

INFLUENCE OF DEFORMATION ON QUANTUM OSCILLATIONS IN LOW-DIMENSIONAL SEMICONDUCTOR

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In this article, the effect of deformation on the Landau levels of electrons and holes in quantum semiconductors is considered. The effect of deformation on the temperature dependence of quantum oscillation effects in small-sized semiconductors obeying the quadratic dispersion law has been applied. Also, the dependence of the surface density of states on temperature and magnetic field for semiconductor heterostructure materials is theoretically explained. A new analytical expression is proposed to calculate the effect of a magnetic field on the surface density of states at the semiconductor-dielectric interface. A mathematical model is developed to determine the effect of a strong magnetic field on the temperature dependence of the surface density of states in semiconductor heterostructures. As a result, the separation of continuous energy spectra measured at room temperature under the influence of a strong magnetic field into discrete levels at low temperatures is explained on the basis of the proposed model.

Keywords: Semiconductor; Conductivity; Quantum well; Magnetoresistance; Magnetic field

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INTRODUCTION

The electronic, optical, and magnetic properties of quantum-scale semiconductor materials are being systematically studied by many scientists, including the effects of deformation, temperature, and volume pressure on these semiconductors, in terms of their different sizes and structural geometries. One of the main features of nanostructured semiconductors is that they can dramatically change the physical, thermal, electrical, optical, and magnetic properties of these materials by doping them with different concentrations [1-5]. That is, dopants radically change the energy band structure of quantum-scale semiconductors, which can be observed in the changes in the electronic, optical, and magnetic properties of the quantum well. In addition, it is possible to observe the formation of new energy levels (doped levels) in the band gap of the quantum well. Based on this, it is clear that the inclusions are used to tune the optoelectronic properties of quantum-walled semiconductor structures [6-11]. At the same time, controlling the inclusion binding energy is important for ensuring the stability and durability of quantum-scale heterostructure materials. In conclusion, it can be said that the susceptibility (resistance) of inclusion quantum-structured materials to external factors (hydrostatic pressure, deformation, magnetic fields) indicates that the study of such materials is relevant both from a theoretical and practical point of view.

MODEL

Explaining the dependence of the quantum band gap on deformation by means of the Schrodinger equation

The effect of deformation on the basic parameters of quantum well materials has been theoretically considered. The Hamiltonian equation for the effect of volumetric deformation and magnetic field on the allowed band of a quantum well can be written as a function of $H(T, \varepsilon)$ using the effective mass approximation as follows [1]:

$$H = \frac{1}{2m^*(\varepsilon, T)} \left[\vec{p} + \frac{e}{c} \vec{A}(\vec{r}) \right]^2 + V(z, \varepsilon, T) - \frac{e^2}{\varepsilon^*(\varepsilon, T)r} \quad (1)$$

where, \vec{p} is the momentum of the electron, $\vec{A}(\vec{r})$ is the vector potential of the magnetic field, which is applied perpendicular to the direction of magnetic field growth (z-direction), i.e., the magnetic field and vector potential have the forms $\vec{B} = (B, 0, 0)$ and $\vec{A} = (0, B_z, 0)$, and c is the speed of light.

The effective mass $m^*(\varepsilon, T)$ and the dielectric constant $\varepsilon^*(\varepsilon, T)$ are functions of the distance between the electron and donor particles in the XOY plane, expressed by $r = \sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2}$. z and z_i are the coordinates of the electron and donor. The effective mass for charged particles as a function of deformation and temperature was found by scientists in [12-18]:

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$$m^*(\varepsilon, T) = \frac{m_0}{1 + E_p^\Gamma \left[\frac{2}{E_g^\Gamma(\varepsilon, T)} + \frac{1}{E_g^\Gamma(\varepsilon, T) + \Delta_0} \right]} \quad (2)$$

where m_0 is the free electron mass, $E_p^\Gamma = 7.51 \text{ eV}$ is the energy associated with the momentum matrix element for $T=0$, Δ_0 is the spin-orbit splitting. For *GaAs*, the spin-orbit splitting parameter is $\Delta_{\text{SO}}=0.34 \text{ eV}$ [20]. And $E_p^\Gamma(\varepsilon, T)$ is the deformation and temperature-dependent energy band for the quantum well in units of Γ -eV, which was found by scientists in works [19-24]. Here, Γ -eV denotes the deformation- and temperature-dependent energy shift of the band edges expressed in electron-volts.

