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ELECTRON STATES IN A FIVE-LAYER SEMICONDUCTOR STRUCTURE. PART 1

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Transcendental equations have been obtained to determine the electron energy spectrum in a five-layer semiconductor structure with an energy dip at its center for various energy ranges. It is shown that the presence of this dip leads to an increase in the energy gaps calculated within first-order perturbation theory. It is pointed out that the origin of the energy-level shift is associated with the dependence of the electron Hamiltonian not only on the potential-energy operator but also on the kinetic-energy operator, which depends on the effective masses in each layer of the structure. As has been shown, the modification of the potential profile of a simple well due to the dip should result in a lowering of the level, whereas the difference in kinetic energies for $m_3 < m_2$ promotes an upward shift of the levels, where m_i is the effective electron mass in the i-th layer.
Keywords: *Five-layer semiconductor structure; Electron energy spectrum; Transcendental equations; Effective mass approximation; Perturbation theory; Energy level shift*

INTRODUCTION

In semiconductor micro- and nanoelectronics, multilayer structures are increasingly employed, in which individual semiconductor layers are characterized by different electrical conductivities or a qualitative modification of the energy spectrum of charge carriers occurs [1–3]. Therefore, classical and quantum-physical investigations of electronic phenomena in such structures provide an opportunity to enhance the efficiency and improve the operating parameters of devices based on them.

At the present stage of micro- and nanoelectronics development, in view of the substantially increased use of multilayer crystals, both classical and quantum-mechanical studies of the electronic phenomena occurring in them are of current interest.

In recent years, the characteristic layer thicknesses in multilayer structures formed from different semiconductors have been in the range of 1–100 nm [4–9]. Accordingly, layered structures based on nanostructures are used in electronics as a fundamentally new type of artificial materials with unusual physical properties. In turn, interest in nanostructures stimulates the development of modern atom-level technologies and research directions associated with surface-structure studies. In this regard, investigating electronic kinetic phenomena in multilayer homo- and heterostructures is of considerable interest from both experimental and theoretical viewpoints [6–11]. On the one hand, this opens the possibility of creating resonant-tunneling devices; on the other hand, it enables observation of unique properties of multilayer structures arising due to interference of de Broglie waves [12–14].

METHODS

Wave Functions of the States and the Energy Spectrum of Charge Carriers in a Multilayer Structure.

At present, the resonant-tunneling diode (RTD) forms the basis of promising nanoelectronic devices. In particular, multilayer structures with an additional rectangular potential well in the central region (Fig. 1) are used to create new generations of RTDs, for example, heterolasers with separate electronic and optical confinement [6,16]. Owing to the lowering of the potential energy, new opportunities arise for controlling the positions of quantum levels in the wide main part of the potential well.

Let us consider, in the five-layer structure with a potential well at the center shown in Fig. 1, the states of charge carriers, e.g., the wave functions, as well as the energy spectrum. In what follows, we take into account the differences in the geometrical dimensions of each layer and the variation of the effective masses of charge carriers depending on the potential-energy profile within them. In the structure whose schematic is shown in Fig. 1, the effective mass of a charge carrier in the layer is $m_n(d_n)$, where n denotes the layer thicknesses.

Throughout the paper we adopt the following unified notation. The structure consists of five layers, numbered from left to right: layer 1 (the left outer barrier, $x \leq 0$); layer 2 (the left inner well, $0 < x \leq d_2$); layer 3 (the central dip, $d_2 < x \leq d_2 + d_3$); layer 4 (the right inner well, $d_2 + d_3 < x \leq d_2 + d_3 + d_4$); and layer 5 (the right outer barrier, $x > d_2 + d_3 + d_4$). The thicknesses of the three inner layers are denoted d_2, d_3, d_4; the corresponding effective masses are m_1, m_2, m_3, m_4, m_5; and the wave numbers k_1, k_2, k_3, k_4, k_5 are defined by Eq. (5). The barrier height is $U_1 > 0$,

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while $U_2 > 0$ denotes the depth (magnitude) of the central dip, so that the potential takes the value $-U_2$ in layer 3. With this convention, the structure is symmetric when $d_2 = d_4$ (and consequently $k_2 = k_4, m_2 = m_4$).

