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THEORY OF ELECTRON TRANSPORT IN TWO-BARRIER FIVE-LAYER SEMICONDUCTOR STRUCTURES

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The dependence of the transparency coefficient of a five-layer two-barrier structure on the electron energy and the ratio of the widths of two neighboring potential barriers is calculated. It is shown that the extremum of the transparency coefficient significantly depends on the geometric dimensions of the structure layers. In a symmetric five-layer two-barrier semiconductor structure, the condition for the occurrence of "resonant" electron transitions is defined. It is demonstrated that the mechanism of such (resonant) transitions is explained by the interference of de Broglie waves of electrons in the potential well, where the phases of de Broglie waves are determined by the geometric dimensions of the structure, and their amplitudes - by the ratio of the carrier energy to the height of the potential barrier. It has been established that with an increase in the effective mass of charge carriers, the number of intersections of the quantities $f_R(\xi)$ and $\frac{(1-2\xi)}{\sqrt{\xi-\xi^2}}$ increases. These intersections determine the dimensionally-quantized levels where electrons are localized.
Keywords: *Potential Barrier; Potential Well; Two-Barrier Five-Layer Structure; Transmission coefficient; Size Quantization*
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INTRODUCTION

The investigation of charge carrier transport through multilayer semiconductors considering the symmetry of the structure is a relevant task due to its applications in the field of solid-state physics, particularly in nanoelectronics [1-5]. In works [6-9], the dynamic conductivity σ(ω) or the current j(ω) response of the system to external stimuli in a semiconductor multilayer structure has been calculated. The theory has been developed using various models and mathematical methods to solve the full Schrödinger equation [10] for a system of electrons interacting with the electromagnetic field in a structure with delta-shaped potential barriers. In works [1-10], electronic transport through multilayer structures has been investigated without considering the Bastard condition [11], i.e., the difference in the effective masses of electrons in the layers of the structure has not been taken into account.

In the studies we have examined, computations are primarily conducted on computers, where it is difficult to analyze intermediate calculations [7-9], while analytical calculations have been performed [13-18], where changes in the effective masses of electrons when transitioning from one layer to another are not considered.

Based on the results of works [1, 2, 14-20], it can be concluded that the transmission coefficient of electrons through an isolated potential barrier is less than unity and does not depend on whether the electron passes through the potential barrier from the left or the right. Based on this conclusion, it follows that in systems consisting of a periodically arranged sequence of "potential well + potential barrier," the resulting transmission coefficient of electrons through the potential barrier may be less than unity. However, it is not always possible to consider the resulting transmission coefficient through such structures as the sum of the transmission coefficients of electrons through individually isolated potential barriers. This is because the de Broglie waves belonging to electrons in a fixed well consist of components approaching the barrier, scattered from the barrier, and passing through the barrier, the first and second components of which interfere since they differ in amplitude and phase. As a result, not only the nature of the physical analysis of the problem changes but also the theoretical calculations applied to electron transport in multilayer semiconductor structures.

QUANTUM-MECHANICAL ANALYSIS OF ELECTRON TRANSPORT

Therefore, let us consider the two-barrier five-layer structure below, where each barrier is located between two adjacent potential wells (Fig. 1). In solving this problem, unlike simple quantum mechanical approximation [10], we take into account the change in the effective mass of the electron when transitioning from one layer to another, that is, we consider the carrier masses to be different in all layers [16-18].

It is worth noting that from Fig. 1, heterostructures with different energy structures can be obtained by choosing the magnitude and sign of the potential barrier heights.

In particular, it provides the energy structure of ladder-cascade and other heterostructures, in which the height of the potential barriers increases, i.e., $U_1 > U_2 > U_3 > U_4$, or decreases, i.e., $U_1 < U_2 < U_3 < U_4$. For all the cases mentioned

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above, by solving the Schrödinger equation with the Bastard condition [11-12, 16-18], one can determine characteristic parameters such as the transmission coefficient of the structure. However, depending on whether the electron's energy is significantly higher or lower than the height of the considered potential barrier, the electron's wave vector can be either a real or an imaginary quantity. Therefore, in intermediate calculations, especially when separating the wave function into real and imaginary parts in the initial stages of the calculation, one must be extremely careful to avoid confusion in the analysis of the final results.

