Physics – Uspekhi **50** (3) 293 – 299 (2007)

METHODOLOGICAL NOTES PACS number: 03.65.Ge

Impedance model for quantum-mechanical barrier problems

E A Nelin

DOI: 10.1070/PU2007v050n03ABEH006091

Contents

Abstract. Application of the impedance model to typical quantum-mechanical barrier problems, including those for structures with resonant electron tunneling, is discussed. The efficiency of the approach is illustrated. The physical transparency and compactness of the model and its potential as a teaching and learning tool are discussed.

1. Introduction

'Barrier' problems of quantum mechanics — that is, problems on quantum-mechanical motion in a medium with jumps in the potential — are used as model problems in many scientific and technical applications. They are extremely important both from the methodical and pedagogical viewpoints, especially in connection with modern R&D in nanotechnology.

The special features of barrier problems stem from the interaction of the fields of waves reflected from the potential jumps. When the interference of the reflected waves is in phase, the barrier penetration coefficient is zero for an infinite periodic structure and is minimal for a finite one. When the interference of the reflected waves is in antiphase, the waves fully compensate each other, so that the incident wave resonantly penetrates (by either tunneling through or passing above) the barrier structure. Such interaction of the reflected waves leads to the formation of forbidden and allowed bands in natural crystals and artificial crystal-like structures (semiconductor superlattices, photon and phonon crystals). Artificial crystal-like structures form the base of various new nanoelectronic signal-processing devices.

E A Nelin National Technical University of Ukraine
'Kiev Polytechnical Institute',
prosp. Pobedy 37, 03056 Kiev, Ukraine
Tel. (38-044) 241 86 87
E-mail: ye_nelin@rtf.ntu-kpi.kiev.ua

Received 24 March 2006, revised 15 December 2006
Uspekhi Fizicheskikh Nauk **177** (3) 307 – 313 (2007)
Translated by E Yankovsky; edited by A Radzig

The common solution to barrier problems by joining the solutions in regions with different potentials and accounting for the boundary conditions requires carrying out cumbersome transformations. Khondker et al. [1, 2] proposed using the impedance concept for a quantum-mechanical wave. This model has important physical meaning, possesses sweeping generality, being based on the impedance concept, and makes it possible to use the tools of the theory of transmission lines, thus simplifying the solution process. Despite the obvious merits, such an approach to solving quantum-mechanical problems has not gained wide acceptance. In the present note, I use the impedance model to solve typical barrier problems, including those involving structures with resonant electron tunneling. Such tunneling forms the base of signal-processing nanoelectronic devices. Figure 1 illustrates the problems examined in this paper.

2. Quantum-mechanical impedance

Impedance (from the Latin *impedio*, meaning opposing) characterizes the reaction of a medium to a wave perturbation. At the boundary between media with different impedances the forces of the wave perturbation and medium reaction differ, which results in the emergence of a reflected wave.

To define quantum-mechanical impedance, let us examine the passage of an electron through the boundary between two media, I and II, with different potentials. We place the boundary between the media with a potential step of height V at point $x = 0$ (Fig. 1a). In medium I, the electron wave function is given by the formula

$$\psi = \exp(\mathrm{i}kx) + r\exp(-\mathrm{i}kx)\,. \tag{1}$$

Here, $k = \sqrt{2mE}/\hbar$, with m the effective electron mass and E the electron energy, and r is the reflection coefficient. The first term on the right-hand side of Eqn (1) represents the incident wave, and the second represents the reflected wave. According to Ref. [3], $r = (1-\rho)/(1+\rho)$, where $\rho = \sqrt{(E-V)/E}$ (the case considered in Ref. [3] corresponds to $E > V$, but the formula is valid for $E < V$, too). If the effective electron

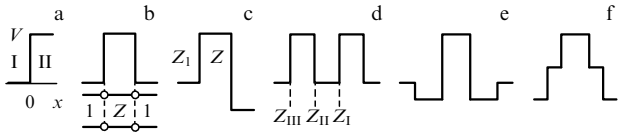

Figure 1. Various barrier problems (the behavior of the potential is shown by the solid line). (a) Potential step. (b) Symmetric potential barrier and the transmission line that models it; 1 and Z are the normalized impedances of the ambient and the barrier. (c) Potential barrier with different base heights; Z_1 is the normalized impedance of the ambient to the left of the barrier. (d) Symmetric double-barrier structure with resonant electron tunneling; $Z_I - Z_{III}$ are the normalized input impedances at the barrier boundaries. (e) and (f) Symmetric single-barrier structures with resonant electron tunneling.

masses m_I and m_{II} in media I and II differ, then $\rho = \sqrt{m_I(E-V)/m_{II}E}$ [1].