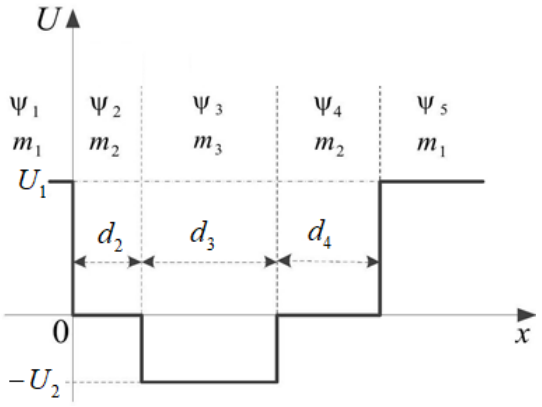

Figure 1. Potential profile of a five-layer semiconductor structure. The labels in the figure follow the unified notation introduced above: layer thicknesses d_2, d_3, d_4 (left inner well, central dip, right inner well, respectively); effective masses $m_1 - m_5$ in layers 1–5; barrier height U_1; well depth U_2.

$$\begin{cases} m_1, & x \le 0, \\ m_2, & 0 < x \le d_2, \\ m_3, & d_2 < x \le d_2 + d_3, \\ m_4, & d_2 + d_3 < x \le d_2 + d_3 + d_4 \\ m_5, & x > d_2 + d_3 + d_4, \end{cases} \tag{1}$$

$U_1 > 0$ and $U_3 > 0$ are the heights of the potential barrier in the outer layers, and $U_2 < 0$ is the depth of the potential well in the central layer, i.e.,

$$U_n = \begin{cases} U_1, x \le 0, x > d_2 + d_3 + d_4 \\ 0, 0 < x \le d_2, d_2 + d_3 < x \le d_2 + d_3 + d_4 \\ -U_2, d_2 < x \le d_2 + d_3 \end{cases} \tag{2}$$

The energy spectrum of charge carriers and their wave functions in such a structure are determined by solving the following Schrödinger equation:

$$\frac{\hbar^2}{2m_n^*} \cdot \frac{\partial^2 \psi_n(x)}{\partial x^2} + (E - U_n)\psi_n = 0, n = 1,2, \dots ,5. \tag{3}$$

Equation (3) is to be understood as the layer-wise (piecewise) form of the more general one-dimensional effective-mass Schrödinger equation with position-dependent mass $m^*(x)$, namely

$$-\left(\frac{\hbar^2}{2}\right)\left(\frac{d}{dx}\right)\left[\left(\frac{1}{m^*(x)}\right)\left(\frac{d\psi(x)}{dx}\right)\right] + U(x)\,\psi(x) = E\,\psi(x) \tag{3a}$$

in which the operator $1/m^*(x)$ is placed between the two derivatives in order to preserve the Hermiticity of the kinetic-energy operator when $m^*(x)$ is piecewise-constant [20, 21]. Within each layer $m^*(x)$ is constant and equation (3a) reduces to (3); the difference between the two formulations is therefore manifested entirely through the matching conditions at the heterointerfaces. The Bastard condition has been recently applied by the present authors to the analysis of asymmetric multilayer semiconductor structures [25] and is a standard ingredient in modern envelope-function calculations for resonant-tunneling heterostructures [22–24]. Integrating (3a) across an interface located at $x = x_i$ between layers n and $n + 1$ yields the so-called Bastard (BenDaniel–Duke) boundary conditions:

$$\psi_{\mathrm{n}}(x_{\mathrm{i}}) = \psi_{\mathrm{n}}{}^{+1}(x_{\mathrm{i}}),\ \left(\frac{1}{m_n}\right)\frac{d\psi_{\mathrm{n}}}{dx}\Big|_{x=x_i} = \left(\frac{1}{m_{n+1}}\right)\frac{d\psi_{n+1}}{dx}\Big|_{x=x_i}, \tag{3b}$$

i.e. continuity of the envelope function and continuity of the probability current $(1/m^*)\,d\psi/dx$ at every interface $x_{\mathrm{i}} \in \{0, d_2, d_2 + d_3, d_2 + d_3 + d_4\}$. The matching conditions (3b) are precisely those that lead to the homogeneous linear system (6) for the coefficients $A_{\mathrm{n}}, B_{\mathrm{n}}$, in which the symbol $\hat{k}$ appearing in the original derivation should be read as the operator $\hat{k} = -i\,(1/m^*(x))\,d/dx$ acting on the envelope. The transcendental equations (7)–(11) of the present work are obtained from the determinant of this system.

