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MODELING THE TEMPERATURE AND MAGNETIC FIELD DEPENDENCE OF THE BAND GAP IN NARROW-ZONE QUANTUM WELL SEMICONDUCTORS

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The fundamental physical parameter of both bulk and low-dimensional semiconductor structures is the band gap (E_g^{3d}, E_g^{2d}), whose energetic width allows the prediction of the operational parameters of semiconductor-based devices in advance. Therefore, the determination of E_g^{3d} and E_g^{2d} (in cases where the band gap of newly synthesized materials is not known) is considered one of the primary tasks in semiconductor heterostructure technology. Furthermore, another important feature of E_g is its strong sensitivity to external influences. Indeed, variations in E_g resulting from such effects can fundamentally alter the physical and chemical properties of semiconductor devices.

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

There are several methods to determine the dependence of the band gap of semiconductors on external factors [1-14]. In particular, in works [15-21], a methodology for determining $E_g(T)$ was proposed based on the model of the temperature dependence of surface state density. In this approach, a mechanism for explaining $E_g(T)$ was developed through the penetration of the "tail" of the density of states into the forbidden gap with increasing temperature. However, these works did not examine the influence of a quantizing magnetic field. In works [22-27], the dependence of the band gap of bulk and quantum-dimensional semiconductors on temperature, magnetic field, and hydrostatic pressure was studied. In particular, in work [28], $E_g^{3d}(B,T)$ was theoretically calculated by changing the allowed bands of bulk semiconductor structures with temperature and magnetic field. It was proved that when the $B \to 0$ condition is met, it turns into$E_g^{3d}(B,T) \to E_g\ (T)$, that is, classical methods. This theory is mainly suitable for wide-bandgap 3D materials. In work [29], a model was developed for $E_g^{2d}(B,T,d)$ in quantum well semiconductors obeying the parabolic dispersion law. A mechanism was proposed for describing the variation of the conduction band minimum and valence band maximum (i.e., the band edges) of a rectangular quantum well as a function of quantizing magnetic field and temperature. The $E_g^{2d}(B,T,d)$ model was proposed as a result of the tail of $N_{cs}^{2d}(B,T,d)$ and $N_{vs}^{2d}(B,T,d)$ entering E_g^{2d}. In this case, the $E_g^{2d}(B,T,d)$ of wide-gap quantum well semiconductors were also determined.

In addition, in work [30], the dependence of the energy density of states of the conduction band of narrow-zone semiconductor materials on magnetic field and temperature was theoretically determined. In this work, an analytical expression for the nonparabolic dispersion law $N_{cs}^{3d(n)}(B,T)$ was derived. The experimental results were interpreted for different T using the obtained theoretical reports. However, in these works, a perfect mathematical model for determining $N_{vs}^{2d(n)}$, $N_{cs}^{2d(n)}$ was not developed.

The main purpose of the work:

- To develop a method for determining the dependence of the allowed bands $N_{vs}^{2d(n)}$ and $N_{cs}^{2d(n)}$ of narrow-zone quantum well semiconductors on the magnetic field *B* and temperature *T*.

- To determine the dependence of the forbidden band width of a narrow-zone quantum well on the magnetic field *B* and temperature *T* using this method.

MODEL

Effect of magnetic field on the energy of light holes at the valence band ceiling of a narrow-band quantum well

The problem is treated within a simplified multiband approximation, where the interaction between conduction, light-hole, and split-off bands is considered. This terminology avoids the misleading interpretation of a 3×3 Hamiltonian and is fully consistent with the subsequent use of the 8×8 Kane matrix. Although the full Hamiltonian is represented in an 8×8 Kane matrix, the physically relevant subspace describing the conduction and light-hole bands is obtained through standard Löwdin partitioning, which results in a reduced effective band model. This approximation is intended to find a

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convenient solution to the equation for narrow-band quantum-well semiconductors. In the considered approximation, the 8×8 interaction matrix can be written using H_{kp} and H_1 as follows [31]:

$$\begin{pmatrix} \mathsf{H} & 0 \\ 0 & \mathsf{H} \end{pmatrix}. \tag{1}$$

Here,

$$\mathsf{H} = \begin{pmatrix} E_c & 0 & Pk_+ & 0 \\ 0 & E_v - \frac{\Delta}{3} & \frac{\sqrt{2}}{3}\Delta & 0 \\ Pk_- & \frac{\sqrt{2}}{3}\Delta & E_v & 0 \\ 0 & 0 & 0 & E_v + \frac{\Delta}{3} \end{pmatrix}. \tag{2}$$

In this formula, $k_\pm = -i\left(\partial_x \pm i\partial_y\right) + \frac{e}{\hbar}\left(A_x \pm iA_y\right)$

In contrast to the previous version, the wave vector in Eq. (2) is now treated as an operator that includes the magnetic vector potential, ensuring the correct description of magnetic-field effects within the Kane model.