Equation (1) is similar to that for the current in a transmission line with distributed parameters (a long transmission line). Here, $\rho = Z_{load}/Z$, with Z_{load} being the load impedance, and Z the wave impedance of the line. Comparison of the expressions for ρ in the cases of quantum-mechanical and electromagnetic waves suggests that the quantum-mechanical impedance $Z \sim \sqrt{(E-V)/m}$. The absolute value of the quantum-mechanical impedance can be found by equating the probability density flux in the quantum-mechanical medium to the mean power in the equivalent transmission line [1, 2]: $Z = 2\sqrt{2(E-V)/m}$.

Let us clarify how the wave penetrates through the boundary between media I and II (e.g., quantum-mechanical waves with $E > V$). The penetration coefficient t_{II}, equal to the amplitude of the transmitted wave for a unit amplitude of the incident wave, is determined from the boundary conditions: $t_{II} = 1 + r = 2/(1+\rho)$. In accordance with energy conservation law, the amplitude of the wave transmitted from medium I to medium II from the side of medium I is $t_I = \sqrt{1-r^2} = 2\sqrt{\rho}/(1+\rho)$. Clearly, $t_{II} = t_I/\sqrt{\rho}$. Thus, in view of the difference in the impedances of the media, the amplitude of the transmitted wave undergoes a transformation at the boundary between the media, and the coefficient of this transformation is equal to the square root of the impedance ratio. The transformation of the transmitted wave is accompanied by the generation of a reflected wave.

The formula that expresses the reflection coefficient in terms of the impedance ratio is universal for waves of different origins. The sign in front of the expression depends on the physical quantity characterized by the wave. For waves with a reflection coefficient equal to $-r$ (for example, the voltage in the transmission line or the normal component of the electric field strength vector in an electromagnetic wave), $t_{II} = 2\rho/(1+\rho) = \sqrt{\rho}\, t_I$. In this case, the transformation coefficient is equal to $\sqrt{\rho^{-1}}$.

Within the framework of the impedance model, the regions of quantum-mechanical media with different potentials and effective electron masses are modelled by segments of a transmission line with different impedances. Analysis of the quantum-mechanical structure is reduced to an analysis of a nonuniform transmission line. Since the characteristics of reflection and transmission depend not on the absolute values of the impedances of the media but also on their ratios, the use of normalized impedances simplifies calculations.

The impedance model based on the concept of quantum-mechanical impedance and on transmission-line theory is a physical one, in contrast to the commonly used mathematical matrix model.

3. Classical barrier problems

3.1 Single-barrier structures

Let us discuss some typical educational problems, namely, the passage of an electron through symmetric and asymmetric single-potential barriers. Within the framework of the impedance model, the expression for the reflection coefficient is derived very simply, in contrast to the much more complicated calculations that have to be done in the traditional model. In analyzing the results, we will focus on an important physical effect, viz. the resonant above-barrier passage of electrons.

Figure 1b illustrates the case of a symmetric single barrier. The regions occupied by the barrier and the ambient have different impedances. Let us normalize the barrier impedance to the ambient impedance. The normalized input impedance at the barrier's boundary for a wave propagating from left to right is given by

$$Z_I = \frac{Z - Z^2 A}{Z - A}\,. \tag{2}$$

Here, $Z = \sqrt{m(E-V)/m_1 E}$ is the normalized barrier impedance, with m and m_1 being the effective electron masses in, respectively, the ambient and the barrier, while V being the barrier height, and $A = \tanh(\mathrm{i}k_1 a)$, with $k_1 = \sqrt{2m_1(E-V)}/\hbar$ being the wave number in the barrier domain, and a the barrier thickness. Notice that $Z = k_1 m/k m_1$, where $k = \sqrt{2mE}/\hbar$ is the wave number in the ambient. The ratio corresponding to Z is present in the well-known final expressions for barrier problems. Thus, by normalizing the impedance at the beginning of calculations we achieve compactness of the solution. For $E < V$, the impedance and the wave number in the barrier domain are imaginary quantities, which corresponds to electron tunneling.

The reflection coefficient is represented by the formula $R = (1 - Z_I)/(1 + Z_I)$. Substituting expression (2) into this formula, we get

$$R = \frac{(Z^2 - 1)A}{2Z - (Z^2 + 1)A}\,. \tag{3}$$

Equation (3) generalizes tunneling and above-barrier passage of electrons and also takes into account the difference in the effective electron masses in the ambient and the barrier domain. It is also valid for a potential well if k and m, and k_1 and m_1 are interchanged in the expressions for Z and A.

If $m = m_1$, we have $Z = k_1/k$, and since $\tanh \mathrm{i}x = \mathrm{i}\tan x$, Eqn (3) becomes

$$R = \frac{(k^2 - k_1^2)\sin k_1 a}{(k^2 + k_1^2)\sin k_1 a + 2\mathrm{i}k k_1 \cos k_1 a}\,.$$

This is the well-known expression for reflection from a potential barrier [3].