$$E_p^\Gamma(\varepsilon, T) = E_g^\Gamma(0, T) + 1.26 * 10^{-2} \varepsilon - 3.77 * 10^{-5} \varepsilon^2 \quad (3)$$

Here, $E_g^\Gamma(0, T) = 1.519 - (5.405 * 10^{-4} T^2) / (T + 204) \text{ eV}$

Deformation and temperature (K) depend on the static dielectric constant [19-24].

$$\varepsilon^*(\varepsilon, T) = \begin{cases} (i) 12.74 e^{-1.7 * 10^{-3} \varepsilon} e^{9.4 * 10^{-5} (T - 75.6)}; & \text{for } T < 200 \text{ K} \\ (ii) 13.18 e^{-1.7 * 10^{-3} \varepsilon} e^{20.4 * 10^{-5} (T - 300)}; & \text{for } T \geq 200 \text{ K} \end{cases} \quad (4)$$

However, these derived equations do not consider the dependence of the energy density of states of a quantum well on deformation and magnetic field.

The effect of deformation on the cyclotron frequency of charged particles in a quantum well

One of the physical effects that depends on the change in the energy spectra of charged particles under the influence of deformation is the cyclotron frequency. The cyclotron frequency is a quantity that depends on the energy of the Landau levels of charged particles: $E_N = \hbar \omega_c \left(N_L + \frac{1}{2} \right)$. That is, the cyclotron frequency is represented by the electron spectrum in a strong magnetic field. To calculate this spectrum, it is necessary to solve the Schrödinger equation in a quantizing magnetic field.

$$(H(K) + H_s - E)F = 0 \quad (5)$$

where, $K = k + \frac{e}{c\hbar} A$ is the total momentum, $H = \text{rot}A$; the wave function in the F-effective mass approximation [25].

In the effective mass approximation (5), it is sufficient to restrict the expression $H(K)$ in the Schrödinger equation to quadratic terms in K , and it is not necessary to take into account the dependence of the g -factor on K . In addition, in the approximation in (5), the cyclotron frequency is the same for all charged particles, which indicates that the spin effect can be ignored. In this case, the Schrödinger equation (5) reduces to the following expression for the effective mass tensor in the principal coordinate axes:

$$\left(\sum_i \frac{\hbar^2}{2m_i} K_i^2 - E \right) F = 0 \quad (6)$$

If equation (6) is applied to the quantum field and a solution is found, then E_N will have the following form:

$$E_N = \hbar \omega_c \left(N + \frac{1}{2} \right) + \frac{\pi^2 \hbar^2}{2md^2} n_z^2, \quad (7)$$

here,

$$\omega_c = \frac{eB}{m^*} \quad (8)$$

It is known from work [26] that the cyclotron effective mass varies with deformation. For example, in work [26], the graph of the $\frac{m_c^*}{m_0}(\varepsilon)$ function is presented (Fig. 1).

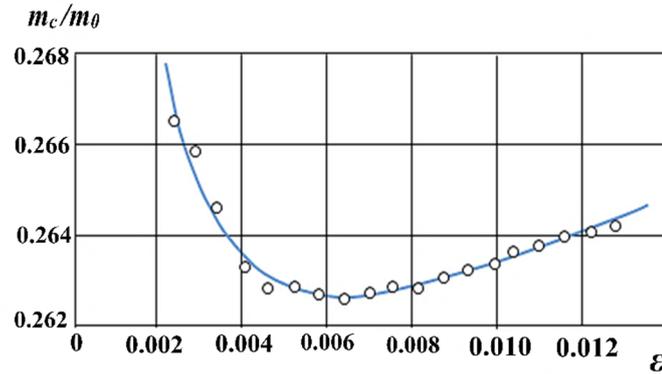


Figure 1. Cyclotron mass dependence of p-type silicon on deformation [26]

This figure shows the dependence of p-type germanium on $\frac{m_c^*}{m_0}(\varepsilon)$. It can be seen from this figure that $\frac{m_c^*}{m_0}(\varepsilon)$ is linearly dependent on strain (ε) at large strains.

It can be seen from this figure that the Landau levels of the quantum wells are significantly affected by large deformation.