The wave functions corresponding to the layers of the structure in the Schrödinger equation can be written in the following form:

$$\begin{cases} \psi_1 = A_1 \cdot \exp(k_1 x) \\ \psi_2 = A_2 \cdot \cos(k_2 x) + B_2 \cdot \sin(k_2 x) \\ \psi_3 = A_3 \cdot \cos\big(k_3(x-d_2)\big) + B_3 \cdot \sin\big(k_3(x-d_2)\big) \\ \psi_4 = A_4 \cdot \cos\big(k_4(x-d_2-d_3)\big) + B_4 \cdot \sin\big(k_4(x-d_2-d_3)\big) \\ \psi_5 = B_5 \cdot \exp\big(-k_5(x-d_2-d_3-d_4)\big) \end{cases} \tag{4}$$

here

$$k_1 = \big(2m_1\hbar^{-2}(U_1 - E)\big)^{1/2}, k_2 = (2m_2\hbar^{-2}E)^{1/2}, k_3 = \big(2m_3\hbar^{-2}(E+U_2)\big)^{1/2} \cdot \tag{5}$$

For the general (asymmetric) structure, the wave numbers in the right inner well and in the right outer barrier are defined analogously: $k_4 = (2m_4E/\hbar^2)^{1/2}$ and $k_5 = [2m_5(U_1 - E)/\hbar^2]^{1/2}$. In the symmetric case considered below ($d_2 = d_4, m_2 = m_4, m_1 = m_5$) we have $k_2 = k_4$ and $k_1 = k_5$.

From the boundary conditions, which follow from the requirements of continuity of the wave function and the probability current density, we obtain the following results:

$$\begin{aligned} &A_1 - A_2 = 0, \cdot\, \tilde{k}_1 A_1 - \tilde{k}_2 B_2 = 0, A_2\cos(k_2 d_2) + B_2\sin(k_2 d_2) - A_3 = 0, \\ &-\tilde{k}_2 A_2 \sin(k_2 d_2) + \tilde{k}_2 B_2 \cos(k_2 d_2) - \tilde{k}_3 B_3 = 0, \cdot\, A_3\cos(k_3 d_3) + B_3\sin(k_3 d_3) - A_4 = 0, \\ &-\tilde{k}_3 A_3 \sin(k_3 d_3) + \tilde{k}_3 B_3 \cos(k_3 d_3) - \tilde{k}_4 B_4 = 0, A_4\cos(k_4 d_4) + B_4\sin(k_4 d_4) - B_5 = 0, \\ &-\tilde{k}_4 A_4 \sin(k_4 d_4) + \tilde{k}_4 B_4 \cos(k_4 d_4) + \tilde{k}_5 B_5 = 0. \end{aligned} \tag{6}$$

As a result, the energy spectra of the charge carriers are determined from the system of equations (6) by setting to zero the determinant of the matrix composed of the coefficients multiplying the unknown quantities A_n and B_n, and are expressed as follows:

$$\begin{aligned} &\big[\tilde{k}_4\sin(k_2 d_2) - \tilde{k}_3\cos(k_2 d_2)\big]\big[-\tilde{k}_2\big(\tilde{k}_1 - \tilde{k}_3\big)\cos(k_2 d_2) + \big(\tilde{k}_1\tilde{k}_3 + \tilde{k}_2^2\big)\sin(k_2 d_2)\big] \times \\ &\times \big[\tilde{k}_4\cos(k_4 d_4) + \tilde{k}_5\sin(k_4 d_4)\big] = 0 \end{aligned} \tag{7}$$

