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Electronic Spectrum of Complex One-Dimensional Superlattices (based on semiconductor heterostructures in the Al/Ga/As system)

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A one-dimensional superlattice with a complex unit cell consisting of two potential wells and two barriers with different widths and heights is studied within the Kronig–Penney model. A dispersion equation for such a structure is obtained. A numerical analysis of this equation is carried out and the behavior of the electron spectrum of the superlattice $GaAs/Al_{0.5}Ga_{0.5}As/GaAs/Al_xGa_{1-x}As$ is investigated depending on the ratio of the wells and barriers widths, as well as barriers heights

Keywords: superlattice, Kronig–Penney model, potential well, potential barrier, band structure.

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Introduction

Research of the electronic spectra of the periodic structures is of undoubted interest, since various types of superlattices (SL) are widely applied in modern micro-, nano- and opto-electronics [1–15]. The classic article by R. de Kronig and W. Penney [16] was the first to solve a quantum-mechanical problem of finding an electron spectrum in the field of a periodic potential of the crystal lattice and to obtain an analytical expression for the dispersion equation, whose solutions determine the spectrum of electrons. The solution of this equation shows that the energy electron spectrum originates band gaps, i.e. intervals of the energy values, which can not belong to free electrons. In other words, the electron spectrum of the superlattice is characterized by a band structure [16], while a corresponding model that is used in theoretical study of such problems in the solid state physics is called the Kronig–Penney model (KPM) [17,18]. In spite the fact that the article [16] was published in the early 30s of the twentieth century, the model proposed therein has been successfully used for calculating various one-dimensional periodic structures up to now [19–22].

Almost all the publications dedicated to KPM application investigate two-component superlattices, whose elementary cell (EC) is formed by one potential barrier (PB) and one potential well (PW).

But, it has been already noted in the paper [23] that it was promising to study complex multi-component structures that are called polytype superlattices, which are characterized by more diverse physical properties. An example of these structures is, for instance, biperiodic superlattices [24–27]. One should mention papers, which have obtained general formulas for finding the superlattice spectra, whose elementary cell contain N layers [28–30] (see also the review article [31]). The articles [28,31] investigate, as an example, the superlattices with four elements in the elementary cell, namely, with two potential wells and two potential barriers. They have numerically analyzed dependences of the electron energy on widths of the wells and the barriers in the studied structures. However, these publications failed to take into account influence of the barrier height on the electron spectra in the superlattice. It should be expected that the difference in the potential barriers heights, along with the widths of the wells and the barriers will also be essentially important for forming the electron spectra of the superlattices. For example, in the paper [32] the transfer matrix method was used to obtain a dispersion equation for the biperiodic superlattice that is obtained by introducing an additional barrier of another height into the potential well. As shown in this article [32], this complication of the superlattice elementary cell makes it possible to control characteristics of minibands.

These studies are necessary for searching new structures that can be applied as an elementary base of next-generation nanoelectronics devices. Recent years' achievements in obtaining new functional media with pre-programmable properties allow creating complex heterostructures that consists of alternating layers of different materials. These structures can be modelled by generalizing the KPM that is developed for the binary superlattices [16] to the superlattices with a large number of elements in the elementary cell, which, for example, contain several potential wells and potential barriers. It will allow increasing a number of independent parameters for predicting new specific features

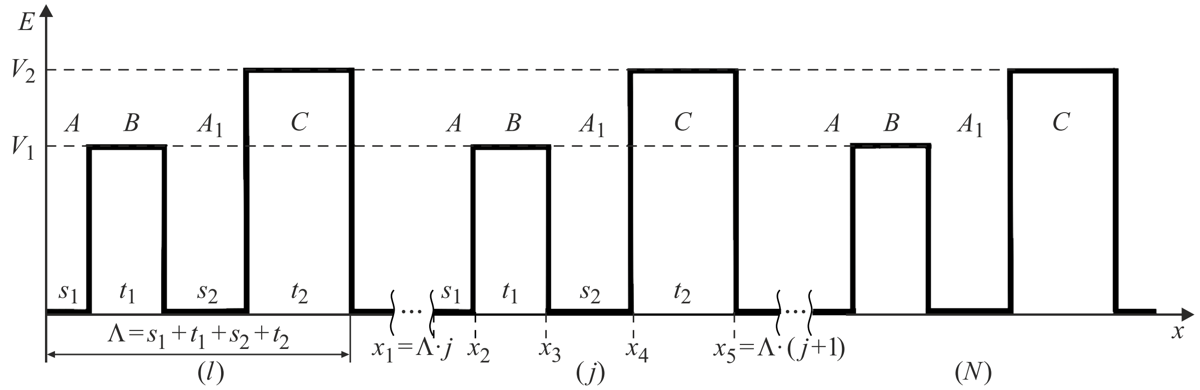

Figure 1. Potential profile of the superlattice with a elementary cell that consists of the two potential wells and the two potential barriers, where j is a number of the elementary cell.

in the electron properties of these heterostructures with predefined widths of minibands and minislots.

The goal of the present study is to investigate the dependence of the electron spectra in the superlattice with the four elements (the two potential wells and the two potential barriers) within the elementary cell on variation of not only the widths of the wells and the barriers, but on the heights of the barriers as well. As far as we know, no such investigations have been carried out before.