To ensure dimensional consistency, equation (2) has been corrected so that both the Hamiltonian matrix and the basis vector are expressed in the proper 4-component form, following the standard Kane model representation.

The right-hand column in the matrix (2) represents the energy states associated with H.

If we calculate the initial energy with the bottom of the conduction band of the quantum well, ($E_c=0$), then the following equation is obtained:

$$\left(E' + E_g\right)\left[E'\left(E' + E_g\right)\left(E' + E_g + \Delta\right) - k^2P^2\left(E' + E_g + 2\Delta/3\right)\right] = 0\,. \tag{3}$$

Here, $E'(k) = E(k) - \frac{\hbar^2 k^2}{2m_0}$.

The fourth-order form of Eq. (3) is consistent with the fact that the effective Hamiltonian obtained after Löwdin partitioning corresponds to a reduced 4-band model derived from the original 8×8 Kane Hamiltonian.

From equation (3) it is known that for k=0 the function $E`(k)$ has four eigenvalues: $E_1=0$; $E_2= E_3= -E_g$ and $E_4=- E_g- \Delta$. The condition $E_1=0$ means that the counting starts from the bottom of the conduction band. The energies E_2 and E_3 represent the ceilings of the valence bands of the heavy (E_{v1}) and light (E_{v2}) holes. The energy E_4 shows the spin-orbit effect on the ceiling of the valence band.

To solve the problem, we use the following approximations:

1. Ignoring the spin-orbit effect on the allowed bands of a narrow-zone semiconductor.
2. Ignoring the interaction with heavy holes, since the effective masses of light holes are close to the effective masses of free electrons.

In this case, $Eg>>\Delta$ and according to work [31], the energy of light holes is determined as follows:

$$E'_{v2}(k) = -\frac{E_g}{2}\left\{1 + \left[1 + \frac{4k^2p^2}{E_g^2}\right]^{1/2}\right\}. \tag{4}$$

From equation (4), it is clear that k^2p^2 (a P-matrix element, which is equal to $P = -\frac{i\hbar}{m_0} < S\left|\hat{P}\right|x >$) is considered the energy, since the condition that the $\frac{k^2p^2}{E_g^2}$ term is a dimensionless quantity must be met. In this case, taking into account the above matrix element equation and the dimensionless quantities $\frac{k^2p^2}{E_g^2}$, (4) can be written in the following form.

$$E_{v2}(\vec{k}) = -\frac{E_g}{2}\left\{1 + \left[1 + \frac{4\hbar^2\vec{k}^2_{xyz}}{2m^*_{xyz}} * \frac{1}{E_g^2}\right]^{1/2}\right\} \tag{5}$$

In equation (5), the energy of light holes in narrow-zone bulk semiconductors at the valence band ceiling is determined mainly by the effective masses and wave numbers of the light holes in the XYZ axes. In this case, the band gap (E_g) of the narrow-zone bulk semiconductor is assumed to be constant. From equation (5), natural questions arise:

1. How to use (5) if the material under the influence of the magnetic field is a quantum-enclosed narrow-zone, heterostructure semiconductor?

2. It is known that the E_g of narrow-zone bulk or small-sized semiconductors is very sensitive to external factors. In this case, how are $E_v^{3d}(k,E_g)$ and $E_v^{2d}(k,E_g,d)$ determined?

How does the change in $E_v^{2d}(k,E_g,d)$ affect the density of energy states in the valence band of a quantum well?

To solve these problems, it is necessary to create a new mathematical model.

Applying equation (5) to narrow-zone semiconductors with quantum wells, the following equation is obtained:

$$E_v^{2d}(k,d) = -\frac{E_g}{2}\left\{1+\left[1+4\frac{\frac{\hbar^2\vec{k}_x^2}{2m_x}+\frac{\hbar^2\vec{k}_y^2}{2m_y}+\frac{\pi^2\hbar^2}{2md^2}n_z^2}{E_g^2}\right]\right\} \tag{6}$$

Equation (6) is the energy of light holes in a narrow-zone quantum well at the valence band ceiling.

Here, n_z is the number of dimensional quanta, d is the thickness of the narrow-zone quantum well, and m^* is the effective mass of the light hole.