According to energy conservation law, $|R|^2 + |T|^2 = 1$, where T is the penetration coefficient. In the case of tunneling, $|T| \ll 1$, so that $|R|^{-2} \approx 1 + |T|^2$. Simple transformations in

formula (3) yield

$$|T| \approx 2\,\frac{|Z|\sqrt{\widetilde{A}^{-2}-1}}{|Z|^2+1}\,,$$

where $\widetilde{A} = \tanh \chi a$, with $\chi = \sqrt{2m_1(V-E)}/\hbar$. At $m = m_1$, bearing in mind that $\cosh^2 x - \sinh^2 x = 1$ and $\chi a \gg 1$, we arrive at the well-known formula [3]

$$|T| \approx 4\,\frac{\sqrt{E(V-E)}}{V}\exp(-\chi a)\,,$$

which we can write down as

$$|T| \approx 4\sqrt{\hat{E}(1-\hat{E})}\,\exp\left(-5.1\sqrt{1-\hat{E}}\,\sqrt{V}a\right). \qquad (4)$$

Here, $\hat{E} = E/V$, $m = m_0$, where m_0 is the electron rest mass, the height of barrier V is measured in electron-volts, and the barrier width a is measured in nanometers. At $\hat{E} = 0.5$, we have $|T| \approx 2\exp\left(-3.6\sqrt{V}a\right)$. The values of $V = 0.4$ eV, $\hat{E} = 0.5$, and $a = 6$ nm correspond to $|T| \approx 2 \times 10^{-6}$.

When electrons pass above the barrier ($E > V$), we obtain $A = \mathrm{i}\tan k_1 a$. If $a = n\lambda_1/2$, where $n = 1, 2, \ldots$, and λ_1 is the electron wavelength in the barrier domain, we have $A = 0$ and $R = 0$, which constitutes the condition for resonant above-barrier passage of electrons in the general case. It should be noted that at $k_1 = 0$ the reflection coefficient $R \neq 0$.

In the particular case where $m_1 < m$, at an appropriate value of E the impedance $Z = 1$, which also corresponds to resonant above-barrier passage of electrons.

Resonant passage of waves is of utmost importance in the formation of the characteristics of wave structures. Let us focus on the physical features of the conditions necessary for such passage. The key issue here is the presence of a standing wave. The jumps in the barrier potential form a cavity. At the cavity's eigenfrequencies which correspond to resonant passage, a standing wave forms in the cavity. A cavity with a standing wave is a source of waves proper with respect to the potential barrier (to the wave structure in the general case). At the cavity's eigenfrequencies, the wave reflected from the barrier is compensated for by the antiphase wave emitted by this source. Thus, in the case of resonant passage, the compensation of the nonuniformities in the wave perturbations of the incident wave at the medium boundaries stems from the perturbations of the standing wave, so that the incident wave penetrates through these boundaries as if the medium was uniform and no reflections occurred.

To put it differently, the jumps in the properties at the boundaries of the media act as intrinsic sources of waves, viz. reflected waves. In resonant passage, the action of (the radiation emitted by) the intrinsic sources is compensated for by the action of (the radiation emitted by) the natural source (or sources). This conclusion is universal for wave structures of different origins. Resonant tunneling, which is considered below, can also be explained by such self-compensation.

In the case of a potential barrier with different base heights (Fig. 1c), we allow for relationship (2) and get

$$R = \frac{Z_1 - Z_\mathrm{I}}{Z_1 + Z_\mathrm{I}} = \frac{Z_1 - 1 - (Z_1/Z - Z)A}{Z_1 + 1 - (Z_1/Z + Z)A}\,. \qquad (5)$$

This solution generalizes the particular solutions that depend on the ratio between the electron energy and the heights of the barrier and bases. In Ref. [4], where the traditional method was employed, these solutions are cumbersome, were derived as a result of cumbersome transformations, and hold only for equal effective electron masses in the different regions. In the process, the conditions necessary for resonant above-barrier passage of electrons remained unnoticed.

If the potential barrier is asymmetric (and generally this is the case), the conditions necessary for resonant passage are violated. The coefficient of reflection from one boundary is smaller than that from the other boundary. In view of such a decrease, the Q-factor of the natural source is too small to compensate for the perturbations of the incident wave at a boundary with a large reflection coefficient. Equation (5) shows that generally the reflection coefficient cannot be equal to zero, since the term $Z_1 - 1$ in the numerator is real-valued, and the next term is imaginary.

