi_d^2}\left((1+\beta^2)\left(1 + \frac{15}{4\beta^2} - \frac{3}{4\beta^3}(5+3\beta^2)\alpha\right) + \frac{C_{11}}{4C_{44}}\left(-13 - \frac{15}{\beta^2} + \frac{3(1+\beta^2)}{\beta^3}(5+\beta^2)\alpha\right)\right), \tag{3}$$

where $\alpha = arctg\,\beta$, $\beta^2 = \frac{m_{||} - m_{\perp}}{m_{\perp}}$.

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Розрахунок рухливості електронів для напруженої наноплівки германію

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На основі теорії пружності було проведено розрахунки величин відносних деформацій, які виникають в наноплівці германію, вирощеній на підкладці $Ge_{(x)}Si_{(1-x)}$ (001), в залежності від її компонентного складу. Для такої орієнтації підкладки наноплівка германію в кристалографічних напрямках [100], [010] (в площині підкладки) зазнає двохосьового стиску, а в кристалографічному напрямку [001] – одновісного розтягу. Показано, що у випадку підкладки з кремнію величини внутрішніх механічних напружень досягають 4 %. Проведені розрахунки зонної структури для напруженої наноплівки германію показують, що при збільшені величини внутрішніх механічних напружень (за рахунок збільшення вмісту Si в підкладці) чотири мінімуми Δ_1 зони провідності будуть опускатися вниз, а мінімуми

L_1 підніматимуться вгору за шкалою енергій. При цьому валентна зона зазнає розщеплення на дві вітки, верхньою з яких стає валентна зона «важких» дірок. При вмісті Ge в підкладці менше як 60 %, в енергетичному спектрі напруженої наноплівки германію найнижчими стають чотири мінімуми Δ_1 зони провідності. Проведені на основі теорії анізотропного розсіяння на акустичних фононах розрахунки рухливості електронів показують, що збільшення відносного вмісту германію в підкладці призводить до зростання рухливості електронів в наноплівці. Це пояснюється деформаційний перерозподіл електронів між чотирма мінімумами L_1 з більшою рухливістю та чотирма мінімумами Δ_1 з меншою рухливістю. Встановлено, що для наноплівок германію товщиною $d > 7$ нм рухливість електронів не залежить від їх товщини. Одержані результати можуть бути використані при моделюванні електричних властивостей напружених наноплівок германію, на основі яких можуть бути створені різні електронні прилади сучасної наноелектроніки з прогнозованими робочими характеристиками.

Ключові слова: Одновісна деформація, Наноплівка германію, Механічні напруження, Анізотропне розсіяння, Зонна структура германію.