As can be seen from equation (6), the energy of a light hole at the valence band ceiling of a quantum well depends on the thickness of the quantum well, the effective mass of the light hole, and the number of dimensional quanta.

Now, let us consider the effect of a strong magnetic field on a narrow-zone quantum well. In particular, let the direction of the magnetic field induction vector $(\vec{B})$ be along the Z axis and perpendicular to the XOY plane. This is called a longitudinal quantizing magnetic field. In this case, Landau theory [32] and according to the laws of the quantizing magnetic field, the $\left[\frac{\hbar^2\vec{k}_x^2}{2m_x}+\frac{\hbar^2\vec{k}_y^2}{2m_y}\right]$ terms of the free light hole at the ceiling of the valence band of the quantum well are replaced by the $\left[\left(N_{Lv}+\frac{1}{2}\right)\hbar\omega_{cv}\right]$ term.

Here N_{Lv} is the number of Landau levels in the valence band of the narrow-band quantum well, ω_{cv} is the cyclotron frequency of light holes.

It follows that equation (6) under the influence of a longitudinal quantizing magnetic field takes the following form:

$$E_v^{2d}\left(B,d,n_z,N_{Lv}\right) = -\frac{E_g}{2}\left\{1+\left[1+4\frac{\left(N_{Lv}+\frac{1}{2}\right)\hbar\omega_{cv}+\frac{\pi^2\hbar^2}{2md^2}n_z^2}{E_g{}^2}\right]^{1/2}\right\} \tag{7}$$

From the derived equation (7) it is clear that the light hole energy at the valence band ceiling of the quantum well is transformed into discrete energy levels in all directions. This, in turn, makes the light hole energy analogous to the quantum dot energy. However, it is also necessary to consider another important physical quantity, E_g, which depends on B and d. The reason is that the change in the function $E_g(B, d)$ is considered monotonically. From this, the function $E_v^{2d}\left(B,d,n_z,N_{Lv}\right)$ becomes $E_v^{2d}\left(E_g(B,d),B,d,n_z,N_{Lv}\right)$. In this case, the equation takes the following form:

$$E_v^{2d,nonparab}\left(E_g(B,d),B,d,n_z,N_{Lv}\right) = -\frac{\left(E_g(0)+\frac{1}{2}\hbar\omega_{cv}+\frac{1}{2}\frac{\pi^2\hbar^2}{2md^2}n_z\right)}{2}\times\left\{1+\left[1+4\frac{\left(N_{Lv}+\frac{1}{2}\right)\hbar\omega_{cv}+\frac{\pi^2\hbar^2}{2md^2}n_z^2}{\left(E_g(0)+\frac{1}{2}\hbar\omega_{cv}+\frac{1}{2}\frac{\pi^2\hbar^2}{2md^2}n_z^2\right)^2}\right]^{1/2}\right\} \tag{8}$$

The resulting equation (8) equation the dependence of the light hole energy at the valence band ceiling of the quantum well on the magnetic field, the band gap width, the quantum well thickness, and the number of dimensional levels. Let us analyze equation (8) numerically and graphically [33], the Shubnikov de Haas oscillations of a narrow-zone InAs quantum well semiconductor were determined. In this case, the InAs quantum well thickness was taken to be $d = 4$ nm, $B = 0 \div 12$ T in the range, $E_g(0) = 0.35$ eV and n_z.

By substituting these experimental values into (8), it is possible to obtain the $E_v^{2d}\left(B,d,E_g(B,d)\right)$ graph. Fig.1 shows the dependence of the energy of light holes in the vacancy ceiling of the InAs quantum well on the magnetic field for different Landau levels. As can be seen from this figure, the curve of the graph is reflected according to the non-quadratic dispersion law of the narrow-zone InAs quantum well.

In addition, using equation (8), it is possible to calculate the two-dimensional energy density of states in the valence band of the narrow-zone quantum well.

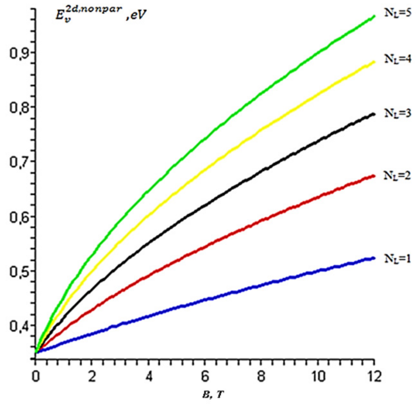


Figure 1. Magnetic field dependence of the energy of light holes in the valence band of an InAs quantum well for Landau levels

Effect of magnetic field on the energy of free electrons at the bottom of the conduction band of a narrow-zone quantum well

Now, let us consider the dependence of the free electron energy at the bottom of the conduction band of a narrow-zone quantum well on the magnetic field.