The paper is organized as follows. In the first section, we analitically obtained the dispersion equation for the one-dimensional superlattice with the four-component EC which in the limiting case coincides with the corresponding dispersion equation for the standard KPM for binary SL. In the second section, we presented the results of numerical simulations and graphical interpretation of dispersion equation obtained in section one for the complex SL with four-component EC $GaAs/Al_0.5Ga_0.5As/GaAs/Al_xGa_{1-x}As$ for different concentration x of Al. In Conclusion, we summarized the obtained results.

1. Dispersion equation: analytical solution

The most common approach for determining the electronic states in lamellar semiconductor structures is an envelope wave function approximation (an effective mass approximation) [33,34]. The main advantage of this method is relative simpleness of computing both volume and surface electron states when using experimental data for structure component parameters. Besides, for the periodic structures with multi-component elementary cells a scope of the numerical calculations is quite small and results in adequate results.

Let us consider the one-dimensional endless superlattice shown in Fig. 1. It consists of elementary cells, wherein each of them contains four layers with respective thicknesses, potential barriers and effective masses. In the layers A and A_1 of the thicknesses s_1 and s_2, the potentials $V_A = V_{A_1} = 0$, and the effective electron mass is m_A^*. In the layers B and C of the thicknesses t_1 and t_2, the potentials V_B and $V_C = V_B + \Delta$, and the effective electron masses are equal to m_B^* and m_C^*, respectively. We will assume for the sake of certainty that $V_B < V_C$. A period of each elementary cell is $\Lambda = s_1 + s_2 + t_1 + t_2$.

The stationary states of electrons in the superlattice are determined from solutions of the one-dimensional Schrödinger equation [17] for each element in the elementary cell.

$$-\frac{\hbar^2}{2m_i^*}\frac{d^2\psi_i(x)}{dx^2} + V_i(x)\psi_i(x) = E\psi_i(x), \quad (1)$$

where E, $\psi_i(x)$ — the energy and the wave function in each i-th layer of the elementary cell $(i = A, B, A_1, C)$, respectively [17]. The potential $V(x)$ is as follows

$$V(x) = \sum_i V_i(x), \quad (2)$$

wherein one sums across all the elementary cells of the superlattice, while the potential $V_j(x)$ in each elementary cell can be presented as

$$V_i(x) = \begin{cases} 0, & \Lambda j < x < \Lambda j + s_1, \\ V_B, & \Lambda j + s_1 < x < \Lambda j + s_1 + t_1, \\ 0, & \Lambda j + s_1 + t_1 < x < \Lambda j + s_1 + t_1 + s_2, \\ V_C, & \Lambda(j+1) - t_2 < x < \Lambda(j+1). \end{cases} \quad (3)$$

The solution of the Schrödinger equation (1) at the section $x \in [\Lambda j, \Lambda(j+1)]$ is described by the Bloch function [17,18]:

$$\psi(x + \Lambda) = \exp(iK\Lambda)\psi(x), \quad (4)$$

where K — the Bloch wave number in the superlattice.

The dispersion equation for finding the spectrum of the electronic states in the considered structure is obtained in a standard way from solving the equation (1) with the potential (2), (3)by generalizing the KPM for the four-component elementary cell using Bastard boundary conditions [12] (see Appendix).

For the superlattice with the four layers in the period, with the energies from the interval $E \in (0, V_B)$, the dispersion equation has the following form:

$$\cos K\Lambda = \operatorname{ch}\gamma_B t_1 \operatorname{ch}\gamma_C t_2 \cos\gamma_A(s_1+s_2) + \left(\frac{\gamma_B^{*2}-\gamma_A^{*2}}{2\gamma_A^*\gamma_B^*}\operatorname{sh}\gamma_B t_1 \operatorname{ch}\gamma_C t_2 + \frac{\gamma_C^{*2}-\gamma_A^{*2}}{2\gamma_A^*\gamma_C^*}\operatorname{ch}\gamma_B t_1 \operatorname{sh}\gamma_C t_2\right) \times \sin\gamma_A(s_1+s_2) + \frac{\operatorname{sh}\gamma_B t_1 \operatorname{sh}\gamma_C t_2}{4\gamma_A^{*2}\gamma_B^*\gamma_C^*}\Big\{-(\gamma_B^{*2}-\gamma_A^{*2})(\gamma_C^{*2}-\gamma_A^{*2}) \times \cos\gamma_A(s_1+s_2) + (\gamma_A^{*2}+\gamma_B^{*2})(\gamma_A^{*2}+\gamma_C^{*2})\cos\gamma_A(s_1-s_2)\Big\}, \tag{5}$$

where

$$\gamma_A = \hbar^{-1}\sqrt{2m_A^* E}, \ \ \gamma_l = \hbar^{-1}\sqrt{2m_l^*(V_l - E)}$$

$(l = B, C)$ — the wave numbers in the elementary cells and the barriers, respectively, whereas $\gamma_i^* = \gamma_i/m_i^*$, $i = A, B, C$.