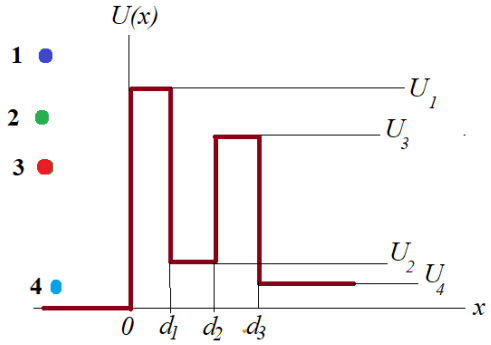

Figure 1. Carrier transport through a five-layer semiconductor structure. 1 corresponds to carrier transport above the potential, 4 - below the potential, 2, 3 - transport below the first and above the second potential. In case 1, the energy of the carriers exceeds all potential barrier heights, in case 4, the energy of the carriers is less than all potential barrier heights, and in the remaining cases, the energy is higher than some potential barrier height and lower than the height of another.

Thus, let us denote the solution of the Schrödinger equation for case 1 in the potential depicted in Fig. 1, i.e., the electron transition above the potential, as follows:

$$\boldsymbol{\psi_1(x) = A_i\, exp(\, ik_i x) + B_i\, exp(-ik_i x)},\tag{1}$$

where $k_1 = \sqrt{\frac{2m_1}{\hbar^2}E}$, $k_i = \sqrt{\frac{2m_i}{\hbar^2}(E - U_i)}$, $i = 2,3,4$ are quantities determined by the boundary conditions of the problem, such as continuity and finiteness conditions of the wave functions at the interface of two adjacent layers.

If the energy of the electron is lower than the heights of the potential barriers in all layers, then the solution of the Schrödinger equation can be written in the form (1), where one needs to make the substitution $k_i = i\kappa_i$, which for an electron with energy $E\langle U_i$ takes the form:

$$\psi_i(x) = A_i exp(\kappa_i x) + B_i\, exp(-\kappa_i x) D_i.\tag{2}$$

Then, following the work [17], it is not difficult to obtain the expression for the electron transmission coefficient for case 1 as:

$$t_{overbarrier} = 4\frac{\tilde{k}_5}{\tilde{k}_1}\{\Re_1^2 + \Re_3^2 + (\Re_2^2 + \Re_4^2 - \Re_1^2 - \Re_3^2)\, sin^2\left(\tilde{k}_3(d_2 - d_1)\right) +$$

$$+2(\Re_1\Re_2 + \Re_3\Re_4)\, cos\big(k_3(d_2 - d_1)\big)\, sin\left(\tilde{k}_3(d_2 - d_1)\right)\},\tag{3}$$

Here:

$$\Re_1 = \frac{1}{\tilde{k}_1}\left[\tilde{k}_1 + \tilde{k}_5 + \frac{\tilde{\kappa}_4^2\tilde{k}_1 + \tilde{k}_5\tilde{k}_2^2}{\tilde{k}_2\tilde{k}_4} tg\big(k_2(d_2 - d_1)\big) tan\big(k_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, cos\big(k_2(d_2 - d_1)\big)\, cos\big(k_4(d_4 - d_1 - d_2)\big),$$

$$\Re_2 = \frac{1}{\tilde{k}_1\tilde{k}_3}\left[\frac{\tilde{k}_5\tilde{k}_2^2 - \tilde{k}_1\tilde{k}_3^2}{\tilde{k}_2} + \frac{\tilde{k}_4^2\tilde{k}_1 - \tilde{k}_3^2\tilde{k}_5}{\tilde{k}_4} cot\big(k_2(d_2 - d_1)\big) tan\big(k_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, sin\big(k_2(d_2 - d_1)\big)\, cos\big(k_4(d_4 - d_1 - d_2)\big),$$

$$\Re_3 = \frac{1}{\tilde{k}_1}\left[\frac{\tilde{k}_2^2 - \tilde{k}_1\tilde{k}_5}{\tilde{k}_2} + \frac{\tilde{k}_4^2 - \tilde{k}_1\tilde{k}_5}{\tilde{k}_4} cot\big(k_2(d_2 - d_1)\big) tan\big(k_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, sin\big(k_2(d_2 - d_1)\big)\, cos\big(k_4(d_4 - d_1 - d_2)\big),$$

$$\Re_4 = -\frac{1}{\tilde{k}_1\tilde{k}_3}\left[\tilde{k}_3^2 + \tilde{k}_1\tilde{k}_5 - \frac{\tilde{k}_2^2\tilde{k}_4^2 + \tilde{k}_1\tilde{k}_3^2\tilde{k}_5}{\tilde{k}_2\tilde{k}_4} tanh\big(k_2(d_2 - d_1)\big) tan\big(k_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, cos\big(k_2(d_2 - d_1)\big)\, cosh\big(k_4(d_4 - d_1 - d_2)\big).\tag{4}$$