It is known that for narrow-zone semiconductors, using the condition $m_n \ll m_0$, the $\frac{\hbar^2 k^2}{2m_0}$ term given in equation (3) is not taken into account ($E' \ll E_g$). In this case, in the presence of a magnetic field, a cubic equation of energy levels for three energy bands similar to equation (3) is formed:

$$E_{N\pm}(E_{N\pm}+E_g)(E_{N\pm}+E_g+\Delta)-P^2\left[k_z^2+(2N+1)\frac{1}{L^2}\right]\times\left(E_{N\pm}+E_g+\frac{2}{3}\Delta\right)\pm\frac{P^2\Delta}{3L^2}=0. \qquad (9)$$

Here: $E_{Nk_z\pm}=E_{N\pm}$

In equation (9), the main energy level starts at the bottom of the conduction band. If, when *B→0*, equation (9) changes to the form (3).

If the spin distribution of electrons is not taken into account and the $E_N \ll E_g$ condition is satisfied, the cubic equation in (9) transforms into a quadratic equation for conduction band electrons, which has the following form:

$$E_{N\pm}(B,\,E_g)=-\frac{E_g}{2}+\frac{1}{2}\sqrt{E_g^2+4E_g\left[\left(N+\frac{1}{2}\right)\hbar\omega_c^0+\frac{\hbar^2k_z^2}{2m_n}\right]}. \qquad (10)$$

It is known that in the absence of a strong magnetic field, the free electron energy is discrete due to dimensional quantization along the OZ axis, but consists of a continuous spectrum in the XOY plane. That is,

$$E_c^{parab}(k,d)=\frac{P_x^2}{2m_{nx}}+\frac{P_y^2}{2m_{ny}}+\frac{\pi^2\hbar^2}{2m_{nz}d^2}n_z^2 \qquad (11)$$

Eq. (11) is valid for wide-band quantum fields (for the quadratic dispersion law).

Equation (10) expresses the dependence of the free electron energy in the conduction band of semiconductors with a narrow band gap on the magnetic field. That is, the magnetic field strength is directed along the Z axis, perpendicular to the XOY plane. In this case, the energy of charge carriers, according to Landau theory, forms discrete levels in the XOY plane. Along the OZ axis, the free electron energy forms a continuous spectrum. Of course, this gives an analogy to the quantum string. The question arises; how does this scientific hypothesis work in semiconductors based on a narrow band quantum well? How does the energy of free electrons in the conduction band of a narrow band quantum well depend on the magnetic field? What about the valence band of the quantum well?

For narrow-zone quantum wells, the equation in work [31] is applied: That is, if the condition $\Delta \ll E_g$ is met

$$E_c^{nonparab}(k)=-\frac{E_g}{2}\left\{1-\left[1+\frac{4P^2}{E_g^2}\times\frac{2m_{nxyz}}{\hbar^2}\times\frac{\hbar^2k_{xyz}^2}{2m_{nxyz}}\right]^{1/2}\right\}. \qquad (12)$$

Equation (12) can be written as follows for a narrow-zone quantum well:

$$E_c^{2d,nonparab}(k,d) = -\frac{E_g}{2}\left\{1-\left[1+\frac{4P^2}{E_g^2}\times\frac{2m_n}{\hbar^2}\left(\frac{\hbar^2k_x^2}{2m_{nx}}+\frac{\hbar^2k_y^2}{2m_{ny}}+\frac{\pi^2\hbar^2}{2m_{nt}}n_z^2\right)\right]^{1/2}\right\}. \tag{13}$$

Here, $P=-\frac{i\hbar}{m_0}<S\left|\hat{P}_x\right|x>$.

Equations (11) and (13) express the energy of free electrons in the conduction band of a quantum well at $B=0$ for quadratic and non-quadratic dispersion laws. If the condition $B\neq 0$ is met, equation (11) transforms into the following equation:

$$E_c^{parab}(B,d)=\left(N_{Lc}+\frac{1}{2}\right)\hbar\omega_{cc}+\frac{\pi^2\hbar^2}{2m_nd^2}n_z^2. \tag{14}$$