It should be noted that the solutions of equation (6) make it possible to determine the energy spectrum under the condition $U_1 > E > 0$. Similarly, to simplify the solution of the problem, if one assumes $d_2 = d_4$ and $k_2 = k_4$, then relation (6) can be written in the following form:

$$\begin{aligned} &\big[\tilde{k}_2^2\big(\tilde{k}_3^2 - \tilde{k}_1^2\big) + \big(\tilde{k}_1^2\tilde{k}_3^2 - \tilde{k}_2^4\big)tg(k_2 d_2)\big]\mathrm{tg}(k_3 d_3) + 2\tilde{k}_1\tilde{k}_2^2 k_3 \cdot [th^2(k_2 d_2) - 1] + \\ &+\tilde{k}_2\big[\tilde{k}_3\big(\tilde{k}_2^2 - \tilde{k}_1^2\big) + \tilde{k}_1\big(\tilde{k}_3^2 + \tilde{k}_2^2\big)\mathrm{tg}(k_3 d_3)\big]\big(\mathrm{tg}(k_2 d_2) + \mathrm{tg}(k_2 d_4)\big) = 0. \end{aligned} \tag{8}$$

If the last expression is treated as consisting of three terms, $f_1 = f_{11} + f_{12} + f_{13}$, then their dependences on the energy, taken in units of U_2, are shown in Fig. 2, and each of them passes through zero.

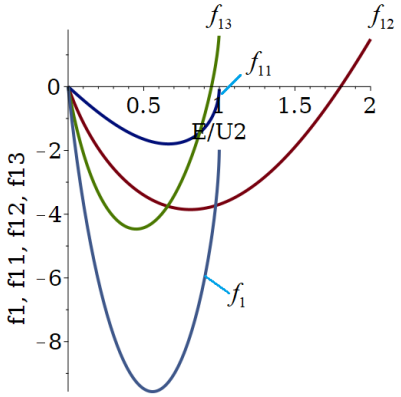

Figure 2. Dependences of the quantities f_{11}, f_{12}, and f_{13}, representing the 1st, 2nd, and 3rd terms of relation (8), as well as the quantity f_1, equal to their sum, on the energy taken in units of U_2.

However, the energies of the charge carriers inside the structure are determined from the condition $f_1 = 0$. It can be seen from this figure that, in a symmetric structure satisfying the condition $d_2 = d_4, k_2 = k_4$, no electron-confined energy

levels are formed. Here and in the subsequent numerical calculations (unless stated otherwise) [19], the following values were chosen: $d_2 = d_4 = 0.9$ nm, $d_3 = 1.84$ nm, $U_2 = 0.24$ eV, $m_2 = 0.046m_0$, $m_3 = 0.023m_0$.

From expression (7), the quantization conditions for the energies of bound states satisfying $0 \geq E > U_2$ can be written as follows:

$$\left[\tilde{k}_2^2\left(\tilde{k}_1^2 - \tilde{k}_3^2\right) + \left(\tilde{k}_2^4 - \tilde{k}_1^2\tilde{k}_3^2\right)\mathrm{th}(k_2d_2)\right]\mathrm{tg}(k_3d_3) + 2\tilde{k}_1\tilde{k}_2^2\tilde{k}_3 \cdot [1 + th^2(k_2d_2)] +$$

$$+\tilde{k}_2\left[\tilde{k}_3\left(\tilde{k}_2^2 + \tilde{k}_1^2\right) + \tilde{k}_1\left(\tilde{k}_2^2 - \tilde{k}_3^2\right)\mathrm{tg}(k_3d_3)\right]2\mathrm{th}(k_2d_2) = 0, \quad (9)$$

Remark on equations (8) and (9). The repeated factors of the type $(\mathrm{t}g(k_2d_2))^2$ and $(\mathrm{th}(k_2d_2))^2$ appearing in (8) and (9) are not typographical errors: they are obtained from the corresponding general expressions $tg(k_2d_2) \cdot tg(k_4d_4)$ and $th(k_2d_2) \cdot th(k_4d_4)$, valid for an asymmetric structure, after substituting the symmetry conditions $d_2 = d_4$ and $k_2 = k_4$ stated above. They may equivalently be written as $tg^2(k_2d_2)$ and $th^2(k_2d_2)$. The fully general (asymmetric) form, in which the corresponding factors appear as $tg(k_2d_2) \cdot tg(k_4d_4)$ and $th(k_2d_2) \cdot th(k_4d_4)$, is given in Part 2 of the present series, equation (6); the present equations (8) and (9) reduce to that expression in the symmetric limit $d_2 = d_4, k_2 = k_4$.

