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Boundary conditions for smooth envelopes of wave functions in type-II heterojunction structures

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A model problem is considered, the solutions of which imply some constraints on the possible boundary conditions in the method of smooth envelope wave functions. The results of this paper may be important for describing structures with type II heterojunctions, which are currently widely used in semiconductor electronics. According to our model results, to obtain the lowest energy values of quantum confinement levels in such structures, different boundary conditions should be used for electrons and holes. The calculations of the energies of size quantization levels show a significant difference in results when using different boundary conditions. This provides an opportunity for experimental verification of the results obtained using the proposed model problem.

Keywords: type II heterojunctions, boundary conditions, quantum well, effective mass.

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1. Introduction

According to the rules of quantum mechanics, the continuity of the total wave function and its derivative shall occur at an abrupt hetero-interface. In this case, the total wave function is the product of the Bloch amplitude and the smooth envelope [1]. Since the Bloch amplitudes turn out to be different in different semiconductor compounds, it is impossible, by and large, with a strict problem solution to obtain any general rules for stitching the smooth envelopes.

However, it is often convenient to use the concept of effective mass to describe the spectrum of dimensional quantization levels, the probabilities of interband and intraband junctions, carrier mobility, and many other properties. At that, it is quite often for the envelope wave function $\Psi(z)$ at $(z = 0)$ hetero-interface when Bastard [2–4]. boundary conditions are used.

$$\Psi_1(z - 0) = \Psi_2(z + 0), \tag{1}$$

$$\frac{1}{m_1}\frac{d\Psi_1(z - 0)}{dz} = \frac{1}{m_2}\frac{d\Psi_2(z + 0)}{dz}. \tag{2}$$

These equations (1) and (2) satisfy the condition of conservation of particle flow through the hetero-interface. Despite many years of use, the scope of their application remains uncertain.

2. The model of indirect determination of boundary conditions

In the absence of a rigorous solution to the boundary conditions problem for the smooth envelopes functions, the approaches that allow obtaining these conditions from model are of particular interest. In this paper, we consider a model problem, the solution of which imposes restrictions on the possible range of applicability of the equations (1) and (2). Our method also predicts the need to use different boundary conditions for a number of compounds. The results obtained below may be important for describing the structures with type II heterojunctions, which are currently widely used in semiconductor electronics, e.g., in the creation of quantum wells and superlattices where precise control of electron and hole levels is necessary, as well as for understanding the charge transfer mechanisms in such heterojunctions and achieving further success in the field photocatalysis [5,6]. Also, composites with II heterojunctions like CdS/AgI, studied in paper [7], or CdS NP−ZnO NF from paper [8], may be used in recovery of the environment due to simplicity of synthesis and excellent photocatalytic activity.

Our approach relates to heterostructures in which levels of dimensional quantization arise. The possibility of its application to single heterojunctions will be discussed further. The main model assumption made in this paper is that the boundary conditions for the smooth envelope functions correspond to the realization of electronic states with the lowest energy values in a quantum well. This condition has no physical justification, since boundary conditions are peculiar to a hetero-interface and should not obey any energy spectrum requirements. Nevertheless, it can be noted that the minimum energy requirement is widely used in various branches of physics, and the results obtained below do not contradict the available data on the properties of heterostructures. As will be seen from the following, the presence of a second hetero-interface does not affect the qualitative results obtained. In this sense, we

can assume that they relate precisely to the properties of a separate heterojunction. At the same time, the proposed approach makes it possible to obtain the quantitative ratios implying that it is possible to compare experimental results with the calculations within this model problem. It is the experiment that may confirm or deny the possibility of using the model results obtained below to describe the properties of real heterostructures.

We assume that the boundary conditions for smooth envelopes generally have the following form:

$$\frac{1}{m_b^{\alpha}}\Psi_b = \frac{1}{m_w^{\alpha}}\frac{d\Psi_w}{dz}, \tag{3}$$

$$\frac{1}{m_b^{1-\alpha}}\frac{d\Psi_b}{dz} = \frac{1}{m_w^{1-\alpha}}\frac{d\Psi_w}{dz}. \tag{4}$$

Conditions (3) and (4) are fulfilled on the hetero-interface. Ψ_i, m_i, where $i = b,\ w$ — wave function and effective mass in the area of barrier and well, respectively. The equations (2) and (3) correspond to the continuity of the particle flow passing through the heterostructure. It is reasonable to assume that the parameter α varies from zero to one, i.e.