Fig.2 shows the graph of the oscillatory dependence of the above-barrier transmission coefficient on the electron energy (in electron-volts) and the ratio of the widths of the two potential barriers $ns = \frac{d2}{d4}$), where $d2$ is the thickness of the second layer (first potential barrier), $d4$ is the thickness of the fourth layer (second potential barrier). In the calculations, it was assumed that the effective masses of electrons in the 1st, 2nd, 3rd, and 4th layers are respectively equal to $m_1 = 0.15 \cdot m_0$, $m_2 = 0.0623 \cdot m_0$, $m_3 = 0.0122 \cdot m_0$, $m_4 = 0.12 \cdot m_0$, and the width of the potential wells is 25 nm. In this case, a) 0.47 eV < E < 0.59 eV; b) 0.80 eV < E < 0.95 eV corresponds to the energy range. From this figure, it can be seen that the amplitude values of $t_{overbarrier}(E, ns)$ significantly depend on the ratio of the thicknesses of the potential barriers and the electron energy, and the oscillatory dependence is described by the interference of de Broglie waves approaching the barrier and scattered from it. Since the interfering waves differ in amplitude and phase, the oscillation in $t_{overbarrier}(E, ns)$ as a function of both E and ns is asymmetric.

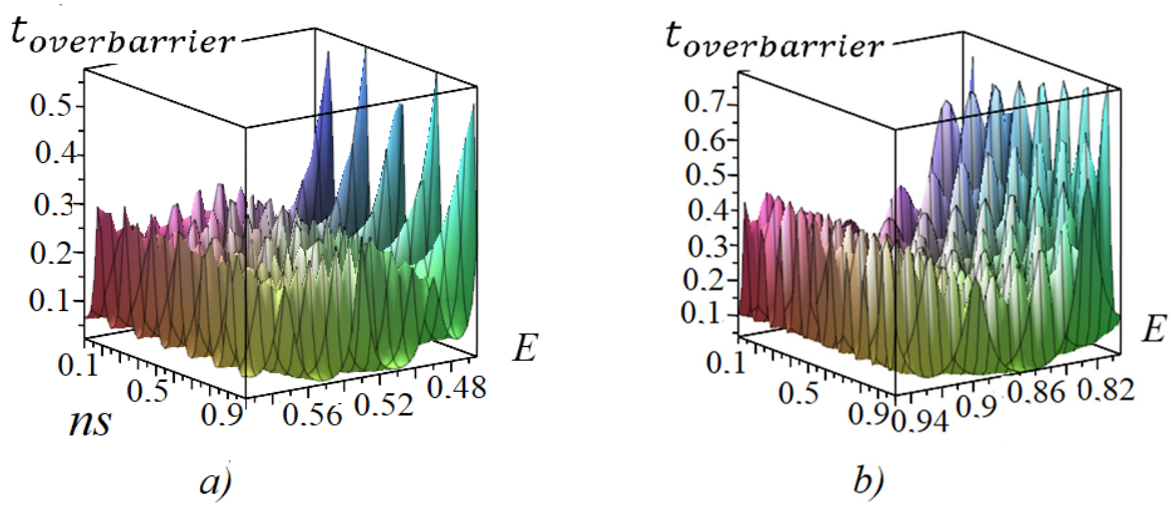

Figure 2. Graph of the dependence of the transparency coefficient of the potential barrier on the electron energy (in electron-volts) and the ratio of the widths of the two potential barriers ($ns = \frac{d2}{d4}$) when electrons pass through the potential barrier:
a) 0.47 eV < E < 0.59 eV; b) 0.80 eV < E < 0.95 eV.