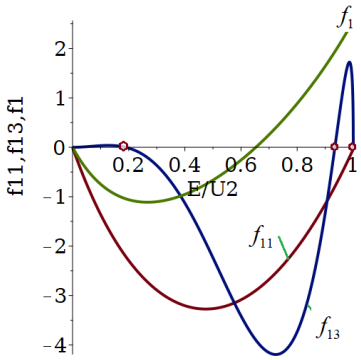

Figure 3. The quantities f_{11}, f_{12}, and f_{13} represent the 1st, 2nd, and 3rd terms of relation (9), respectively; f_1 is equal to their sum.

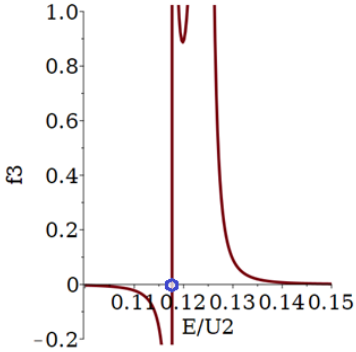

Figure 4. Dependence of the quantity f_3 on the relative energy E/U_2 (see expression (10)).

If expression (9) is regarded as consisting of three components, $f_1 = f_{11} + f_{12} + f_{13}$, then it follows from Fig. 3 that their dependences on the energy, taken in units of U_2, are such that, in a symmetric structure satisfying the condition $d_2 = d_4$, $k_2 = k_4$, three electron energy levels are formed (they are marked by red dots). If the height of the potential barrier U_1 is significantly greater in magnitude than the depth of the potential well, then the energies of the charge carriers:
a) under the condition $E > 0$

$$f3 = \left[\tilde{k}_2^2 - \tilde{k}_3^2\mathrm{tg}(k_2d_2)\mathrm{tg}(k_2d_4)\right]\mathrm{tg}(k_3d_3) + \tilde{k}_2\tilde{k}_3[\mathrm{tg}(k_2d_2) + \mathrm{tg}(k_2d_4)] = 0, \quad (10)$$

b) under the condition $0 \geq E > |U_2|$

$$f4 = \left[\tilde{k}_2^2 + \tilde{k}_3^2\mathrm{th}(k_2d_2)\mathrm{th}(k_2d_4)\right]\mathrm{tg}(k_3d_3) + \tilde{k}_2\tilde{k}_3[\mathrm{th}(k_2d_2) + \mathrm{th}(k_2d_4)] = 0 \quad (11)$$

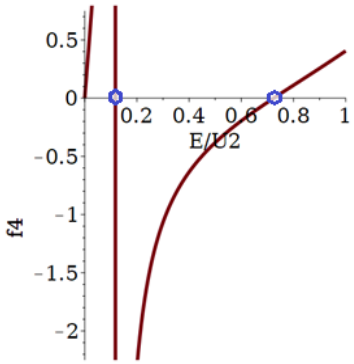

Figure 5. Dependence of the quantity $f_4$on the relative energy E/U_2 (see expression (11)).

These relations make it possible to determine them. In this case, Figs. 4 and 5 show that, in the first case, one energy level is formed, whereas in the second case, two energy levels are formed. In addition, for a structure with an infinitely high potential barrier, the coefficients in the charge-carrier wave functions (satisfying the orthonormality condition) can be determined as follows:

$$A_1 = A_2 = B_5 = 0, B_2 = A, A_3 = A \cdot \sin(k_2 d_2),$$

$$A_4 = A\left[\tilde{k}_{23}\cos(k_2 d_2)\sin(k_3 d_3) + \sin(k_2 d_2)\cos(k_3 d_3)\right], B_3 = A\tilde{k}_{23}\cos(k_2 d_2),$$

$$B_4 = -A\mathrm{ctg}(k_2 d_4)\left[\tilde{k}_{23}\cos(k_2 d_2)\sin(k_3 d_3) + \sin(k_2 d_2)\cos(k_3 d_3)\right], \quad (12)$$

here $\bar{k}_{n'n} = \frac{\bar{k}_{n'}}{\bar{k}_n} = \frac{m_n k_{n'}}{k_n m_{n'}}$. As a result, it has been established that the probability of finding charge carriers in a selected layer depends on the geometrical dimensions of the potential wells, their mutual arrangement, and also on the effective masses of the charge carriers in the layers.