$$0 \le \alpha \le 1. \tag{5}$$

Outside of this interval, both the wave function and its derivative are characterized by „jumps“ in opposite directions. Within the framework of the considered model, this looks unnatural. For a more detailed discussion of this assumption, see „Discussion of results“. Consider the application of boundary conditions (3) and (4) to solve the classical quantum mechanics problem of a symmetric quantum well with a width of a and a potential barrier height of u_0 [9]. For the selected boundary conditions, we obtain the following equations for the spectrum

$$\mathrm{tg}\ \frac{ka}{2} = \frac{q}{k}\left(\frac{m_w}{m_b}\right)^{1-2\alpha}, \tag{6}$$

$$\mathrm{tg}\ \frac{ka}{2} = -\frac{k}{q}\left(\frac{m_w}{m_b}\right)^{2\alpha-1}, \tag{7}$$

for symmetric and antisymmetric states, respectively. Here, $k=\sqrt{2m_wE}/\hbar a$, $q=\sqrt{2m_b(u_0-E)}/\hbar a$. It follows from equations (6) and (7) that the minimum energy value of the ground state level is obtained for $\alpha = 0$ if $m_b > m_w$, and for $\alpha = 1$ in the opposite case. Moreover, for the considered structure, the same conditions are fulfilled to obtain the lowest energy values for all excited levels of dimensional quantization of carriers in the potential well. Thus, at $m_b > m_w$, the Bastard boundary conditions [3] correspond to the lowest energy values, and at $m_w > m_b$ — another type of boundary conditions — continuity of the derivative and a jump in the wave function at the interface:

$$\frac{1}{m_b}\Psi_b = \frac{1}{m_w}\Psi_w, \tag{8}$$

$$\frac{d\Psi_b}{dz} = \frac{d\Psi_w}{dz}. \tag{9}$$

This kind of boundary conditions has also been repeatedly discussed in the literature. However, as far as we know, the criterion for the transition from one type of boundary conditions to another for finding the lowest values of the energy of dimensional quantization has not been previously obtained. For $m_w = m_b$, the question of the type of boundary conditions for smooth envelopes does not arise. For different values of effective masses, within the framework of the proposed model, only two boundary conditions are possible: (1) and (2) or (8) and (9). There are no intermediate values for the parameter α in our model.

This result was obtained when solving the problem of a specific form of potential energy in the quantum well region. However, we believe that it has a much broader scope. Indeed, the equation for the spectrum of states localized in a quantum well within the framework of our model is expressed as follows:

$$\frac{d(\ln\Psi_b)}{dz} = \gamma^{1-2\alpha}\frac{d(\ln\Psi_w)}{dz}, \tag{10}$$

where parameter $\gamma = m_w/m_b$. The optimal value of parameter α is determined from the condition that the mass ratio dependent coefficient γ on the right side of equation (10) is maximal. It is this condition that corresponds to the minimum value of the energy level in the quantum well. This can be seen in cases where the dependence of the wave function in the well or barrier is known. So, in the case of rectangular barriers with a potential pit of arbitrary shape, the left side of equation (10) is limited simply to the value $q = \sqrt{2m_b(u_0-E)}/\hbar$. Thus, for any given value of the carrier wave function in the quantum well, the minimum energy value corresponds precisely to the maximum value of the coefficient $\gamma^{1-2\alpha}$ in the right-hand side of equation (10). A similar result is also obtained for a rectangular shape with any shape of the barriers. In general, it can be argued that choosing the maximum possible coefficient on the right side of equation (10) is equivalent to effectively increasing the height of the barriers. In this case, the energy value of the dimensional quantization levels turns out to be the lowest one.

In semiconductors, as a rule, there is a correlation between the band gap width and the effective mass of the carriers. In compounds with a larger band gap, the effective carrier masses turn out to be larger. It means that in heterostructures with I junctions it generally turns out that $m_b > m_w$, i.e. coefficient $\gamma < 1$, which leads to Bastard boundary conditions [2].