Dependence of the forbidden band width on the density of states in the conduction band of a quantum well

Various experiments are being conducted to study the influence of pressure, deformation, and temperature on quantum oscillation effects in new types of bulk and quantum-based semiconductors, and new scientific and practical results are being obtained. For example, the fact that the oscillation processes of the energy density of states lead to oscillations of all quantum effects was shown in these works [27-39] proposed a new model of the temperature dependence of magnetoresistance, magnetic absorption and quantum Hall effect oscillations of bulk and nanostructured semiconductors. In this work, theoretical mechanisms for the temperature dependence of magnetoresistance and magnetic absorption oscillations were developed, taking into account the thermal expansion of discrete Landau levels. However, in these works, the dependence of the energy density of states, magnetoresistance and magnetic absorption oscillations on deformation for parabolic dispersion laws was not considered at all.

The main purpose of this work is to theoretically determine the method for calculating the effect of deformation on Landau levels in the conduction band of quantum-enclosed semiconductors.

Let us consider the effect of temperature and strain on the Landau levels in the conduction band of a rectangular quantum well for the parabolic dispersion law. Here, the magnetic field induction is directed along the Z axis, parallel to the thickness of the quantum well, perpendicular to the XOY plane. Let us choose the ceiling of the valence band of the quantum well as the starting point for the energy spectrum of charge carriers. In this case, the energy spectra of free electrons and holes under the influence of a quantizing magnetic field are calculated by the following equations:

$$E_c^{2d}(B, N_L, n_z, d) = E_g^{2d} + (N_L + \frac{1}{2})\hbar\omega_c + \frac{\pi^2 \hbar^2}{2m_e d^2} n_z^2 \tag{9}$$

$$E_v^{2d}(B, N_L, n_z, d) = - \left((N_L + \frac{1}{2})\hbar\omega_v + \frac{\pi^2 \hbar^2}{2m_p d^2} n_z^2 \right) \tag{10}$$

For the quadratic dispersion law [40]:

$$E = \hbar^2 k^2 / 2m, \text{ then } S = \pi k_{\perp}^2 = \pi(k^2 - k_z^2),$$

$$m_c = \frac{\hbar^2}{2\pi} \frac{\partial S}{\partial E} = m. \tag{11}$$

In previous works, the equation for the temperature dependence of the density of energetic states for the parabolic dispersion law of a quantum-walled heterostructure has been presented. In this case, based on condition (9), the density of energetic states can be written as follows:

$$N_S^{2d}(E, B, T, d) = \sum_{N_L, n_z} \frac{eB}{\pi \hbar} \cdot \frac{1}{kT} \cdot \exp \left[- \frac{\left(E - \left(E_g^{2d} + \left(N_L + \frac{1}{2} \right) \hbar\omega_c + \frac{\pi^2 \hbar^2}{2m_e d^2} n_z^2 \right) \right)^2}{(kT)^2} \right] \tag{12}$$

The difference between equation (12) and the previous equations is that the two-dimensional density of states depends on the band gap of the quantum well.

The effect of deformation on the energy density of states of a quantum well.

Now let us consider the effect of deformation on the energy density of states in the conduction band of a quantum well. It is known that when a semiconductor structure is subjected to deformation, its resistance changes. The resistance that changes under the influence of this deformation is called the tensorsistance. The tensorsistance effect divides the types of elastic deformation into 2 classes, mainly depending on the change in the symmetry of the crystal lattice of semiconductor structures. The symmetry of the crystal lattice of semiconductors practically does not change due to the overall deformation. Therefore, the fact that the crystal lattice remains unchanged from a symmetrical point of view cannot change the resistance component of any material when this deformation is applied. Usually, when the effect of deformation is applied to semiconductor structures, volumetric (all-round) compression is considered [41]. Under the influence of volumetric deformation, the deformation tensor (u_{ii}) of the crystal lattice becomes a scalar (u), and the lattice constant changes as follows:

$$a' = a(1-u), \quad (13)$$

where a' is the lattice constant after deformation, a is the lattice constant before deformation, u is the relative deformation.

A decrease in the interatomic distance of semiconductor structures increases the degree of "coverage" of the wave functions of charge carriers. This, in turn, leads to a change in the interatomic interaction potential energy $W(a)$ of the crystal lattice of the material. If the $W_{\min}(a) = W(a_0)$ condition is introduced, then the value of the potential energy W should also increase in the special limits $a < a_0$ and $a > a_0$. A change in the interatomic potential energy W of the crystal lattice of semiconductor structures leads to a shift in the allowed boundary zones of the quantum well. This, in turn, causes a change in the forbidden band width of the quantum well.