In two particular cases, resonant passage is possible only for one energy value (different in these two cases). Here, the effective electron mass to the left of the barrier must be smaller than that to the right, and the following conditions must be met: $Z_1 = 1$, $A = 0$ or $Z = Z_1 = 1$. The last conditions assume that the effective electron mass in the barrier domain is smaller than in the region to the left of the barrier.

Resonant passage through an asymmetric barrier is of a single-mode nature (occurs at a single energy value), in contrast to the multimode nature of such passage through a symmetric barrier. The single-mode nature of resonant passage makes it possible to realize a single-band transmission characteristic in applications.

3.2 Double-barrier structure with resonant electron tunneling

The symmetric double-barrier structure is central to understanding the physical bases of the formation of band diagrams, of the principles on which nanoelectronic devices work, and of the methods of designing such devices. A remarkable phenomenon occurs in this structure, namely, resonant electron tunneling in which penetration coefficient is equal to unity. When tunneling occurs through a single potential barrier, the penetration coefficient is extremely small, equal to about 10^{-6}. It would seem that adding another barrier should decrease penetration coefficient. However, at certain energies the penetration coefficient of the double-barrier structure is equal to unity. In textbooks, only the particular case of a delta-function barrier is examined [3]. The impedance model leads to new results, i.e., to analytical expressions for the reflection coefficient and the eigenvalues of the double-barrier structure.

When examining the double-barrier structure (Fig. 1d), we must find, in succession, the normalized input impedances $Z_\mathrm{I} - Z_\mathrm{III}$ at the barrier boundaries. Doing the necessary transformations, we obtain

$$Z_\mathrm{III} = Z\,\frac{Z^3A^2B - Z^2AB + 2Z^2A - ZA^2 + ZB - Z - AB}{-Z^3AB - Z^2A^2 + Z^2B - Z^2 - ZAB + 2ZA + A^2B}\,,$$

where $B = \mathrm{i}\tan kb$, with b being the width of the potential well.

The reflection coefficient

$$R = \frac{1 - Z_\mathrm{III}}{1 + Z_\mathrm{III}} = \frac{(1-Z^2)\left[2Z + (Z^2+1)AB\right]A}{(Z^4+1)A^2B + 2Z\left\{\left[(Z^2+1)A - Z\right](1-B) - ZA^2\right\}}\,. \qquad (6)$$

The condition $R = 0$ determines the expressions for the eigenvalues

$$AB = -\frac{2Z}{Z^2+1}\,, \qquad E > 0\,, \tag{7}$$

and $A = 0$ or $Z = 1$, for $E > V$. The last expressions correspond to the eigenvalues for a single barrier. Notice that at $E = 0$ the reflection coefficient $R = 1$.

Incidentally, Eqn (7) can be transformed to the form $AB = (r^2-1)/(r^2+1)$, where $r = (1-Z)/(1+Z)$ is the coefficient of reflection from a potential jump of height V. Thus, within the framework of the impedance model, the eigenvalues of the symmetric double-barrier structure are determined by the relative barrier impedance or the coefficient of reflection from the potential jump. This conclusion illustrates the fact that the physics of the impedance model is clear-cut.

At $m = m_1$, Eqn (7) yields

$$\tanh \chi a \, \tan kb = \frac{2\eta}{1-\eta^2} = \frac{\sqrt{E(V-E)}}{E-0.5V}\,, \tag{8}$$

where $\eta = \chi/k$. In the tunneling range, which is of the most interest to us and is examined below, χ is real.

For wide barriers, where $\chi a \gtrsim 1$, which corresponds to $a \gtrsim \lambda_1/\pi$, $\tanh \chi a \approx 1$ and formula (8) is consistent with the well-known expression for a potential well [5].

In the case of narrow barriers, where $\chi a \ll 2$, we have $\tanh \chi a \approx \chi a$, and Eqn (8) becomes $\tan kb = k\hbar^2/\bigl[am(2E-V)\bigr]$. For a delta-function barrier, described by the function $\alpha\delta(x)$ (here, $\alpha > 0$ is a constant), one finds $V = \alpha/a$, $a \to 0$. Here, $\tan kb = -k\hbar^2/\alpha m$, which coincides with the results obtained in Ref. [3].