Then, if we replace $\frac{\hbar^2k_z^2}{2m_n}$ in equation (10) with $\frac{\pi^2\hbar^2}{2m_nd^2}n_z^2$ in accordance with the narrow-zone quantum well condition (Louis de Broglie relation, $\lambda_d\approx d$), we obtain the following equation:

$$E_n^{2d,nonparab}(E_g(B,d),B,d,n_z,N_{Lc})=-\frac{E_g(B,d)}{2}+\frac{1}{2}\sqrt{(E_g(B,d))^2+4E_g(B,d)[(N_{Lc}+\frac{1}{2})\hbar\omega_{cc}+\frac{\pi^2\hbar^2}{2md^2}n_z^2]} \tag{15}$$

This equation expresses the dependence of the energy of free electrons in the conduction band of a narrow-zone quantum well on the magnetic field. The newly obtained equation (15) is important because until now, regardless of the forbidden band width of the quantum well, $E_N(B,d)$ has been calculated only according to (14). However, according to (15), the energy E_N is nonlinearly related to *B*. Here, $\omega_c=\frac{eB}{m_n}$.

Let us apply equation (15) to semiconductors based on narrow-zone quantum wells. Let us analyze this theoretical idea graphically. Fig. 2 shows the dependence of the free electron energy in the conduction band for the *InAs/AlSb* quantum well semiconductor $E_c^{nonparab}$ on *B*. Here, $E_g(InAs)=0.35$ *eV*, $d=12$ nm [33]. Fig. 3 shows the $E_c^{parab}(B,d)$ graph for the *GaAs/Al$_x$Ga$_{1-x}$/GaAs* [37] quantum well. As can be seen from this figure, linear and nonlinear graphs obey the dispersion laws. In addition, according to equation (15), it is possible to obtain the dependence of the narrow-zone quantum well thickness *d* from $E_c^{parab}(B,d)$.

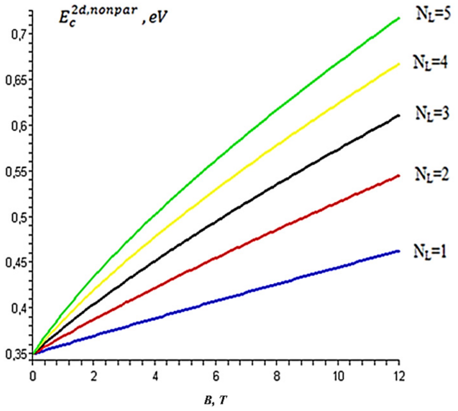


Figure 2. Effect of magnetic field on the energy of free electrons in the conduction band of an *InAs/AlSb* quantum well

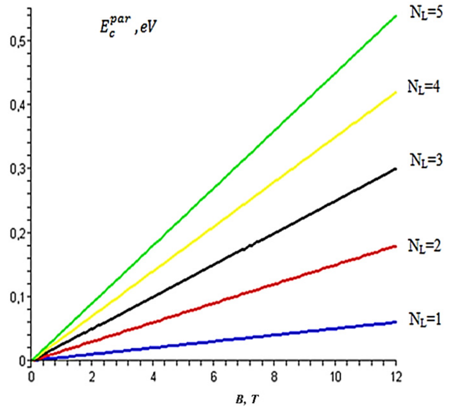


Figure 3. Effect of magnetic field on the energy of free electrons in the conduction band of a GaAs/Al$_x$Ga$_{1-x}$/GaAs quantum well

Mathematical modeling of the temperature and magnetic field dependence of the density of two-dimensional energy states in the allowed zones of a narrow-band quantum coil

It is known from the scientific literature that the change in the energy of charge carriers in the allowed zones of a narrow-zone quantum well under the influence of a strong magnetic field has a strong effect on the two-dimensional energy density of states $N_s^{2d}(E)$. This allows us to obtain sufficient information on the location of electrons and holes in the quantum well at discrete levels and the distribution of current carriers.

However, to date, the dependence of the energy density of states of a narrow-zone quantum well on the magnetic field and temperature has not been sufficiently studied in the available literature. The energy of electrons and holes in a narrow-zone quantum well obeys the non-quadratic dispersion law.