That is, in this [41] work:

$$\alpha = -\frac{1}{\Delta\varepsilon_0} \frac{\partial \Delta\varepsilon_0}{\partial P}. \quad (14)$$

Then

$$\Delta\varepsilon(P) = \Delta\varepsilon_0(1 - \alpha P). \quad (15)$$

The change in the forbidden band width of the quantum well under the influence of volumetric deformation is formed by the shifts of the bottom of the quantum well conduction band E_c and the ceiling of the valence band E_v .

Under the influence of weak deformation

$$\begin{aligned} E_c(\varepsilon) &= E_c(0) + \Delta_c \varepsilon \\ E_v(\varepsilon) &= E_v(0) + \Delta_v \varepsilon \end{aligned} \quad (16)$$

Using the condition $E_g(\varepsilon) = E_c(\varepsilon) - E_v(\varepsilon)$ and according to (16), the following equation is derived:

$$E_g(\varepsilon) = E_g(0) + \Delta\varepsilon, \quad (17)$$

where Δ_c and Δ_v are the deformation results in the conduction and valence bands of the quantum well.

One of the main components of volumetric deformation is the compression (stretching) of the crystal lattice from all sides. Therefore, a change in the concentration of electrons and holes associated with volumetric deformation must be observed in all cases. A change in the concentration of charge carriers $n(\varepsilon)$ leads to a change in the energy density of states of this quantum well. Then, substituting (17) into (12), we obtain the following $N_s^{2d}(E, \varepsilon, B, T)$:

$$N_s^{2d}(E, B, T, \varepsilon, d) = \sum_{N_L, n_z} \frac{eB}{\pi\hbar} \cdot \frac{1}{kT} \cdot \exp \left[-\frac{\left(E - \left(E_g^{2d}(E_g^{2d}(0) + \Delta\varepsilon) + \left(N_L + \frac{1}{2} \right) \hbar\omega_c + \frac{\pi^2 \hbar^2}{2m_c d^2} n_z^2 \right) \right)^2}{(kT)^2} \right] \quad (18)$$

Thus, a new analytical expression for the dependence of the energy density of states of a quantum well on B , T and d under the influence of volumetric deformation was derived.

According to the new analytical expression (18), one can see the graph of the dependence of the oscillations of the density of states in the conduction band of a quantum well on deformation (Fig. 2). Fig. 2 shows the effect of deformation on the states in a GaAs quantum well. Here, $E_g(0) = 1.52$ eV [42-43], $B = 7$ T, $\varepsilon = 0.001$. With these parameters, the $N_s^{2d}(E, B, \varepsilon)$ under the effects of $\varepsilon = 0$ and $\varepsilon = 0.001$ are compared. As can be seen from the graphs in this figure, a slight shift of the discrete Landau levels to the right is observed under the influence of deformation. This, of course, reflects the effect of free electrons on the energy spectrum.

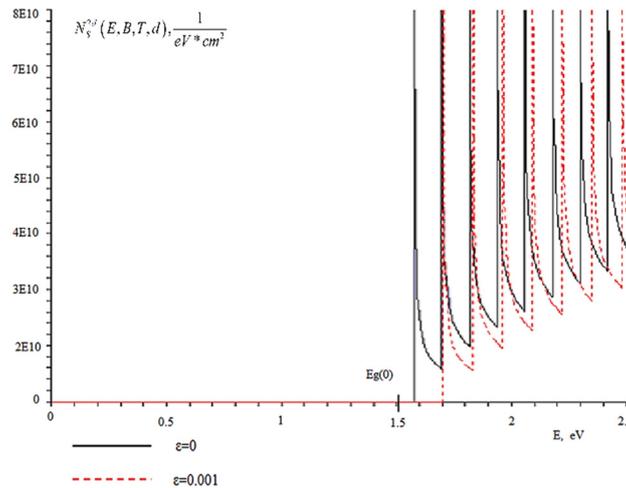


Figure 2. Effect of deformation on the density of states in a GaAs quantum well according to the parabolic dispersion law

Dependence of deformation on quantum oscillation effects in quantum-walled semiconductor structures