In case 2, i.e., when the energy of the electrons is lower than the height of the first barrier and higher than the height of the second barrier, the transition coefficient can be determined using (3), where the quantities $\Re_j (j = 1,2,3,4)$ should be replaced by $\Re_j' (j = 1,2,3,4)$:

$$\Re_1' = \frac{1}{\tilde{k}_1}\left[\tilde{k}_1 + \tilde{k}_5 - \frac{\tilde{k}_1\tilde{k}_4\tilde{\kappa}_4 + \tilde{k}_5\tilde{\kappa}_2^2}{\tilde{\kappa}_2\tilde{\kappa}_4} tanh\big(\kappa_2(d_2 - d_1)\big) tan\big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, ch\big(\kappa_2(d_2 - d_1)\big)\, cos\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

$$\Re_2' = \frac{1}{\tilde{k}_1\tilde{k}_3}\left[\frac{\tilde{k}_5\tilde{\kappa}_2^2 - \tilde{k}_1\tilde{k}_3^2}{\tilde{\kappa}_2} - \frac{\tilde{k}_4^2\tilde{k}_1 + \tilde{k}_3^2\tilde{k}_5}{\tilde{k}_4}\left(\frac{K_4}{K_3} + \frac{K_3}{K_1}\frac{K_5}{K_4}\right) coth\big(\kappa_2(d_2 - d_1)\big) tg\big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, sinh\big(\kappa_2(d_2 - d_1)\big)\, cos\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

$$\Re_3' = \frac{1}{\tilde{k}_1}\left[\frac{\tilde{\kappa}_2^2 - \tilde{k}_1\tilde{k}_5}{\tilde{\kappa}_2} - \frac{\tilde{k}_4^2 + \tilde{k}_1\tilde{k}_5}{\tilde{k}_4} coth\big(\kappa_2(d_2 - d_1)\big) tg\big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, sinh\big(\kappa_2(d_2 - d_1)\big)\, cos\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

$$\Re_4' = -\frac{1}{\tilde{k}_1\tilde{k}_3}\left[\tilde{k}_3^2 + \tilde{k}_1\tilde{k}_5 - \frac{\tilde{\kappa}_2^2\tilde{\kappa}_4\tilde{k}_4 - \tilde{k}_1\tilde{k}_3^2\tilde{k}_5}{\kappa_2\tilde{\kappa}_4} tanh\big(\kappa_2(d_2 - d_1)\big)\, t\, g\, \big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$

$$\times\, cosh\big(\kappa_2(d_2 - d_1)\big)\, \cos\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

Here: $k_i = \sqrt{2m_i E_i \hbar^{-2}}$.

In case 4, i.e., if the energy of the electrons is lower than the heights of both potential barriers, the transition coefficient is also determined using (3), but in this case, the expressions $\Re_j (j = 1,2,3,4)$ should be replaced by the quantities $\Re_j'' (j = 1,2,3,4)$, given below:

$$\Re_1'' = \frac{1}{\tilde{k}_1}\left[\tilde{k}_1 + \tilde{k}_5 + \frac{\tilde{\kappa}_4^2\tilde{k}_1 + \tilde{k}_5\tilde{\kappa}_2^2}{\tilde{\kappa}_2\tilde{\kappa}_4} tanh\big(\kappa_2(d_2 - d_1)\big)tanh\big(\tilde{\kappa}_4(d_4 - d_1 - d_2)\big)\right] \times$$
$$\times cosh\big(\kappa_2(d_2 - d_1)\big)cosh\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

$$\Re_2'' = \frac{1}{\tilde{k}_1\tilde{k}_3}\left[\frac{\tilde{k}_5\tilde{\kappa}_2^2 - \tilde{k}_1\tilde{k}_3^2}{\tilde{\kappa}_2} + \frac{\tilde{\kappa}_4^2\tilde{k}_1 - \tilde{k}_3^2\tilde{k}_5}{\tilde{\kappa}_4} cath\big(\kappa_2(d_2 - d_1)\big)th\big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$
$$\times sinh\big(\kappa_2(d_2 - d_1)\big)cosh\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

$$\Re_3'' = \frac{1}{\tilde{k}_1}\left[\frac{\tilde{\kappa}_2^2 - \tilde{k}_1\tilde{k}_5}{\tilde{\kappa}_2} + \frac{\tilde{\kappa}_4^2 - \tilde{k}_1\tilde{k}_5}{\tilde{\kappa}_4} cath\big(\kappa_2(d_2 - d_1)\big)tanh\big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$
$$\times sinh\big(\kappa_2(d_2 - d_1)\big)cosh\big(\kappa_4(d_4 - d_1 - d_2)\big),$$