We rewrite Eqn (8) in the form

$$0 = \cosh \chi a \, \cos kb - \frac{1-\eta^2}{2\eta} \, \sinh \chi a \, \sin kb\,. \tag{9}$$

The right-hand side of Eqn (9) is the dispersion characteristic of a periodic superlattice formed by alternating barriers and wells [6]. The dispersion characteristic, viz. the function $E(K)$, where K is the Bloch wave number, represents the band energy spectrum of the superlattice. The left-hand part of the dispersion characteristic contains $\cos K\Lambda$, where $\Lambda = a + b$ is the structure's period. At the edges of the forbidden bands, one has $|\cos K\Lambda| = 1$, or $K\Lambda = n_\mathrm{f}\pi$ (where $n_\mathrm{f} = 1, 2, \ldots$ is the number of the forbidden band). Equation (9) corresponds to the values of the dispersion characteristic near the middles of the allowed bands at $\cos K\Lambda = 0$, or $K\Lambda = (2n_\mathrm{a} - 1)\pi/2$ (with $n_\mathrm{a} = 1, 2, \ldots$ being the number of the allowed band). The above conditions imposed on $K\Lambda$ in the forbidden and allowed bands correspond to in-phase and antiphase interference of the reflected waves. Antiphase interference conforms to resonant electron tunneling. Thus, the expression obtained for the eigenvalues of the double-barrier structure — the base cell of a superlattice — is directly related to the superlattice's dispersion characteristic.

Let us recast Eqn (8) to the form

$$\operatorname{thg} p\pi x \, \tan \pi x = \frac{\sqrt{\hat{E}\,|\hat{E}-1|}}{\hat{E}-0.5}\,, \tag{10}$$

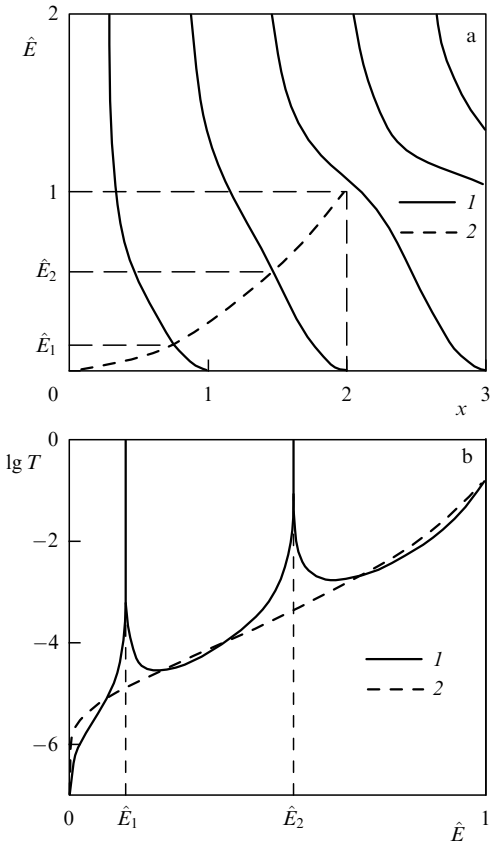

Figure 2. Characteristics of the symmetric double-barrier structure. (a) Dependence of the normalized eigenvalues (curves *1*) on x and the function $x(\hat{E})$ (curve 2). (b) Penetration coefficient of the double-barrier structure as a function of the normalized electron energy (curve *1*) and that of a barrier of double thickness (curve *2*).

where

$$\operatorname{thg} x = \begin{cases} \tanh x\,, & \hat{E} < 1\,, \\ \tan x\,, & \hat{E} \geqslant 1\,. \end{cases}$$

Here, $x = kb/\pi$ and $p = |\hat{E}^{-1} - 1|^{1/2}\, a/b$. Since $x = 2b/\lambda$ (λ is the electron wavelength in the potential well), $x = 1, 2, \ldots$ is the number of electron half-waves that fit into the potential well. If we allow for the E-dependence of k, we arrive at $x(\hat{E}) = x(V)\hat{E}^{1/2}$, where $x(V) = \sqrt{2mV}\,b/\pi\hbar$.

Figure 2a depicts the dependence of the normalized eigenvalues of the double-barrier structure according to expression (10) at $a = b$, and the function $x(\hat{E})$ at $x(V) = 2$. In their entire range, the eigenvalues vary from values that are approximately equal to the eigenvalues of the structure's potential well to values determined by the condition of mutual compensation for the four waves reflected from each potential jump of the structure: $x = n/4$, with $n = 1, 3, \ldots$. The $\hat{E} < 1$ range conforms to resonant electron tunneling. The complete spectrum of the eigenvalues of the double-barrier structure also incorporates the eigenvalues of a single barrier in the form of vertical lines located at the points $x = 1, 2, \ldots$ in the $\hat{E} > 1$ range.

The points where curves *1* and *2* intersect determine the eigenvalues $\hat{E}_1 = 0.14$ and $\hat{E}_2 = 0.54$ at $x(V) = 2$. This value of $x(V)$ corresponds to, say, the following parameters: $V = 0.24$ eV, $a = b = 25$ Å, and $m = m_1 = m_0$.