Oscillations in the magnetoresistance and magnetoreductive effects arise when the energy density of states in quantum well heterostructures changes. Using equation (18), we determine the dependence of the oscillations in the magnetoresistance and magnetoreductive effects on the overall deformation. The dependence of the Fermi level on the overall deformation can be written as follows:

$$E_F(\epsilon, T) = -\frac{Eg(\epsilon)}{2} + \frac{3}{4}kT \ln\left(\frac{m_h^*}{m_e^*}\right), \tag{19}$$

$$\frac{\partial f_0(E, E_F(\epsilon, T), T)}{\partial E} = -\frac{1}{kT} \frac{\exp\left(\frac{E - \left(-\frac{Eg(\epsilon)}{2} + \frac{3}{4}kT \ln\left(\frac{m_h^*}{m_e^*}\right)\right)}{kT}\right)}{\left[1 + \exp\left(\frac{E - \left(-\frac{Eg(\epsilon)}{2} + \frac{3}{4}kT \ln\left(\frac{m_h^*}{m_e^*}\right)\right)}{kT}\right)\right]^2}. \tag{20}$$

The dependence of effective masses on deformation can be expressed as follows [44-45]:

$$m_c^*(\epsilon) = m_c^*(0) \cdot \left(1 - \frac{\Delta E_g}{E_g(0)}\right) = m_c^*(0) \cdot \frac{E_g(\epsilon)}{E_g(0)} \tag{21}$$

$$\omega_c(\epsilon) = \frac{eB}{m_c^*(\epsilon)} \tag{22}$$

Using (18), (19), (20), (21) and the $\rho_H^{2d}(B, T)$ and $\chi_H^{2d}(B, T)$ mathematical models in [46-47], the following expression is derived:

$$\rho_H^{2d}(B, T, \epsilon) = A \cdot \hbar \omega_c(\epsilon) \int_{\hbar \omega_c(\epsilon)}^{\infty} \sum_{N_L, n_z} \frac{eB}{\pi \hbar} \cdot \frac{1}{kT} \cdot \exp\left(-\frac{\left(E - \left(E_g^{2d}(E_g(0) + \Delta\epsilon) + \left(N_L + \frac{1}{2}\right)\hbar \omega_c + \frac{\pi^2 \hbar^2}{2m_e^* d^2} n_z^2\right)\right)^2}{(kT)^2}\right) \times \left(-\frac{\partial f_0(E, E_F(\epsilon, T), T)}{\partial E}\right) \tau_n(E) d \tag{23}$$

$$\chi_H^{2d}(B, T, \epsilon) = 2\mu_B^2 \int_0^\infty \sum_{N_L, n_z} \frac{eB}{\pi\hbar} \cdot \frac{1}{kT} \cdot \exp \left[-\frac{\left(E - \left(E_g^{2d}(E_g(0) + \Delta\epsilon) + \left(N_L + \frac{1}{2} \right) \hbar\omega_c + \frac{\pi^2 \hbar^2}{2m_e d^2} n_z^2 \right) \right)^2}{(kT)^2} \right] \times \left(-\frac{\partial f_0(E, E_F(\epsilon, T), T)}{\partial E} \right) \tau_n(E) d \tag{24}$$

If the deformation is equal to or greater than the critical value ($\epsilon \geq \epsilon_k$), then the Landau levels begin to shift towards the edges of the conduction band. Using equations (23) and (24), we obtain graphs of the magnetoresistance and magnetoresistance oscillations of the quantum well. Fig. 3 shows the dependence of the magnetoresistance and magnetoresistance oscillations of the GaAs quantum well material on the overall deformation. As can be seen from this figure, the appearance of the oscillations of charged particles changes significantly with increasing deformation.

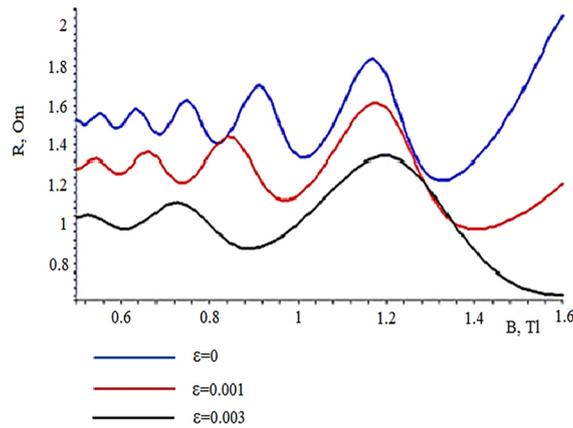


Figure 3. Oscillations of $\rho(B, T, \epsilon)$ in a GaAs quantum well at various deformations

Figures 4 and 5 show three-dimensional images of the magnetoresistance and magnetoresistance oscillations of the GaAs quantum well at various deformations. As the strain in a GaAs quantum well increases to 0.004, a slight decrease in the number of discrete Landau levels of free electrons is observed in the magnetoresistance and magnetoresistance effects at a constant low temperature.