$$\Re_4'' = -\frac{1}{\tilde{k}_1\tilde{k}_3}\left[\tilde{k}_3^2 + \tilde{k}_1\tilde{k}_5 - \frac{\tilde{\kappa}_2^2\tilde{\kappa}_4^2 + \tilde{k}_1\tilde{k}_3^2\tilde{k}_5}{\kappa_2\tilde{\kappa}_4} tanh\big(\kappa_2(d_2 - d_1)\big)tanh\big(\kappa_4(d_4 - d_1 - d_2)\big)\right] \times$$
$$\times cosh\big(\kappa_2(d_2 - d_1)\big)cosh\big(\kappa_4(d_4 - d_1 - d_2)\big).$$

Fig. 3 presents the graphs of the dependence of the transparency coefficient of the potential barriers on the electron energy (in electron-volts) and the ratio of the widths of the two potential barriers when electrons pass below the potential barrier in a five-layer structure considering the Bastard condition, where: in Fig. a) the range of electron energy values is 0.47 eV < E < 0.59 eV, and in Fig. b) it is 0.80 eV < E < 0.95 eV. The following values are used in the calculations: $m_1 = 0.15 \cdot m_0$, $m_2 = 0.0623 \cdot m_0$, $m_3 = 0.0122 \cdot m_0$, $m_4 = 0.12 \cdot m_0$, where is the effective mass of electrons in the 1st, 2nd, 3rd, and 4th layers, respectively, and the widths of the potential wells are 25 nm.

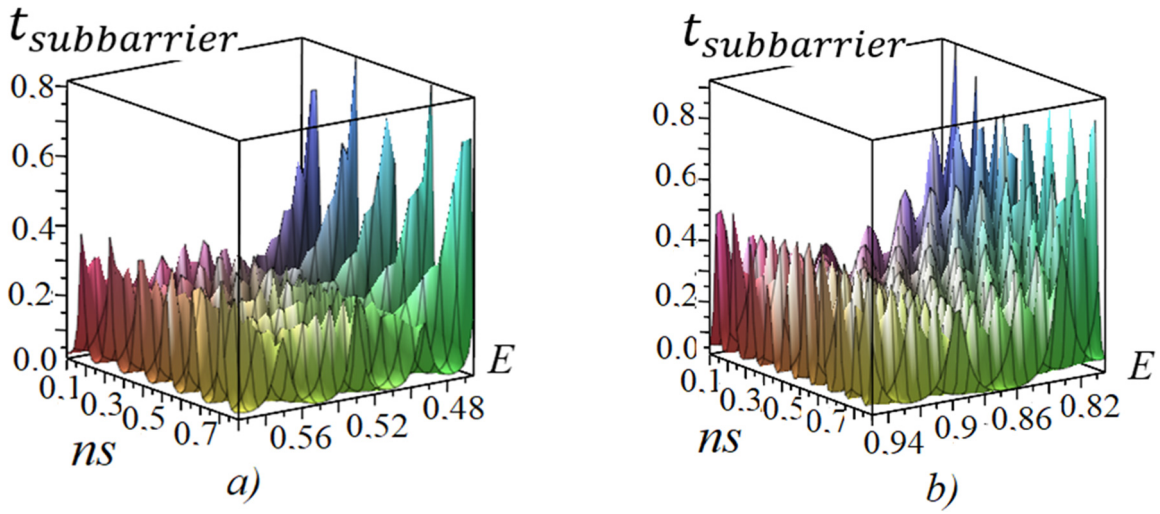

Figure 3. Graph of the dependence of the transparency coefficient of the potential barrier on the electron energy and $\boldsymbol{ns = \frac{d2}{d4}}$ when electrons pass below the potential barrier: a) 0.47 eV < E < 0.59 eV; b) $\boldsymbol{0.80\ eV < E < 0.95\ eV}$. In the calculations, the effective masses of electrons in the 1st, 2nd, 3rd, and 4th layers are respectively $m_1 = 0.15 \cdot m_0$, $m_2 = 0.0623 \cdot m_0$, $m_3 = 0.0122 \cdot m_0$, $m_4 = 0.12 \cdot m_0$, and the widths of the potential wells are 25 nm.