If the electron energy is within the interval $E \in (V_B, V_C)$, then γ_B is an imaginary quantity:

$$\gamma_B = i\hbar^{-1}\sqrt{2m_B^*(E - V_B)} = i\beta_B,$$

and the equation (5) takes the following form

$$\cos K\Lambda = \cos\beta_B t_1 \operatorname{ch}\gamma_C t_2 \cos\gamma_A(s_1+s_2) - \left(\frac{\beta_B^{*2}+\gamma_A^{*2}}{2\gamma_A^*\beta_B^*}\sin\beta_B t_1 \operatorname{ch}\gamma_C t_2 - \frac{\gamma_C^{*2}-\gamma_A^{*2}}{2\gamma_A^*\gamma_C^*}\cos\beta_B t_1 \operatorname{sh}\gamma_C t_2\right) \times \sin\gamma_A(s_1+s_2) - \frac{\sin\beta_B t_1 \operatorname{sh}\gamma_C t_2}{4\gamma_A^{*2}\beta_B^*\gamma_C^*}\Big\{(\gamma_A^{*2}+\beta_B^{*2})(\gamma_A^{*2}-\gamma_C^{*2}) \times \cos\gamma_A(s_1+s_2) - (\gamma_A^{*2}-\beta_B^{*2})(\gamma_A^{*2}+\gamma_C^{*2})\cos\gamma_A(s_1-s_2)\Big\}, \tag{6}$$

For the energies from the interval $E \in (V_C, \infty)$ the parameter γ_C also becomes imaginary

$$\gamma_C = i\hbar^{-1}\sqrt{2m_C^*(E - V_C)} = i\beta_C,$$

and the dispersion law is pre-defined by the equation:

$$\cos K\Lambda = \cos\beta_B t_1 \cos\beta_C t_2 \cos\gamma_A(s_1+s_2) + \frac{\sin\beta_B t_1 \sin\beta_C t_2}{4\gamma_A^{*2}\beta_B^*\beta_C^*}(\Gamma_- - \Gamma_+) - \frac{1}{2\gamma_A^*} \times \left(\frac{\gamma_A^{*2}+\beta_B^{*2}}{\beta_B^*}\sin\beta_B t_1 \cos\beta_C t_2 + \frac{\gamma_A^{*2}+\beta_C^{*2}}{\beta_C^*}\cos\beta_B t_1 \sin\beta_C t_2\right) \times \sin\gamma_A(s_1+s_2), \tag{7}$$

where

$$\Gamma_\pm = (\gamma_A^{*2} \pm \beta_B^{*2})(\gamma_A^{*2} \pm \beta_C^{*2})\cos\gamma_A(s_1 \pm s_2).$$

We note that the equations (5)–(7) are symmetrical in relation to simultaneous replacement of all the parameter pairs V, t and s, namely $V_B \leftrightarrow V_C$, $t_1 \leftrightarrow t_2$, $s_1 \leftrightarrow s_2$. It means that selection of the elementary cell has no effect on the form of the dispersion equations.

If the heights of the potential barriers are the same — $V_B = V_C = V$, then the effective masses in them are equal: $m_B^* = m_C^* = m^*$ and $\gamma_B = \gamma_C = \gamma = \hbar^{-1}\sqrt{2m^*(V-E)}$. Then the equation (5) is written as

$$\cos K\Lambda = \operatorname{ch}\gamma(t_1+t_2)\cos\gamma_A(s_1+s_2) + \frac{(\gamma_A^{*2}+\gamma^{*2})^2}{2\gamma_A^{*2}\gamma^{*2}}\sin\gamma_A s_1 \sin\gamma_A s_2 \operatorname{sh}\gamma t_1 \operatorname{sh}\gamma t_2 + \frac{\gamma^{*2}-\gamma_A^{*2}}{2\gamma_A^*\gamma^*}\operatorname{sh}\gamma(t_1+t_2)\sin\gamma_A(s_1+s_2). \tag{8}$$

When $E > V$, for (8) we have

$$\cos K\Lambda = \cos\beta(t_1+t_2)\cos\gamma_A(s_1+s_2) + \frac{(\gamma_A^{*2}-\beta^{*2})^2}{2\gamma_A^{*2}\beta^{*2}}\sin\gamma_A s_1 \sin\gamma_A s_2 \sin\beta t_1 \sin\beta t_2 - \frac{\beta^{*2}+\gamma_A^{*2}}{2\gamma_A^*\beta^*}\sin\beta(t_1+t_2)\sin\gamma_A(s_1+s_2). \tag{9}$$

When the thicknesses of the layers with the potential wells are the same and the thicknesses of the layers with the potential barriers are the same, then the elementary cell period is $\Lambda = 2(s+t)$. Then, the considered model is similar to the classic KPM [16], but with a double period, and the respective dispersion equation takes the following form

$$\cos K\Lambda = \operatorname{ch}2\gamma t \cos 2\gamma_A s + \frac{\gamma^{*2}-\gamma_A^{*2}}{2\gamma_A^*\gamma^*}\operatorname{sh}2\gamma t \sin 2\gamma_A^* s + \frac{(\gamma_A^{*2}+\gamma^{*2})^2}{8\gamma_A^{*2}\gamma^{*2}}(\operatorname{ch}2\gamma t - 1)(1-\cos 2\gamma_A s). \tag{10}$$

The third summand has appeared in (10) due to the fact that the elementary cell in the above-considered model has the two potential barriers and the two potential wells. It is a principal difference of the considered model from the classic KPM. However, it is possible to transfer from the equation (5) to the KPM equation in a limiting case: $V_B = V_C = V$, $t_1 = t$, $t_2 \to 0$, $s_1 = s_2 = s/2$. As a result of this procedure we obtain

$$\cos K\Lambda = \operatorname{ch}\gamma t \cos\gamma_A s + \frac{\gamma^{*2}-\gamma_A^{*2}}{2\gamma_A^*\gamma^*}\operatorname{sh}\gamma t \sin\gamma_A s, \tag{11}$$

which corresponds to the KPM dispersion equation for the simple superlattice with the two elements in the elementary cell with the period $\Lambda = s + t$.