Figure 2b illustrates the dependence of the penetration coefficient of the double-barrier structure at $x(V) = 2$ and that of a single potential barrier on the normalized electron energy. The $\hat{E}_1$ and $\hat{E}_2$ values comply with those in Fig. 2a. The single barrier is double the thickness of the structure's barrier and conforms to a double-barrier structure without the potential well. Curve *2* was calculated using the approximate formula (4). The results of calculations by the exact and approximate formulas coincide. As expected, comparison of the curves shows that far from the eigenvalues of the double-barrier structure the potential well has practically no effect on the transmitted wave.

4. Single-barrier structures with resonant electron tunneling

Analysis of the features of resonant electron tunneling in the double-barrier structure suggests new simple structures with such tunneling — symmetric single-barrier structures.

Just as with resonant passage of waves, resonant tunneling is caused by the compensation of the reflected waves as a result of the formation of a natural compensating source of waves, namely, a resonance region with a standing wave. In the double-barrier structure, the cavity forming the standing wave is placed inside the barrier, so that two barriers with a potential well between them are formed. We denote such a structure by the abbreviation TCT, where T stands for a tunnel barrier, and C for the cavity corresponding to the potential well. Another solution reduces to placing the barrier in the field of the cavity's standing wave. This results in obtaining symmetric single-barrier structures with potential wells, CTC_w, and with steps, CTC_s (Figs 1e and f).

For a CTC-structure we have

$$R = \left\{ \left[(Z_1^2 - Z^4)A^2 + Z^2(1 - Z_1^2) \right] B - 2ZZ_1(Z^2 - 1)A \right\} \times \left\{ \left[(Z^4 + Z_1^2)A^2 - 2Z(Z^2 + Z_1^2)A + Z^2(Z_1^2 + 1) \right] B + 2ZZ_1 \left[(Z^2 - ZA + 1)A - Z \right] \right\}^{-1}. \quad (11)$$

Similar to a TCT-structure, the outer regions have an impedance Z, a factor A, and a thickness a, while the inner region has Z_1, B, and b. As expected, Eqn (11) coincides with Eqn (6) at $Z_1 = 1$. The eigenvalues are given by the formula

$$B = \frac{2ZZ_1(Z^2 - 1)A}{(Z_1^2 - Z^4)A^2 + Z^2(1 - Z_1^2)}. \quad (12)$$

Let us rearrange Eqn (12) for the case of equal effective masses in different regions. For the CTC_w-structure subject to the condition $V = V_w$, where V is the height of the barrier measured from the top of the potential well, and V_w is the depth of the well, we have

$$\operatorname{thg} p\pi x = \frac{\sqrt{|\hat{E}^{-2} - 1|}\, \sin 2\pi x}{2 - \cos 2\pi x + \hat{E}^{-1}}, \quad (13)$$

where

$$p = \sqrt{\frac{|\hat{E} - 1|}{\hat{E} + 1}}\, \frac{b}{a}.$$

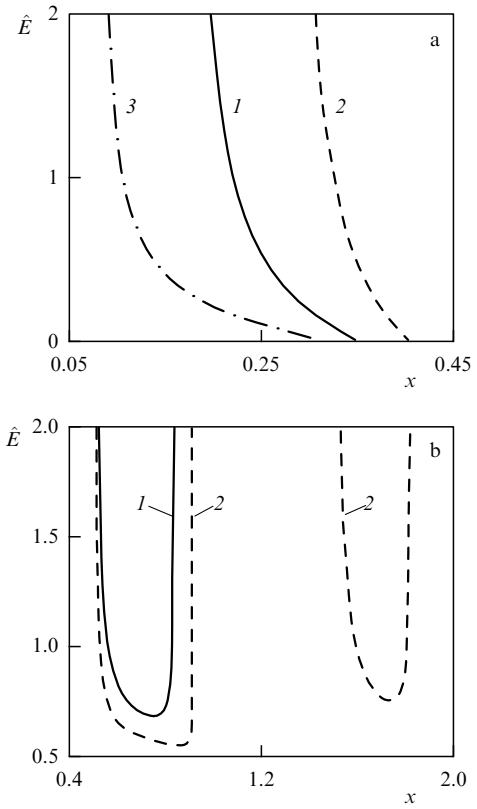

Figure 3. Dependence of the normalized eigenvalues of CTC-structures on x. (a) CTC_w-structures with $a/b = 1$, 2, and 0.6 (curves *1*, *2*, and *3*, respectively). (b) CTC_s-structures with $a/b = 5$ and 10 (curves *1* and *2*, respectively).