ANALYSIS OF THE RESULTS

Now let's consider a five-layer structure with symmetric double potential barriers, i.e., $U_3 = U_5 = 0$, $U_2 = U_4 = U_0$, as shown in Fig. 1, where we assume that the effective masses of charge carriers in all layers are the same. Then the electron transmission coefficient for case 2 is expressed as follows:

$$t_2 = \left\{1 + \frac{\left(k^2+\kappa^2\right)^2 sh^2\big(\kappa(d_2-d_1)\big)\left[2k\kappa - \left(k^2-\kappa^2\right)th\big(\kappa(d_2-d_1)\big)tg(kd_1)\right]^2}{4k^4\kappa^4 ch^{-2}\big(\kappa(d_2-d_1)\big)\cos^{-2}(kd_1)}\right\}^{-1}, \quad (5)$$

where d_1 – is the thickness of the first layer, $\tilde{d}_2 = d_2 - d_1$ is the thickness of the second layer, $k = \sqrt{2m\hbar^{-2}E}$ and $\kappa = \sqrt{2m\hbar^{-2}(U_0 - E)}$

Calculations show that in the aforementioned symmetric five-layer double-barrier semiconductor structure, the transmission coefficient equals unity under the condition.

$$\frac{1-2\xi}{\sqrt{\xi-\xi^2}} = f_R(\xi), \quad (6)$$

where resonant transitions occur, where $f_R(\xi) = 2cth\left(\kappa_0\sqrt{1-\xi}(d_2-d_1)\right)ctg\left(\kappa_0\sqrt{\xi}d_1\right)$, $\xi = \frac{E}{U_0}$, $\kappa_0 = \sqrt{\frac{2m}{\hbar^2}U_0}$. The latter condition is the condition for observing "resonant" transitions through a symmetric five-layer structure, where the phases and amplitudes of de Broglie waves obey this condition, where the phases of de Broglie waves are determined by the geometric dimensions of the structure, and their amplitudes are determined by the ratio of the carrier energy to the height of the potential barrier.

In Fig. 4, graphs of the dependence of the function $f_R(\xi)$ on $\xi = E/U_0$ are shown for $n_S = \tilde{d}_2/d_1 = 1.01$ (Figure 4a) and $n_S = \tilde{d}_2/d_1 = 1.5$ (Figure 4b) for various values of the effective masses of charge carriers. Here, $d_1 = 50nm$ is the thickness of the first layer, $\tilde{d}_2$ is the thickness of the second layer, $U_0 = 0.1eV$ is the height of the first potential barrier, m_0 is the mass of a free electron.

In Fig. 4a, it is shown that with an increase in the effective mass of charge carriers, the number of intersections of the values of $f_R(\xi)$ and $\frac{1-2\xi}{\sqrt{\xi-\xi^2}}$ increases, leading to an increase in the value of the transmission coefficient. Thus, in crystals with large effective masses of charge carriers, the transparency coefficient approaches unity. A comparison of the results in Figures 4a and 4b shows that the number of intersections of $f_R(\xi)$ and $\frac{(1-2\xi)}{\sqrt{\xi-\xi^2}}$ in the low-energy region does not change with the increase in the parameter $n_S = \tilde{d}_2/d_1$ in the range of its values from 1.0 to 1.5.