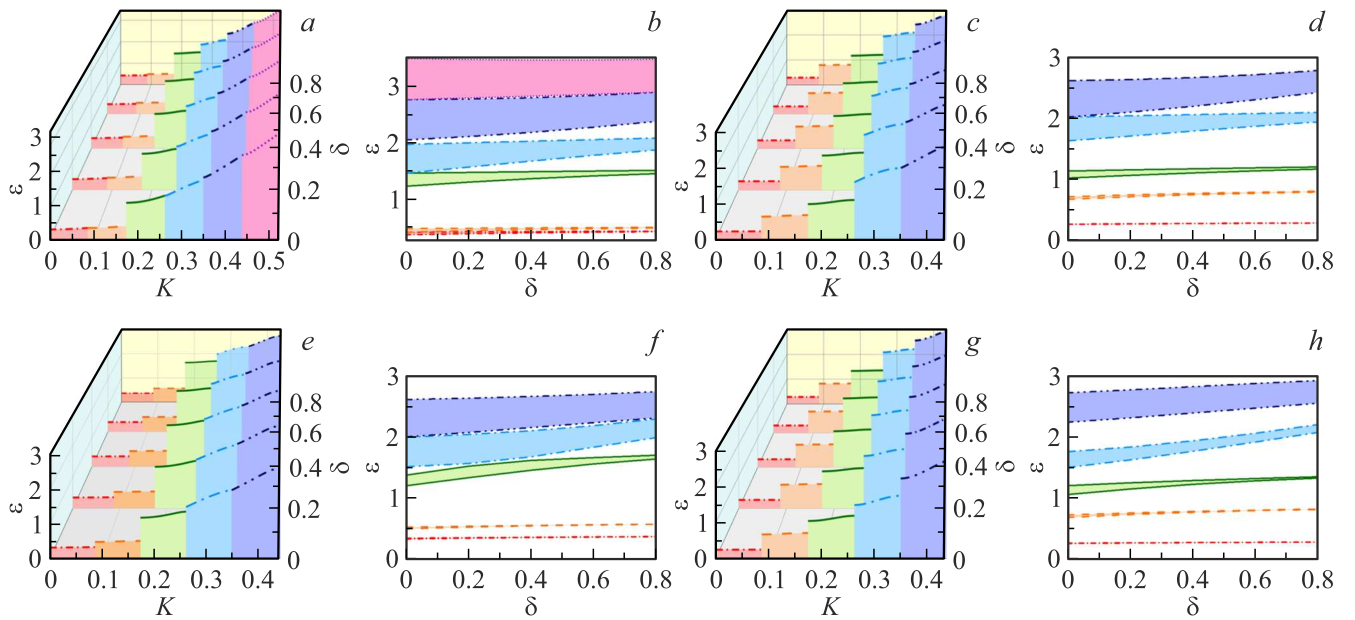

Figure 2. Dependence of the electronic band structure on a relative difference of the heights of the potential barriers δ (11) and on the wave number K for the following parameters of the superlattice: *a, b* — $s_1^* = s_2^* = t_1^* = t_2^* = 9$; *c, d* — $s_1^* = 4.5$, $s_2^* = 13.5$ and $t_1^* = t_2^* = 9$; *e, f* — $t_1^* = 4.5$, $t_2^* = 13.5$ and $s_1^* = s_2^* = 9$; *g, h* — $s_1^* = t_1^* = 4.5$ and $s_2^* = t_2^* = 13.5$.

It should be noted that in the case of the structure with two-well and two-barrier bases the dispersion equations (5)–(7) coincide with a limit case that is obtained in the paper [29]. The next section provides results of numerical analysis of the dispersion equations for the superlattice with the four-component elementary cell that is formed by the two potential wells of a different width and the two potential barriers of a different width and height.

2. Dispersion equations: numerical solutions

As an example, we consider the four-component superlattice with the period of 100 Å, which is formed by the binary compound GaAs (the layers A and A_1) and the ternary alloys — $Al_{0.5}Ga_{0.5}As$ (the layer B, in which the Al concentration is fixed), and $Al_xGa_{1-x}As$ (the layer C), where x determines the Al concentration. As noted in the paper [35], the values of the potential barriers and the effective electron masses in the layers $Al_xGa_{1-x}As$ are determined by the empirical relationships $V(x) = 944x$ meV and $m(x) = (0.067 + 0.083x)m_0$, where m_0 — the mass of a free electron. For numerical calculations, we use parameters of the respective materials from the review [31] and the article [35].

We investigate the dependence of the band structure of this superlattice when varying the widths of the potential wells and the barriers as well as the heights of the potential barriers for various Al concentrations in the layer C.

In order to simplify a procedure finding the numerical solutions it is advisable to proceed to dimensionless variables in the equations (5)–(7)

$$s_{1,2}^* = \hbar^{-1}\sqrt{2m_0V_B}s_{1,2}, \quad t_{1,2}^* = \hbar^{-1}\sqrt{2m_0V_B}t_{1,2}$$

(see details in Appendix). In these units, the period of the considered superlattice is 36.