For the quadratic dispersion law, the dependence of the energy density of states in a quantum well on the magnetic field and temperature has been thoroughly studied in [25]. As a result, a new model for $N_s^{k,2d}(E,B,T,d)$ was proposed [29]:

$$N_{S,Z}^{2d}\left(E,B,T,d\right)=\sum_{N_L,N_Z}^{\infty}\frac{eB}{\pi\hbar}\cdot\frac{1}{kT}\cdot\exp\left(-\frac{\left(E-\left(\left(N_L+\frac{1}{2}\right)\hbar\omega_c+\frac{\pi^2\hbar^2}{2m^*d^2}n_Z^2\right)\right)^2}{\left(kT\right)^2}\right) \tag{16}$$

In creating this model, the method of expanding the density of states delta functions *δ(x)* in a series with respect to energy was used [19]. At absolute zero temperature (*T→0*), the energy derivatives of the Lorentz, Gauss, Fermi-Diract functions $\left(\frac{\partial f_0}{\partial E}\right)$ and GN [35] take the form *δ(E)*. The authors of this work [29] mainly applied the Gaussian (*E,T*) delta function to determine $N_s^{k,2d}(E,B,T)$. In this case, the proposed model was mainly applied to heterostructures with a wide band gap (or classical) quantum well. In addition, the obtained $N_s^{k,2d}(E,B,T)$ model was related to free electrons in the conduction band of a wide band gap quantum well.

Now, using the $E_c^{nk,2d}(E,d,E_g^{2d})$ and $E_v^{nk,2d}(E,d,E_g^{2d})$ connections introduced in the previous paragraphs, let's consider $N_{s,c}^{2d,nk}(E_c^{nk,2d},B,T,d)$ and $N_{s,v}^{2d,nk}(E_v^{nk,2d},B,T,d)$.

A function δ(x) of one real argument is reasonable if the following conditions are met:

$$\delta(x)=\begin{cases}-\infty\,, & x=0\\ 0\,, & x\neq 0\end{cases} \tag{17}$$

$$\int_{-\infty}^{\infty}\delta(x)dx=1$$

In work [36], it is shown that the energy dependence of the density of states for two-dimensional materials consists of a sum of delta functions:

$$N_S^{2d}(E,B)=\frac{eB}{\pi\hbar}\sum_{N_LN_Z}\delta\left(E-E\left(N_L,n_Z\right)\right) \tag{18}$$

This equation (18) is a generalized equation, which has been used to date for all (classical, wide and narrow bandgap) quantum-gap semiconductors. As mentioned above, when the condition *T→0* is met, the Gaussian function transforms into Gaussian(*E,T*) δ(E,T). That is:

$$\lim_{T\to 0}Gauss\left(E,T\right)\to\delta\left(E,T\right),\ Gauss\left(E,T\right)=\frac{1}{kT}\exp\left(-\frac{(E-E_i)}{(kT)^2}\right) \tag{19}$$

The energy E_i given in equation (19) corresponds to the valence band ceiling or the conduction band bottom of a narrow-band quantum well. However, equation (19) does not depend on the magnetic field, and the effect of temperature on equation (18) has not been studied.

The meaning of $E(N_L, n_Z)$ in equation (18) is the discrete energy levels of charge carriers in the allowed bands of the quantum well, that is, it corresponds to (8) and (15). In general, in (18) the quantum well corresponds to the delta function $\delta(E-E(N_L, n_Z))$ due to the magnetic field, while in equation (19) the condition *T→0* is fulfilled and *δ(E, T)* becomes the limit *δ(x)*.

Equation (15) gives the dependence of the free electron energy at the bottom of the conduction band of a narrow-zone quantum well on the magnetic field, the thickness of the quantum well, and the number of quantum levels ($E_{nc}^{2d}(B,d,N_L,n_z)$). This is valid for the nonparabolic dispersion law. Then, taking into account the dependence of $N_S^{2d}(E,B)$ on $E(E_L,n_z)$ in (18) and the substitution of $\left(\left(N_L+\frac{1}{2}\right)\hbar\omega_c+\frac{\pi^2\hbar^2}{2md^2}n_z^2\right)$ in (15) for the $-\frac{E_g(B,d)}{2}+\frac{1}{2}\sqrt{(E_g(B,d))^2+4E_g(B,d)[(N_{Lc}+\frac{1}{2})\hbar\omega_{cc}+\frac{\pi^2\hbar^2}{2md^2}n_z^2]}$ term in (16), the following expression is obtained:

$$N_{s,z}^{c,2d}(E,B,T,d)=\sum_{N_L,n_e}^{\infty}\frac{eB}{\pi\hbar}\cdot\frac{1}{kT}\cdot\exp\left(-\frac{\left(E+\frac{E_g(B,d)}{2}-\frac{1}{2}\sqrt{(E_g(B,d))^2+4E_g(B,d)\left(\left(N_L^e+\frac{1}{2}\right)\hbar\omega_c^e+\frac{\pi^2\hbar^2}{2m^*d^2}n_e^2\right)}\right)^2}{(kT)^2}\right) \quad (20)$$

This expression represents the equation for determining the energy density of states in the conduction band of a narrow-zone quantum well. Fig. 4 compares the dependence of the two-dimensional energy density of states for parabolic (wide-gap quantum well) and non-parabolic (narrow-zone quantum well) on the magnetic field at constant $T = const$. It can be seen from this figure that, due to the energy dependence of the effective mass of free electrons in a narrow-zone quantum well, a “compression” (deformation) of discrete Landau levels in a uniform energy interval is observed.