This is not the case for heterostructures with II junctions [10]. As a rule, a situation is realized for them when the ratio between the masses of electrons and holes in the quantum well and in the barriers turns out to be different. Within the framework of our model, this means that different boundary conditions for electrons and holes should be used to find the lowest energy levels. The table

Examples of heterojunctions in which different boundary conditions should be used

Heterojunction	c-band	v-band
InP−GaAs	(8), (9)	(1), (2)
InP−AlAs	(1), (2)	(8), (9)
InP−GaSb	(8), (9)	(1), (2)
InAs−GaSb	(1), (2)	(8), (9)

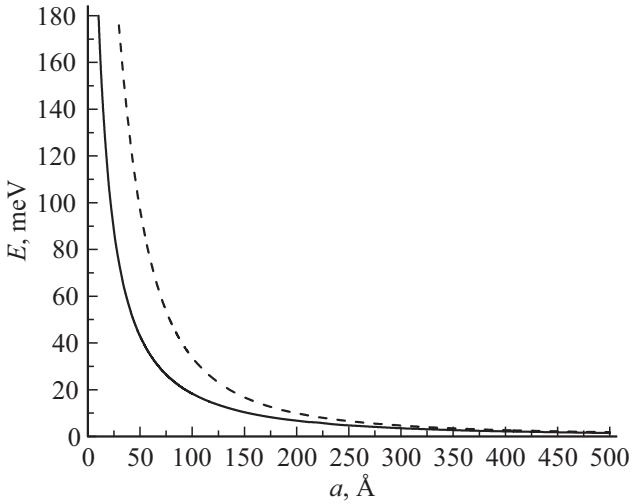

Figure 1. The dependence of the position of energy level E for an electron in the ground state on the width of the quantum well a when using different boundary conditions. Here, the solid line at $\gamma^{-1} = m_b/m_w$ corresponds to the boundary conditions (8) and (9), and dashed line — $\gamma = m_w/m_b$ — corresponds to Bastard conditions (1) and (2).

shows some structures with II heterojunctions and indicates for which carriers the boundary conditions (1) and (2) should be used, and for which the boundary conditions corresponding to equations (8) and (9) are applied if the quantum well is located in the conduction band (c) or in the valence band (v). The applicability of the boundary conditions was analyzed using data from [11].

The use of different boundary conditions naturally leads to significant changes in the calculation of energy levels of dimensional quantization. Figure 1 shows the dependence of the position of the electron ground state energy level E on the width of the quantum well for the structure InP−GaSb.

It can be seen that in sufficiently narrow quantum wells of 20−100 Å the boundary conditions for such a structure obtained in our work give a gain of several tens of MeV. This means that detailed experimental studies of energy levels arrangement in such structures with II type heterojunction may confirm or reject the applicability of the proposed model.

If we consider an ideal single heterojunction, then our model is not directly applicable to it. However, there is often a redistribution of electric charges in heterostructures due to the presence of impurities. In this case, the potential energy near the junction is distorted, which may result in conditions that allow using the results obtained above to realize the lowest values of energy levels.

Quite often, the course of potential energy near the boundary can be approximated by a triangular potential well, the height of the potential barrier of which is defined as

$$u = u_0 \quad \text{by} \quad z < 0,$$

$$u = bz \quad \text{by} \quad z > 0, \tag{11}$$

The value of u_0 stands for the band discontinuity for this heterojunction, and coefficient b is an effective „electrical field“, occurring near the hetero-interface.

Equation (11) has a known solution — for $z > 0$, the wave function is expressed in terms of Airy F function. The equation for determining energy levels can be represented in a dimensionless form.

$$\sqrt{1 - \gamma^{-1}k_1^2} = \beta\gamma^{1-2\alpha}\frac{\Phi'\left(-(k_1^2)/\beta^2\right)}{\Phi\left(-(k_1^2)/\beta^2\right)}, \tag{12}$$

where the dimensionless parameter β is expressed in terms of the barrier height u_0 and the effective „electric field“ b is expressed as follows

$$\beta^3 = \frac{\hbar}{\sqrt{2}}\frac{m_w b}{(m_b u_0)^{3/2}}. \tag{13}$$

The value $k_1 = \sqrt{\gamma E/u_0}$ %. Just as in the case of a symmetric quantum well, the same dependence on the parameterα arises in equation (12). Therefore, in this case, all the conclusions from the previous section are preserved, that is, at $m_w > m_b$, which corresponds to $\gamma > 1$, the lowest energy in the quantum well corresponds to $\alpha = 0$, and at $m_w < m_b$ ($\gamma < 1$) — to the value $\alpha = 1$. Note that in this case, equation (12) describes a certain universal dependence of the energy state values on the „electric field“ b. For each studied heterojunction, it is necessary to substitute specific values of the band parameters of the corresponding materials in equation (12).

Figure 2 provides solutions for the equation (12) for $\alpha = 0$ and $\alpha = 1$. It can be seen that there is a noticeable difference between the values of the parameter k_1 in these cases. The expression (12) allows us to find the corresponding difference in energy levels. For clarity in Figure 2 the values for u_0, m_w and m_b are used for the conduction band of InP−GaSb heterojunction [11].