The results of solving the dispersion equations (A6)–(A8) are given in Fig. 2, *a, c, e, g*, which show the dependence of the electron energy (in dimensionless units) on the wave number K at various values of the relative heights of the potential barriers $\delta = (V_C - V_B)V_B^{-1}$ $(0 < \delta < 0.8)$ for the following cases:

a — the widths of the wells and the barriers are equal to each other ($s_1^* = s_2^* = t_1^* = t_2^* = 9$);

c — the widths of the barriers are equal to each other, while the widths of the wells are different ($s_1^* = 4.5$ and $s_2^* = 13.5$);

c — the widths of the wells are equal to each other, while the widths of the barriers are different ($t_1^* = 4.5$ and $t_2^* = 13.5$);

g — the widths of the wells and the barriers are different ($s_1^* = 4.5$, $s_2^* = 13.5$ and $t_1^* = 4.5$, $t_2^* = 13.5$).

(Compliance of the dimensionless lattice parameters with real dimensions: 4.5 → 12.5 Å, 9 → 25 Å, 13.5 → 37.5 Å).

It is clear from Fig. 2, *a, c, e, g* that at certain values of K the energy electron spectrum exhibits slots, i.e. band gaps. It follows from the results of numerical analysis that when the widths of the wells and the barriers are equal (Fig. 2, *a*), the energy interval originates six minibands. When the wells and the barriers have a different width (Fig. 2, *c, e, g*), then the number of the allowed bands is reduced to five.

The dependence of the band structure on the relative difference of the heights of the potential barriers δ for the various widths of the potential wells and the barriers is shown in Fig. 2, *b, d, f, h*. It is clear that with increase of δ there is narrowing of the allowed bands in the energy electron spectrum. This corresponds to the fact that electron tunneling in this structure will be observed in a narrower energy interval. We also note that the increase of the difference of the heights of the potential barriers results in origination of new allowed minibands with higher energies. It contributes to additional tunneling through the potential barrier in the structure under study.

When the widths of the wells and the barriers are equal to each other, there is observed merging of the adjacent minibands (1 and 2, 3 and 4, 5 and 6) at the equal heights of the barriers ($\delta = 0$) and of the fifth and the sixth bands at the relative difference of the heights of the barriers $\delta = 0.8$ (Fig. 2, *b*). Besides, merging of the fourth and fifth bands when $\delta = 0$ is observed for the same widths of either the wells or the barriers. We note that the similar result was obtained in the papers [31,35] for the two-well and two-barrier bases (with the potential barriers of the equal height) in the four-component superlattice. When the widths of the potential wells and the barriers are different (Fig. 2, *h*), at any δ there are observed wide band gaps that do not merge.

Conclusion

In this paper, we theoretically investigated the electronic spectra of the four-component SLs. The dispersion equations for this structure are obtained in general form. These equations were solved numerically and graphically analyzed for the SL with complex EC composed of binary and ternary semiconductor compounds, namely, $GaAs/Al_{0.5}Ga_{0.5}As/GaAs/Al_xGa_{1-x}As$. The principal results of this paper are presented below:

• The greatest number of the minibands will appear when the widths of the potential wells and the potential barriers are equal (Fig. 2, *a, b*).

• When the potential wells and the barriers are different, the widths of the band gaps increase, whereas the widths of the minibands decrease (Fig. 2, *h*).

• With increase of the difference of the heights of the potential barriers, the widths of the minibands decreases, while the widths of the band gaps increase.

• At certain values of the relative widths of the potential barriers the adjacent minibands can adjoin (Fig. 2, *b, d, f*).

It should be noted that the above-listed results were obtained for the relative widths of the potential wells and the barriers and the relative heights of the potential barriers. It allowed present the calculation results in the general form. Using data for specific compounds [36], it would be possible to predict and model the electronic properties of the predefined heterostructures based on semiconductor materials with the various values of the potential barriers.

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Conflict of interest

The authors declare that they have no conflict of interest.

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Appendix

We consider an energy range from the interval $E \in (0, V_B)$. For each layer in the elementary cell, within the section $x \in [\Lambda j, \Lambda(j+1)]$ the general solution of the equation (1) is written as

$$\psi_A(x) = a_{1j}\cos\gamma_A(x-\Lambda j) + a_{2j}\sin\gamma_A(x-\Lambda j),$$
$$x \in [\Lambda j, \Lambda j + s_1],$$
$$\psi_B(x) = b_{1j}\,\mathrm{ch}\,\gamma_B(x-\Lambda j) + b_{2j}\,\mathrm{sh}\,\gamma_B(x-\Lambda j),$$
$$x \in [\Lambda j + s_1, \Lambda j + s + t_1],$$
$$\psi_{A_1}(x) = a_{11j}\cos\gamma_A(x-\Lambda j) + a_{12j}\sin\gamma_A(x-\Lambda j),$$
$$x \in [\Lambda j + s_1 + t_1, \Lambda j + s_1 + s_2 + t_1],$$
$$\psi_C(x) = c_{1j}\,\mathrm{ch}\,\gamma_C\big(x-\Lambda(j+1)\big) + c_{2j}\,\mathrm{sh}\,\gamma_C\big(x-\Lambda(j+1)\big),$$
$$x \in [\Lambda(j+1) - t_2, \Lambda(j+1)]. \quad \text{(A1)}$$