Using equations (23) and (24), it is possible to calculate both deformation and temperature effects of $\rho^{2d}(B, T, \epsilon)$ and $\chi^{2d}(B, T, \epsilon)$ of quantum coils subject to the law of parabolic dispersion at the same time.

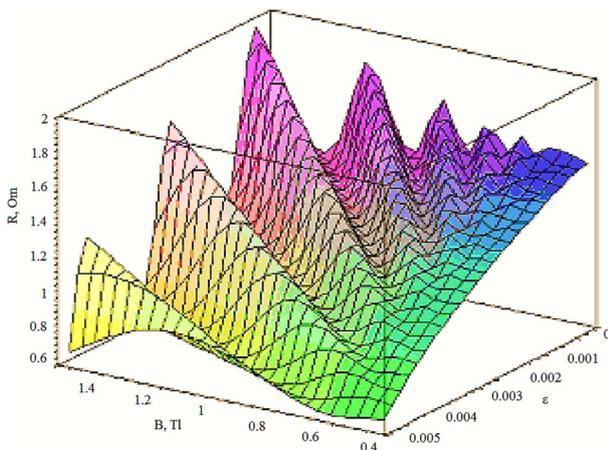


Figure 4. The dependence of the magnetoresistance of a GaAs quantum well on deformation $\rho(B, T, \epsilon)$

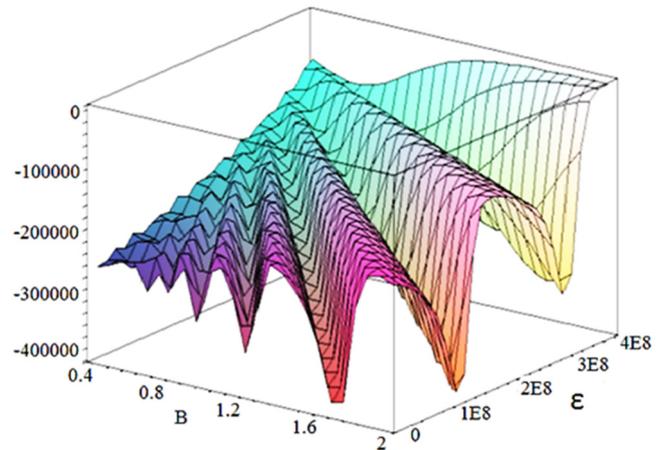


Figure 5. Dependence of magnetic susceptibility of a GaAs quantum well on deformation $\chi(B, T, \epsilon)$

CONCLUSIONS

Based on the results of this study, the following conclusions were drawn:

1. The dependence of the energy density of states in the conduction band of quantum well semiconductors subject to parabolic band dispersion on deformation was introduced.

2. A new analytical expression was found that determines the dependence of the energy density of states of a quantum well on deformation ($N_s^{2d}(E, B, T, \varepsilon)$).

3. The quantum oscillation effects of a quantum well were studied theoretically using the proposed analytical expression.

4. Methods for calculating $\rho^{2d}(B, T, \varepsilon)$ and $\chi^{2d}(B, T, \varepsilon)$ of a quantum well using $N_s^{2d}(E, B, T, \varepsilon)$ were developed.

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ВПЛИВ ДЕФОРМАЦІЇ НА КВАНТОВІ КОЛИВАННЯ В НИЗЬКОВИМІРНИХ НАПІВПРОВІДНИКАХ
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У цій статті розглядається вплив деформації на рівні Ландау електронів та дірок у квантових напівпровідниках. Застосовано вплив деформації на температурну залежність квантових коливальних ефектів у малорозмірних напівпровідниках, що підпорядковуються квадратичному закону дисперсії. Також теоретично пояснено залежність поверхневої густини станів від температури та магнітного поля для напівпровідникових гетероструктурних матеріалів. Запропоновано новий аналітичний вираз для розрахунку впливу магнітного поля на поверхневу густину станів на межі напівпровідник-діелектрик. Розроблено математичну модель для визначення впливу сильного магнітного поля на температурну залежність поверхневої густини станів у напівпровідникових гетероструктурах. В результаті, на основі запропонованої моделі пояснюється розділення неперервних енергетичних спектрів, виміряних при кімнатній температурі під впливом сильного магнітного поля, на дискретні рівні при низьких температурах.

Ключові слова: напівпровідник; провідність; квантова яма; магнітоопір; магнітне поле