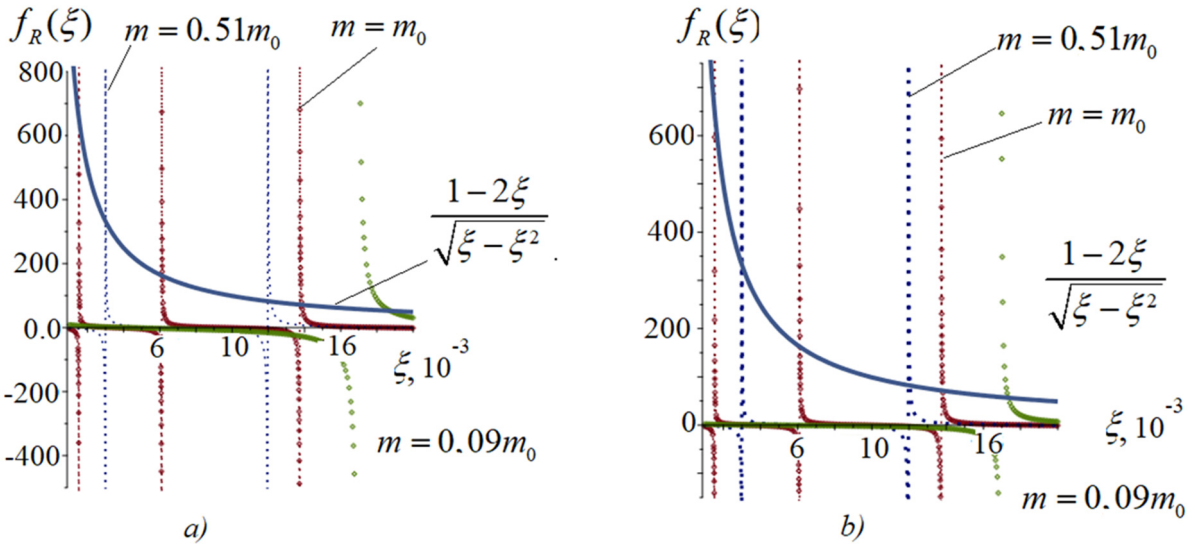

Figure 4. Graphs of the dependence of the function $f_R(\xi)$ on the ratio $\xi = E/U_0$ for $n_S = \tilde{d}_2/d_1 = 1.01$ (a), and $n_S = \tilde{d}_2/d_1 = 1.5$ (b) for various values of the effective masses of electrons. Here, $d_1 = 50nm$ nm is the thickness of the first layer, $\tilde{d}_2$ is the thickness of the second layer, $U_0 = 0.1eV$ is the height of the first potential barrier, m_0 is the mass of a free electron.

CONCLUSIONS

In this way, the dependence of the transparency coefficient of the five-layer double-barrier structure on the electron energy and the ratio of the widths of two adjacent potential barriers has been calculated. It has been demonstrated that the extremum of the transparency coefficient significantly depends on the geometric dimensions of the structure layers. In the symmetric five-layer double-barrier semiconductor structure, a condition has been defined under which the numerical value of the transmission coefficient through the potential barriers is approximately unity, indicating a "resonant" electron transition.

It has been shown that the mechanism of such a "resonant" transition is explained by the interference of de Broglie waves of electrons in the potential well. It has been established that the phases of de Broglie waves are determined by the geometric dimensions of the structure, while their amplitudes are determined by the ratio of the carrier energy to the height of the potential barrier.

It has been determined that with an increase in the effective mass of charge carriers, the number of intersections of $f_R(\xi)$ and $\frac{(1-2\xi)}{\sqrt{\xi-\xi^2}}$, increases, which determine the dimensionally-quantized levels where electrons are localized. It has also been shown that the number of intersections of $f_R(\xi)$ and $\frac{(1-2\xi)}{\sqrt{\xi-\xi^2}}$ in the low-energy region remains unchanged for values of $n_S = \tilde{d}_2/d_1$ ranging from 1.0 to 1.5 in crystals with a large effective mass of electrons.

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ТЕОРІЯ ТРАНСПОРТУ ЕЛЕКТРОНІВ У ДВОБАР'ЄРНИХ П'ЯТИШАРОВИХ НАПІВПРОВІДНИКОВИХ СТРУКТУРАХ

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Розраховано залежність коефіцієнта прозорості п'ятишарової двобар'єрної структури від енергії електронів та відношення ширин двох сусідніх потенційних бар'єрів. Показано, що екстремум коефіцієнта прозорості істотно залежить від геометричних розмірів шарів структури. У симетричній п'ятишаровій двобар'єрній напівпровідниковій структурі визначено умову виникнення «резонансних» електронних переходів. Показано, що механізм таких (резонансних) переходів пояснюється інтерференцією хвиль де Бройля електронів у потенційній ямі, де фази хвиль де Бройля визначаються геометричними розмірами структури, а їх амплітуди – відношення енергії носія до висоти потенційного бар'єру. Встановлено, що зі збільшенням ефективної маси носіїв заряду кількість перетинів величин $f_k(\xi)$ і $(1-2\xi)/\sqrt{(\xi-\xi^2)}$ зростає. Ці перетини визначають розмірно-квантовані рівні, на яких локалізовані електрони.

Ключові слова: *потенційний бар'єр; потенційна яма; двобар'єрна п'ятишарова структура; коефіцієнт пропускання; квантування розміру*