The arbitrary constants a_{1j}, a_{2j}, b_{1j}, b_{2j}, a_{11j}, a_{12j}, c_{1j}, c_{2j} can be found from boundary conditions at respective interfaces. We will use the Bastard conditions as these boundary conditions [12]:

$$\psi_C\big(\Lambda(j+1)\big) = \exp(iK\Lambda)\psi_A(\Lambda j),$$
$$m_C^{*-1}\psi'_C\big(\Lambda(j+1)\big) = \exp(iK\Lambda)m_A^{*-1}\psi'_A(\Lambda j),$$
$$\psi_A(\Lambda j + s_1) = \psi_B(\Lambda j + s_1),$$
$$m_A^{*-1}\psi'_A(\Lambda j + s_1) = m_B^{*-1}\psi'_B(\Lambda j + s_1),$$
$$\psi_B(\Lambda j + s_1 + t_1) = \psi_{A_1}(\Lambda j + s_1 + t_1),$$
$$m_B^{*-1}\psi'_B(\Lambda j + s_1 + t_1) = m_A^{*-1}\psi'_{A_1}(\Lambda j + s_1 + t_1),$$
$$\psi_{A_1}(\Lambda j + s_1 + s_2 + t_1) = \psi_C\big(\Lambda(j+1) - t_2\big),$$
$$m_A^{*-1}\psi'_{A_1}(\Lambda j + s_1 + s_2 + t_1) = m_C^{*-1}\psi'_C\big(\Lambda(j+1) - t_2\big). \quad \text{(A2)}$$

By substituting the functions from (A1) into the boundary conditions (A2), we obtain a system of linear algebraic equations for determining the constants a_j, b_j, c_j, d_j, f_j, g_j, m_j, r_j. In particular, it follows from (A2) that

$$c_{1j} = \exp(iK\Lambda)a_{1j}, \quad c_{2j} = (\gamma_A^*/\gamma_C^*)\exp(iK\Lambda)a_{2j.} \quad \text{(A3)}$$

and these relationships make it possible to decrease the number of the equations for determining the constants a_j, b_j, c_j, d_j, f_j, g_j, m_j, r_j. As a result of simple transformations we obtain a homogeneous system of six linear algebraic equations:

$$\begin{cases} a_{1j}\cos\gamma_A s_1 + a_{2j}\sin\gamma_A s_1 - b_{1j}\,\mathrm{ch}\,\gamma_B s_1 - b_{2j}\,\mathrm{sh}\,\gamma_B s_1 = 0, \\ -a_{1j}\gamma_A^*\sin\gamma_A s_1 + a_{2j}\gamma_A^*\cos\gamma_A s_1 \\ \qquad - b_{1j}\gamma_B^*\,\mathrm{sh}\,\gamma_B s_1 - b_{2j}\gamma_B^*\,\mathrm{ch}\,\gamma_B s_1 = 0, \\ -a_{1j}\exp(iK\Lambda)\,\mathrm{ch}\,\gamma_C t_2 + a_{2j}\exp(iK\Lambda)(\gamma_A^*/\gamma_C^*)\,\mathrm{sh}\,\gamma_C t_2 \\ \quad + a_{11j}\cos\gamma_A(s_1+s_2+t_1) + a_{12j}\sin\gamma_A(s_1+s_2+t_1) = 0, \\ a_{1j}\gamma_C^*\,\mathrm{sh}\,\gamma_C t_2 - a_{2j}\gamma_A^*\,\mathrm{ch}\,\gamma_C t_2 - a_{11j}\gamma_A^*\exp(iK\Lambda)\sin\gamma_A \\ \quad \times(s_1+s_2+t_1) + a_{12j}\gamma_A^*\exp(-iK\Lambda)\cos\gamma_A(s_1+s_2+t_1) = 0, \\ b_{1j}\,\mathrm{ch}\,\gamma_B(s_1+t_1) + b_{2j}\,\mathrm{sh}\,\gamma_B(s_1+t_1) \\ \qquad + a_{11j}\cos\gamma_A(s_1+t_1) - a_{12j}\sin\gamma_A(s_1+t_1) = 0, \\ b_{1j}\gamma_B^*\,\mathrm{sh}\,\gamma_B(s_1+t_1) + b_{2j}\gamma_B^*\,\mathrm{ch}\,\gamma_B(s_1+t_1) \\ \qquad + a_{11j}\gamma_A^*\sin\gamma_A(s_1+t_1) - a_{12j}\gamma_A^*\cos\gamma_A(s_1+t_1) = 0, \end{cases} \quad \text{(A4)}$$

wherein this system of equations has nontrivial solutions, if a determinant of a matrix of its coefficients is zero. This determinant can be presented as a sum

$$\Delta = \sum_{i=1}^{5}\Delta_i,$$

where each of the summands Δ_i is determined by the following expressions:

$$\Delta_1 = -(\gamma_A^{*4}/\gamma_C^*)\,\mathrm{sh}\,\gamma_B t_1\,\mathrm{sh}\,\gamma_C t_2 \sin\gamma_A s_1 \sin\gamma_A s_2,$$

$$\Delta_2 = (\gamma_A^{*3}/\gamma_C^*)(\gamma_C^*\,\mathrm{sh}\,\gamma_B t_1\,\mathrm{ch}\,\gamma_C t_2 + \gamma_B^*\,\mathrm{ch}\,\gamma_B t_1\,\mathrm{sh}\,\gamma_C t_2)$$
$$\times (\sin\gamma_A s_1 \cos\gamma_A s_2 + \cos\gamma_A s_1 \sin\gamma_A s_2),$$