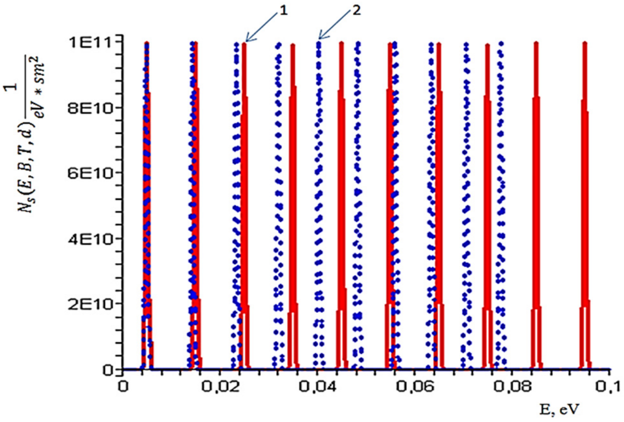
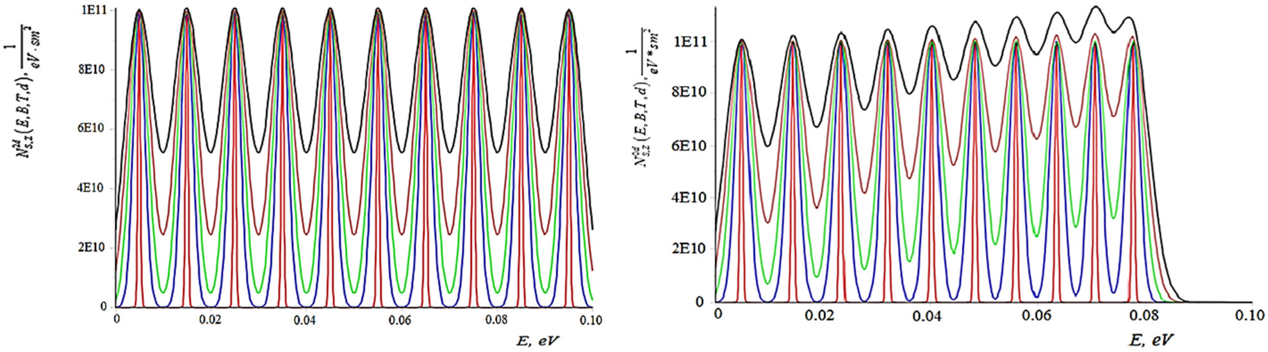


Figure 4. Energy density of states in the conduction band of a wide-band and narrow-zone quantum well for parabolic and nonparabolic dispersion laws

1 - parabolic. $Al_xGa_{1-x}As$ T=4.2 K, B = 10 T, d =5 nm; 2 - non-parabolic. InAs T = 4.2 K, B = 10 T, d =4 nm

Here, graphs of a narrow-zone *InAs* [33] quantum well and a wide-gap *GaAs/Al$_x$Ga$_{1-x}$As/GaAs* (quantum well $Al_xGa_{1-x}As$) [37-39] quantum well are presented. The oscillations were calculated at temperatures T=1.5 K, B=3 T, d=5 nm ($Al_xGa_{1-x}As$) and d=*4* nm (InAs).

Fig. 5 shows the temperature dependence of the two-dimensional energy density of states oscillations in the conduction band of *Al$_x$Ga$_{1-x}$As* and *InAs* quantum well semiconductors. In this case, the quantum well of *Al$_x$Ga$_{1-x}$As* obeys the parabolic dispersion law, and *InAs* obeys the nonparabolic dispersion law. As can be seen from the application of the star-shaped Gaussian function to these materials, it is observed that as the temperature increases, the discrete Landau level “washes out”. However, comparing the graphs a) and b) in Fig.5, it becomes clear that the oscillations of the *InAs* quantum well turn into a continuous spectrum earlier.