For the CTC_s-structure with the step height $V_s = 0.5V$, we obtain

$$\operatorname{thg} p\pi x = \frac{2\sqrt{2|\hat{E}^{-2} - 3\hat{E}^{-1} + 2|}\, \tan \pi x}{4 - \hat{E}^{-1} \tan^2 \pi x + 2\hat{E}^{-1}}, \quad (14)$$

where

$$p = \sqrt{\frac{|\hat{E} - 1|}{\hat{E} - 0.5}}\, \frac{b}{a}.$$

Figure 3 depicts the dependence of the eigenvalues of CTC-structures according to Eqns (13) and (14). The plots make it possible to determine the eigenvalues of a structure in a way similar to Fig. 2a. The curves can also be used to synthesize structures with fixed eigenvalues.

Figure 4 shows the dependence of the reflection coefficient of CTC-structures. The potential wells and barriers are formed by layers of GaAs and $Al_xGa_{1-x}As$, respectively. The effective electron mass in GaAs is $m = 0.0665m_0$, and that in $Al_xGa_{1-x}As$ is $m_1 = (0.0665 + 0.0835)m_0$ [8]. The values of V and x are related as follows: $V = 0.7731x$ [9]. For the sake of comparison, Fig. 4a portrays the dependence of the reflection coefficient of a potential barrier with the parameters of the barrier in the CTC_w-structure. Each CTC-structure exhibits two levels of resonant electron tunneling.

Symmetric single-barrier structures with resonant tunneling are of interest as possible basic structures used in signal-processing devices for various waves. The idea of selective devices based on such structures amounts to the following.

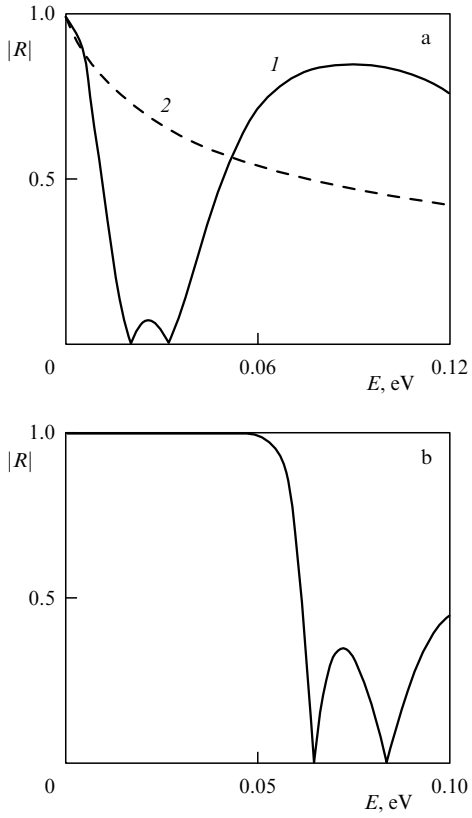

Figure 4. Dependence of reflection coefficients of CTC-structures on electron energy. (a) A CTC_w-structure (curve *1*) and a potential barrier (curve *2*): $a = 48d$, $b = 6d$, where d is the thickness of the GaAs monolayer in the [100] direction ($d = 2.82665$ Å [7]), and $V = V_w = 0.12$ eV. (b) A CTC_s-structure: $a = 40d$, $b = 4d$, and $V = 2V_s = 0.1$ eV.

The transmission band corresponds to resonant tunneling. Penetration coefficient at a resonance frequency is equal to unity. Outside the transmission band, the tunnel barrier has exceptionally low penetrability, which ensures substantial signal attenuation.

5. Modeling crystals and semiconductor superlattices

The modern theory of metals, semiconductors, and insulators proceeds from band theory. The study of the physical grounds and the modeling of band diagrams are of utmost importance in educating specialists in physics and technology. Such knowledge becomes especially significant in connection with intensive R&D in signal-processing nanoelectronic devices.

A deep understanding and the mastering of this subject, as well as the building of constructive physical analogs, are guaranteed if one employs the wave interference approach [10]. Focusing on the similarity of crystals and wave filters is also important [11]. Yariv [6] used the matrix model to develop a theory that explains the propagation of electrons in periodic structures formed by potential barriers and wells. On the basis of this model, Brennan [12] developed, for educational purposes, a computer program based on the FORTRAN programming language in order to be able to model the formation of band diagrams of crystals and the characteristics of semiconductor superlattices. The impedance model reduces the program from five pages to one by using the FORTRAN language, and to half a page by using

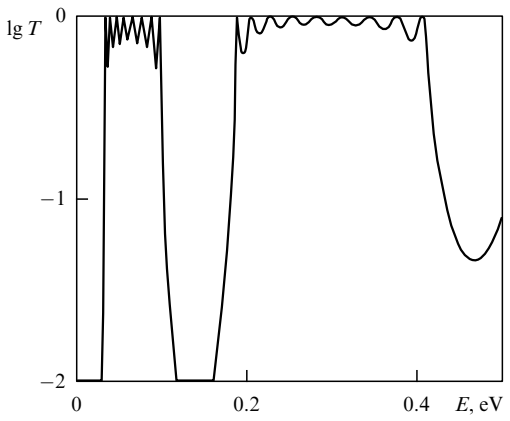

Figure 5. Dependence of the penetration coefficient of a superlattice formed by GaAs and $Al_xGa_{1-x}As$ layers on electron energy. The number of barriers equals 10, $a = 5d$, $b = 20d$, and $V = 0.2$ eV.