$$\Delta_3 = 2\gamma_A^{*2}\gamma_B^*\cos K\Lambda - (\gamma_A^{*2}/\gamma_C^*)\big((\gamma_B^{*2} + \gamma_C^{*2})\,\mathrm{sh}\,\gamma_B t_1\,\mathrm{sh}\,\gamma_C t_2$$
$$\times \cos\gamma_A s_1 \cos\gamma_A s_2 + 2\gamma_B^*\gamma_C^*\,\mathrm{ch}\,\gamma_B t_1\,\mathrm{ch}\,\gamma_C t_2$$
$$\times (\cos\gamma_A s_1 \cos\gamma_A s_2 - \sin\gamma_A s_1 \sin\gamma_A s_2)\big),$$

$$\Delta_4 = -\gamma_A^*\gamma_B^*(\gamma_B^*\,\mathrm{sh}\,\gamma_B t_1\,\mathrm{ch}\,\gamma_C t_2 + \gamma_C^*\,\mathrm{ch}\,\gamma_B t_1\,\mathrm{sh}\,\gamma_C t_2)$$
$$\times (\sin\gamma_A s_1 \cos\gamma_A s_2 + \cos\gamma_A s_1 + \cos\gamma_A s_1 \sin\gamma_A s_2),$$

$$\Delta_5 = -\gamma_B^{*2}\gamma_C^*\,\mathrm{sh}\,\gamma_B t_1\,\mathrm{sh}\,\gamma_C t_2 \sin\gamma_A s_1 \sin\gamma_A s_2. \qquad \text{(A5)}$$

The solution of the equation $\Delta = 0$ determines the electronic spectrum for the energies from the interval $E \in (0, V_B)$.

It is convenient to proceed to dimensionless variables in the equations (5)–(7) for numerical solutions. Let $V_C = V_B + \Delta$, $E/V_B = \varepsilon$, $\delta = \Delta/V_B$, $m_l^* = \alpha_l m_0$, m_0 the mass of the free electron, then for the parameters included in (5)–(7) we obtain:

$$\gamma_j = \hbar^{-1}\sqrt{2m_0V_B}\sqrt{\alpha_j\varepsilon_j}, \quad \gamma_j^* = (\hbar m_0)^{-1}\sqrt{2m_0V_B}\sqrt{\varepsilon_j/\alpha_j},$$
$$s_{1,2}^* = \hbar^{-1}\sqrt{2m_0V_B}s_{1,2}, \quad t_{1,2}^* = \hbar^{-1}\sqrt{2m_0V_B}t_{1,2},$$

where

$$\varepsilon_j = \begin{cases} \varepsilon, & j = A, \\ (1-\varepsilon), & j = B, \\ (1+\delta-\varepsilon), & j = C. \end{cases}$$

After simple transformations the equations (5)–(7) in these variables will take the following form:

I. For $\varepsilon \in (0, 1)$:

$$\cos K\Lambda = \mathrm{ch}\sqrt{\alpha_B\varepsilon_B}t_1^*\,\mathrm{ch}\sqrt{\alpha_C\varepsilon_C}t_2^*\cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*)$$
$$+ \frac{1}{2\sqrt{\alpha_A\varepsilon}}\left(\frac{\alpha_A - (\alpha_A+\alpha_B)\varepsilon}{\sqrt{\alpha_B\varepsilon_B}}\,\mathrm{sh}\sqrt{\alpha_B\varepsilon_B}t_1^*\,\mathrm{ch}\sqrt{\alpha_C\varepsilon_C}t_2^*\right.$$
$$\left.+ \frac{\alpha_A(1+\delta) - (\alpha_A+\alpha_B)\varepsilon}{\sqrt{\alpha_C\varepsilon_C}}\,\mathrm{ch}\sqrt{\alpha_B\varepsilon_B}t_1^*\,\mathrm{sh}\sqrt{\alpha_C\varepsilon_C}t_2^*\right)$$
$$\times \sin\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*) - \frac{\mathrm{sh}\sqrt{\alpha_B\varepsilon_B}t_1^*\,\mathrm{sh}\sqrt{\alpha_C\varepsilon_C}t_2^*}{4\alpha_A\varepsilon\sqrt{\alpha_B\alpha_C\varepsilon_B\varepsilon_C}}$$
$$\times \Big\{\big(\alpha_A - (\alpha_A+\alpha_B)\varepsilon\big)\big(\alpha_A(1+\delta) - (\alpha_A+\alpha_C)\varepsilon\big)$$
$$\times \cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*) - \big(\alpha_A - (\alpha_A-\alpha_B)\varepsilon\big)$$
$$\times \big(\alpha_A(1+\delta) - (\alpha_A-\alpha_C)\varepsilon\big)\cos\sqrt{\alpha_A\varepsilon}(s_1^* - s_2^*)\Big\}. \qquad \text{(A6)}$$