Thus, during tunneling through the structure, the possibility of electron confinement in the region of the potential wells may arise [1,7], which, undoubtedly, reduces the amplitude values of the resonant current. The relative shift of the ground and first excited states can be qualitatively explained on the basis of perturbation theory [7].

In the first approximation, the calculated energy values are determined as follows [LL, Quantum Mechanics]:

$$E_n^{(2)} \approx E_n^{(0)} + \delta E_n^{(1)}, \delta E_n^{(1)} = \left\langle \psi_{n_0}^{(0)} \middle| \hat{V} \middle| \psi_{n_0}^{(0)} \right\rangle, \quad (13)$$

here, $E_n^{(0)}$ and $\psi_{n0}^{(0)}$ are the unperturbed energy and the wave function of the n-th order state, and $\hat{V}$ is the perturbation operator. Now, for the case where the potential wells of width b and depth $-U_2$ are infinitely deep, and the potential well of width d_2 is located at the center of the structure, we obtain the following result:

$$\delta E_1^{(1)} = -U_2\left[\frac{1}{d_{32}+1} + \frac{1}{\pi}\sin\left(\frac{\pi}{d_{32}+1}\right)\right], \quad \delta E_2^{(1)} = -U_2\left[\frac{1}{d_{32}+1} - \frac{1}{2\pi}\sin\left(\frac{2\pi}{d_{32}+1}\right)\right].$$

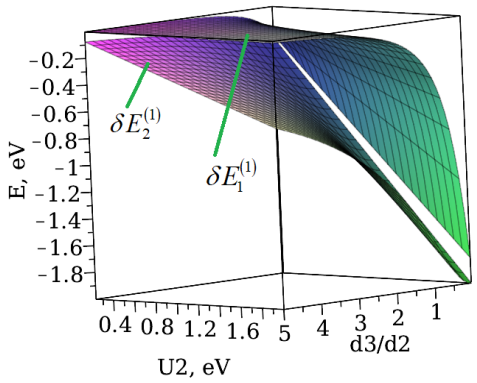

Figure 6. Two types of dependences of the energy quantities $\delta E_1^{(1)}$ and $\delta E_2^{(1)}$ on the depth of the middle potential well (U_2), as well as on the ratio of the thicknesses of the third and second layers (d_3/d_2).

It can be seen from Fig. 6 that the dependences of the energy quantities $\delta E_1^{(1)}$and $\delta E_2^{(1)}$, calculated from expression (13), on the depth of the middle potential well (U_2) and on the ratio of the thicknesses of the third and second layers (d_3/d_2) are as follows: (a) with increasing U_2, the quantity $\delta E_1^{(1)}$ remains almost unchanged quantitatively, whereas $\delta E_2^{(1)}$ decreases; (b) with increasing $d_{32} = d_3/d_2$, both quantities increase.

Expressions (14) show that a displacement of the energy-level positions in the quantum potential well leads to a lowering of the ground and excited-state levels. Obviously, to explain the positive shift of the excited state, it is necessary to take into account the difference in effective masses. In this case, according to the infinite-depth potential-well model:

$$\delta E_n^{(1)} = \frac{2}{d_2+d_3}\int_{d_3/2}^{(d_3+2d_2)/2} \sin\left(\frac{\pi n x}{d_2+d_3}\right)\left(\frac{\vec{p}^2}{2m_3} - \frac{\vec{p}^2}{2m_2} - U_2\right)\sin\left(\frac{\pi n x}{d_2+d_3}\right)dx = \\ = \left[\frac{\pi n^2\hbar^2}{2(d_2+d_3)^2}\left(\frac{1}{m_3} - \frac{1}{m_2}\right) - U_2\right]\cdot\left[\frac{d_2}{d_2+d_3} - \frac{(-1)^n}{n\pi}\sin\left(\frac{2\pi n d_2}{d_2+d_3}\right)\right]. \quad (14)$$

To clarify the problem, Fig. 7 shows the dependence of $\delta E_n^{(1)}$on the index of the energy level, where its possible values on the plot are determined by the intersection points of the curve with vertical lines drawn from the selected value of n. It can be seen from this figure that the energy levels with indices $n = 2$ and $n = 8$ can be confining levels, since they have negative values.