Mathcad. Here, in contrast to Ref. [12], above-barrier passage of electrons is included in the picture. The matrix and impedance models yield identical results, which makes bench tests possible.

Figure 5 displays the dependence of the penetration coefficient of a superlattice calculated by the impedance model. The results illustrate the formation of a band diagram. Sections with penetration coefficients close to unity correspond to allowed bands, and those with small penetration coefficients to forbidden bands. The first allowed band with $E < V$ is formed due to resonant electron tunneling, and the second is formed due to resonant above-barrier passage of electrons.

This characteristic is typical for educational purposes. In their laboratory work involving the study of band diagrams of crystals and semiconductor superlattices, students investigate resonant tunneling and above-barrier passage of electrons, as well as specific characteristics of passage and reflection, depending on the parameters of the structures.

One must bear in mind that resonance effects are narrow-band, so that the density of the computed points must be high. And because this density in the dependence in Fig. 2 taken from Ref. [12] was not sufficiently high, the maximum of the penetration coefficient is noticeably smaller than unity, despite resonant electron tunneling.

Forming the necessary characteristics of superlattices requires apodization, or varying the parameters of the potential wells and barriers. Amplitude apodization of superlattices has been examined in Ref. [13], phase apodization in Ref. [14], and edge apodization in Ref. [15].

6. Conclusion

The impedance model provides a new approach to the barrier problems of quantum mechanics, brings us closer to understanding the peculiarities of the formation of band diagrams of crystals and the characteristics of crystal-like structures, and simplifies modeling. Using this model, a student can write and compile, on their own computer, programs that enable him or her to simulate various scenarios and analyze the results. Programming in the Mathcad medium becomes much simpler: because of the automatic transformation of imaginary arguments there is no need to study resonant tunneling and above-barrier passage of electrons separately. Problems

associated with modeling apodized superlattices and other crystal-like structures and devices based on them form a large body of degree works of students.

References

1. Khondker A N, Khan M R, Anwar A F M *J. Appl. Phys.* **63** 5191 (1988)
2. Anwar A F M, Khondker A N, Khan M R *J. Appl. Phys.* **65** 2761 (1989)
3. Galitskii V M, Karnakov B M, Kogan V I *Zadachi po Kvantovoi Mekhanike* (Problems in Quantum Mechanics) (Moscow: Nauka, 1981)
4. Fromhold A T (Jr.), in *Encyclopedia of Physical Science and Technology* Vol. 13 (San Diego: Academic Press, 2001) p. 359
5. Landau L D, Lifshitz E M *Kvantovaya Mekhanika*: *Nerelyativistskaya Teoriya* (Quantum Mechanics: Non-Relativistic Theory) (Moscow: Fizmatlit, 2002) [Translated into English (Oxford: Pergamon Press, 1977)]
6. Yariv A *An Introduction to Theory and Applications of Quantum Mechanics* (New York: Wiley, 1982) [Translated into Russian (Moscow: Mir, 1984)]
7. Gaylord T K, Glytsis E N, Brennan K F *J. Appl. Phys.* **65** 2535 (1989)
8. Nakamura K et al. *IEEE J. Quantum Electron.* **QE-28** 1670 (1992)
9. Wilson D W, Glytsis E N, Gaylord T X *IEEE J. Quantum Electron.* **QE-29** 1364 (1993)
10. Kittel Ch *Elementary Solid State Physics* (New York: Wiley, 1962) [Translated into Russian (Moscow: Nauka, 1965)]
11. Sproull R L *Modern Physics*: *The Quantum Physics of Atoms, Solids, and Nuclei* 2nd ed. (New York: Wiley, 1963) [Translated into Russian (Moscow: Nauka, 1974)]
12. Brennan K F *IEEE Trans. Education* **E-35** 60 (1992)
13. Nelin E A *Izv. Vyssh. Uchebn. Zaved. Radioelektron.* **38** (5) 33 (1995) [*Radioelectron. Commun. Syst.* **38** (5) 23 (1995)]
14. Nelin E A *Izv. Vyssh. Uchebn. Zaved. Radioelektron.* **47** (7) 87 (2004) [*Radioelectron. Commun. Syst.* **47** (7) 10 (2004)]
15. Nelin E A *Zh. Tekh. Fiz.* **75** (11) 120 (2005) [*Tech. Phys.* **50** 1511 (2005)]