a) Parabolic. $Al_xGa_{1-x}As$. 1) T=5 K, B=10 T, d=5 nm; 2) T=20 K, B=10 T, d=5 nm; 3) T=30 K, B=10 T, d=5 nm; 4) T=40 K, B=10 T, d=5 nm; 5) T=50 K, B=10 T, d=5 nm

b) Nonparabolic. InAs. 1) T=5 K, B=10 T, d=4 nm; 2) T=20 K, B=10 T, d=4 nm; 3) T=30 K, B=10 T, d=4 nm; 4) T=40 K, B=10 T, d=4 nm; 5) T=50 K, B=10 T, d=4 nm

Figure 5. a) Oscillations of the temperature-dependent change in the energy density of states in the conduction band of a wide-band quantum well for the parabolic dispersion law; b) Oscillations of the temperature-dependent change in the energy density of states in the conduction band of a narrow-band quantum well for the nonparabolic dispersion law

Fig. 6 shows the temperature variation of the density of states oscillations of an *InAs* narrow-zone quantum well at B = 10 T and d = 4 nm. It can be seen from this figure that as the temperature increases, the “peaks” of the discrete Landau levels decrease. This, of course, indicates the fulfillment of the condition $kT \approx \hbar\omega_c$ and the laws of “thermal expansion”.

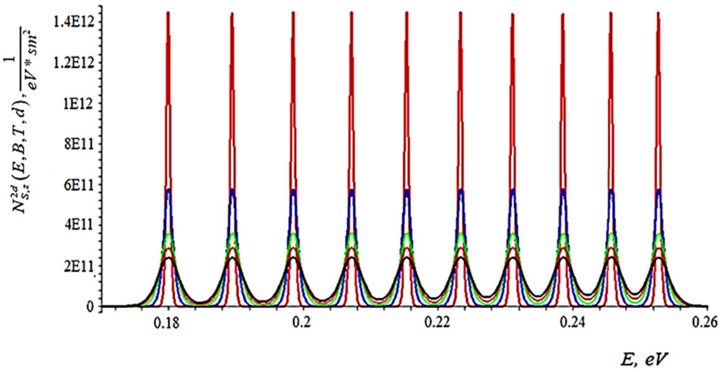


Figure 6. Temperature dependence of the energy density of states oscillations in the conduction band of an InAs narrow-zone quantum well (*d*=4 nm) up to a transverse quantizing magnetic field (*B*=10 T). The energy spectra shown in the figure were calculated by equation (20)
1) *T*=2 K, *B*=10 T, *d*=4 nm; 2) *T*=5 K, *B*=10 T, *d*=4 nm; 3) *T*=8 K, *B*=10 T, *d*=4 nm; 4) *T*=10 K, *B*=10 T, *d*=4 nm; 5) *T*=12 K, *B*=10 T, *d*=4 nm

CONCLUSIONS

In the process of carrying out this research work, the following conclusions were reached:

1. A mathematical model was developed to determine the dependence of the light hole energy $E_v^{2d}\left(E_g(B,d),B,d,n_z,N_{Lv}\right)$ at the valence band ceiling of a narrow-zone quantum well and the free electron energy $E_n^{2d,nonparab}(E_g(B,d),B,d,n_z,N_{Lc})$ at the conduction band bottom of the quantum well on the magnetic field, band gap width, quantum well thickness, and number of dimensional levels.
2. A method was proposed to determine the dependence of the allowed bands $N_{vs}^{2d(n)}$, $N_{cs}^{2d(n)}$ of narrow-zone quantum well semiconductors on the magnetic field *B* and temperature *T*.
3. Using this method, the dependence of the band gap width of a narrow-zone quantum well on the magnetic field *B* and temperature *T* was determined.

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МОДЕЛЮВАННЯ ЗАЛЕЖНОСТІ ШИРИНИ ЗОНИ ВІД ТЕМПЕРАТУРИ ТА МАГНІТНОГО ПОЛЯ У НАПІВПРОВІДНИКАХ З ВУЗЬКОЗОННИМИ КВАНТОВИМИ ЯМАМИ

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Фундаментальним фізичним параметром як об'ємних, так і низьковимірних напівпровідникових структур є ширина забороненої зони E_g^{3d}, E_g^{2d}, енергетична ширина якої дозволяє заздалегідь передбачити робочі параметри напівпровідникових пристроїв. Тому визначення E_g^{3d}, та E_g^{2d} у випадках, коли ширина забороненої зони щойно синтезованих матеріалів невідома вважається одним з першочергових завдань у технології напівпровідникових гетероструктур. Крім того, ще однією важливою особливістю E_g є його сильна чутливість до зовнішніх впливів. Дійсно, зміни E_g, що виникають внаслідок таких ефектів, можуть фундаментально змінити фізичні та хімічні властивості напівпровідникових приладів.

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