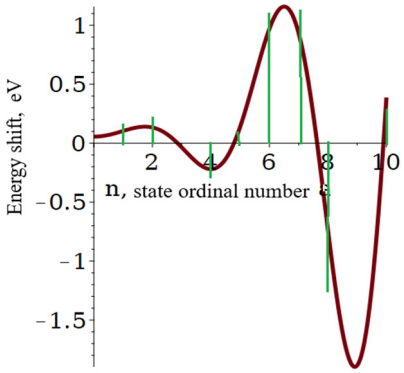

Figure 7. Dependence of the quantity $\delta E_n^{(1)}$ on the energy-level index n for a second-layer thickness $d_2 = 10$ nm.

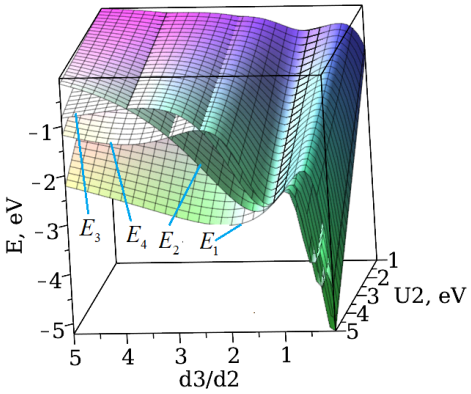

Figure 8. Plots of the state energies with indices $n = 1,2,3,4$ at a second-layer thickness $d_2 = 10$ nm as functions of the depth of the potential well in the middle region (U_2) and of the ratio of the thicknesses of the third and second layers (d_3/d_2).

Figure 8 shows the dependence of the first four energy levels on the depth of the central potential well and the thickness ratio d_3/d_2 at $d_2 = 10$ nm. The nonlinear variation of the energy surfaces demonstrates that both the depth and the relative width of the central dip significantly affect the positions and separation of the confined states.

CONCLUSIONS

The reason for the shift of the excited level is that the particle Hamiltonian in a well with a dip differs not only in potential energy but also in kinetic energy due to the difference in effective masses in different parts of the well. As shown earlier, a modification of the potential profile of a simple well caused by a dip of depth $-U_2$ should lead to a lowering of the level, whereas the difference in kinetic energies for $m_3 < m_2$ promotes an upward shift of the levels. For the first excited state ($n = 2$), the effect of the effective-mass difference is more pronounced; therefore, in a structure consisting of a potential well with an additional dip, the excited level lies higher than the excited level in a simple well (without a dip).

The calculations show that, within the first-order approximation of perturbation theory, the behavior of the energy shifts can be qualitatively explained only for small values of $d_3/(d_2 + d_3 + d_4)$; as the width of the dip increases, higher-order approximations must be taken into account.

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ЕЛЕКТРОННІ СТАНИ У П'ЯТИШАРОВІЙ НАПІВПРОВІДНИКОВІЙ СТРУКТУРІ. ЧАСТИНА 1

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Отримано трансцендентні рівняння для визначення енергетичного спектра електронів у п'ятишаровій напівпровідниковій структурі з енергетичним заглибленням у центрі для різних діапазонів енергій. Показано, що наявність цього заглиблення призводить до збільшення енергетичних щілин, обчислених у межах теорії збурень першого порядку. Зазначено, що походження зсуву енергетичних рівнів пов'язане із залежністю електронного гамільтоніана не лише від оператора потенціальної енергії, але й від оператора кінетичної енергії, який визначається ефективними масами в кожному шарі структури. Як показано, модифікація потенціального профілю простого квантового колодязя внаслідок наявності заглиблення повинна призводити до зниження енергетичного рівня, тоді як різниця кінетичних енергій за умови $m_3 < m_2$ сприяє зсуву рівнів угору, де m_i— ефективна маса електрона в *i*-му шарі.

Ключові слова: *п'ятишарова напівпровідникова структура, енергетичний спектр електронів, трансцендентні рівняння, наближення ефективної маси, теорія збурень, зсув енергетичних рівнів*