From Figure 2 we see that because of the difference in parameter k_1 the difference in positions of the respective energy levels may reach 10 % of the band discontinuity u_0. This also provides an opportunity for experimental verification of the proposed model.

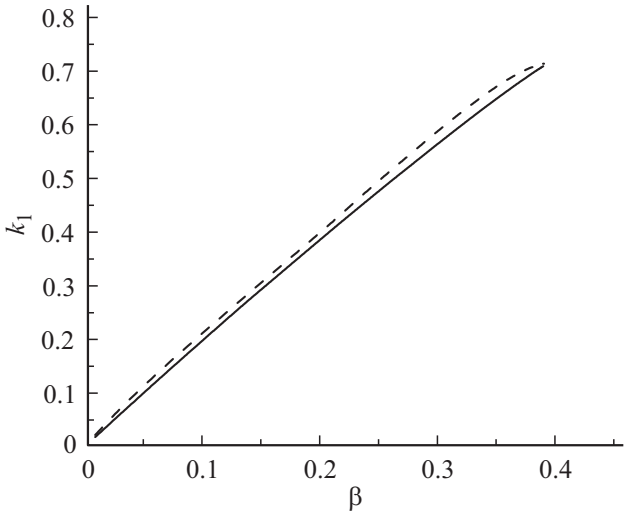

Figure 2. Dependence $k_1(\beta)$ for both ratios of the carriers effective masses in the quantum well and barriers. At that, the solid line corresponds to $\gamma^{-1} = m_b/m_w$ and boundary conditions (8) and (9), and the dashed line — $\gamma = m_w/m_b$ — to conditions (1) and (2).

3. Discussion of results

This study outlines a model problem, the solution of which involves obtaining the lowest energy levels of the charge carriers, which leads to significant limitations in determining possible boundary conditions on a heterointerface when describing electronic states using smooth envelope functions. The field of applicability of the obtained results will be shown by further experimental and theoretical studies of the properties of heterostructures. Within the framework of the considered problem, it is obtained that, depending on the ratio of carrier masses, two types of boundary conditions are possible for smooth envelope functions. For limitations for parameter α from the interval (5) both versions of the boundary conditions are known and have been discussed in the literature many times. The criterion for the transition from one type of boundary conditions to another for determining the lowest energy values was found, and, to our knowledge, it has not been discussed yet. The quantitative calculations show that the results obtained within the framework of the proposed model can be verified experimentally.

Note that the limitations used in the work for parameter α from condition (5) have no effect on the qualitative results obtained. That is, both at $\alpha > 1$ and at $\alpha < 0$, two different types of boundary conditions and the criterion obtained above for the transition from one type of condition to another are preserved. However, this creates rather exotic boundary conditions that differ from both (1) and (2), as well as from (9) and (10). In addition, the minimum energy of the dimensional quantization levels corresponds to the maximum possible values of the parameter modulus α. Within the limit $|\alpha| \to \infty$ a zero energy level arises in the quantum well of any width. This contradicts the known properties of heterostructures. Therefore, it can be assumed that the values α outside of interval (5) contradict modern experimental data, which can be further verified in the experimental study of structures with type II heterojunctions.

Note that the obtained qualitative results are preserved for any finite width of the quantum well. At the same time, the presence of a second heterogeneous boundary is necessary only for the classification of electronic states which is consistent with the conventional approach to describing electronic states in finite-size crystals [1]. For structures with type II heterojunctions, it is found that various boundary conditions for electrons and holes should be used to find the lowest dimensional quantization energies. As far as we know, this circumstance has also not been mentioned anywhere before.

4. Conclusion

In this paper, we considered non-degenerate energy zones for both electrons and holes. For many semiconductor compounds of A^2B^6 and A^3B^5 the valence band in the bulk crystals is a degenerate by itself. Although, in quantum wells grown in the direction of normals to highly symmetric directions, the positions of the energy levels of light and heavy holes can be considered independently. The properties of the structures where the mixing of hole states occurs require an individual review.

The results obtained may be important, first of all, for describing the structures with type II heterojunctions, which are currently widely used in semiconductor electronics, e.g., in the creation of quantum wells and superlattices where precise control of electrons and holes levels is necessary, as well as for better understanding the charge transfer mechanisms in such heterojunctions and achieving further success in photocatalysis.

Conflict of interest

The authors declare that they have no conflict of interest.

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