II. For $\varepsilon \in (1, 1+\delta)$:

$$\cos K\Lambda = \cos\sqrt{-\alpha_B\varepsilon_B}t_1^*\,\mathrm{ch}\sqrt{\alpha_C\varepsilon_C}t_2^*\cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*)$$
$$+ \frac{1}{2\sqrt{\alpha_A\varepsilon}}\left(\frac{\alpha_A - (\alpha_A+\alpha_B)\varepsilon}{\sqrt{-\alpha_B\varepsilon_B}}\sin\sqrt{-\alpha_B\varepsilon_B}t_1^*\,\mathrm{ch}\sqrt{\alpha_C\varepsilon_C}t_2^*\right.$$
$$\left.+ \frac{\alpha_A(1+\delta) - (\alpha_A+\alpha_C)\varepsilon}{\sqrt{\alpha_C\varepsilon_C}}\cos\sqrt{-\alpha_B\varepsilon_B}t_1^*\,\mathrm{sh}\sqrt{\alpha_C\varepsilon_C}t_2^*\right)$$
$$\times \sin\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*) + \frac{\sin\sqrt{-\alpha_B\varepsilon_B}t_1^*\,\mathrm{sh}\sqrt{\alpha_C\varepsilon_C}t_2^*}{4\alpha_A\varepsilon\sqrt{-\alpha_B\alpha_C\varepsilon_B\varepsilon_C}}$$
$$\times \Big\{\big((\alpha_A+\alpha_B)\varepsilon - \alpha_A\big)\big(\alpha_A(1+\delta) - (\alpha_A+\alpha_C)\varepsilon\big)$$
$$\times \cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*) + \big(\alpha_A + (\alpha_B-\alpha_A)\varepsilon\big)$$
$$\times \big(\alpha_A + (\alpha_B-\alpha_A)\varepsilon\big)\big(\alpha_A(1+\delta) - (\alpha_A-\alpha_C)\varepsilon\big)$$
$$\times \cos\sqrt{\alpha_A\varepsilon}(s_1^* - s_2^*)\Big\}. \qquad \text{(A7)}$$

III. For $\varepsilon \in (1+\delta, \infty)$:

$$\cos K\Lambda = \cos\sqrt{-\alpha_B\varepsilon_B}t_1^*\cos\sqrt{-\alpha_C\varepsilon_C}t_2^*\cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*)$$
$$- \frac{1}{2\sqrt{\alpha_A\varepsilon}}\left(\frac{(\alpha_A+\alpha_B)\varepsilon - \alpha_A}{\sqrt{-\alpha_B\varepsilon_B}}\sin\sqrt{-\alpha_B\varepsilon_B}t_1^*\cos\sqrt{-\alpha_C\varepsilon_C}t_2^*\right.$$
$$\left.+ \frac{(\alpha_A+\alpha_C)\varepsilon - \alpha_A(1+\delta)}{\sqrt{-\alpha_C\varepsilon_C}}\cos\sqrt{-\alpha_B\varepsilon_B}t_1^*\sin\sqrt{\alpha_C\varepsilon_C}t_2^*\right)$$
$$\times \sin\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*) + \frac{\sin\sqrt{-\alpha_B\varepsilon_B}t_1^*\sin\sqrt{-\alpha_C\varepsilon_C}t_2^*}{4\alpha_A\varepsilon\sqrt{\alpha_B\alpha_C\varepsilon_B\varepsilon_C}}$$
$$\times \Big\{\big(\alpha_A - (\alpha_A+\alpha_B)\varepsilon\big)\big((\alpha_A+\alpha_C)\varepsilon - \alpha_A(1+\delta)\big)$$
$$\times \cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*) + \big(\alpha_A + (\alpha_B-\alpha_A)\varepsilon\big)$$
$$\times \big(\alpha_A(1+\delta) + (\alpha_C-\alpha_A)\varepsilon\big)\cos\sqrt{\alpha_A\varepsilon}(s_1^* - s_2^*)\Big\}. \qquad \text{(A8)}$$

Similarly, for the superlattices with the equally-high barriers, by taking into account the relationships $\varepsilon = E/V$, $m^* = \alpha m_0$, $m_A^* = \alpha_A m_0$, for the energies $\varepsilon \in (0, 1)$ the equations (8), (9) will take the following form:

$$\cos K\Lambda = \mathrm{ch}\sqrt{\alpha(1-\varepsilon)}(t_1^* + t_2^*)\cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*)$$
$$+ \frac{\big(\alpha_A + (\alpha-\alpha_A)\varepsilon\big)^2}{2\alpha_A\alpha\varepsilon(1-\varepsilon)}\,\mathrm{sh}\,t_1^*\sqrt{\alpha(1-\varepsilon)}\,\mathrm{sh}\,t_2^*\sqrt{\alpha(1-\varepsilon)}$$
$$\times \sin s_1^*\sqrt{\alpha_A\varepsilon}\sin s_2^*\sqrt{\alpha_A\varepsilon} + \frac{(\alpha_A - (\alpha+\alpha_A)\varepsilon)}{2\sqrt{\alpha_A\alpha\varepsilon(1-\varepsilon)}}$$
$$\times \mathrm{sh}\big((t_1^* + t_2^*)\sqrt{\alpha(1-\varepsilon)}\big)\sin\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*). \qquad \text{(A9)}$$

for the energies $\varepsilon \in (1, \infty)$:

$$\cos K\Lambda = \cos\sqrt{\alpha(\varepsilon-1)}(t_1^* + t_2^*)\cos\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*)$$
$$+ \frac{\left(\alpha_A + (\alpha-\alpha_A)\varepsilon\right)^2}{2\alpha_A\alpha\varepsilon(\varepsilon-1)}\sin t_1^*\sqrt{\alpha(\varepsilon-1)}\sin t_2^*\sqrt{\alpha(\varepsilon-1)}$$
$$\times \sin s_1^*\sqrt{\alpha_A\varepsilon}\sin s_2^*\sqrt{\alpha_A\varepsilon} + \frac{\left(\alpha_A - (\alpha+\alpha_A)\varepsilon\right)}{2\sqrt{\alpha_A\alpha\varepsilon(\varepsilon-1)}}$$
$$\times \sin\left((t_1^* + t_2^*)\sqrt{\alpha(\varepsilon-1)}\right)\sin\sqrt{\alpha_A\varepsilon}(s_1^* + s_2^*). \tag{A10}$$