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The bottom of a dimensional subband in a superlattice with strongly coupled shallow quantum wells

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Based on the analytical solution of the dispersion equation, the energy position of the bottom of the dimensional subband in shallow superlattices is estimated. It is shown that for the upper valleys of GaAs/AlAs superlattices used in heterostructures of field-effect transistors, the depth of the bottom of the dimensional subband relative to the top of the barrier is at the level of 0.11−0.13 eV.

Keywords: superlattice, dimensional subbands, potential barrier.

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Experimental data [1] and theoretical estimates [2–4] reveal that the use of short-period GaAs/AlAs superlattices may improve significantly the characteristics of heterostructure field-effect transistors. However, this raises the question as to how hot electrons will behave in the region of the strong field domain when moving into the upper valleys of a semiconductor, given that X and Γ valleys are inverted in $Al_xGa_{1-x}As$ at aluminum molar fraction $x = 0.4$. Thus, while the AlAs layer forms a barrier with a height of 1.04 eV for the GaAs/AlAs heterojunction along the Γ valley, it turns into a quantum well with a depth of approximately 0.26 eV along the X valley of AlAs [5] (Fig. 1). A natural question arises: is it possible that electrons transitioning in a narrow-gap channel to the upper valleys and transitioning further to AlAs quantum wells will relax and be trapped there? Such processes may potentially have a negative impact on the device characteristics. This is essentially a question of how the distance from the lower quantum level in a well along the X valley to the edge of the well relates to the thermal energy of electrons. It is rather easy to estimate the height of quantum levels for one or two barriers [6]. However, this issue is also of interest in the case of a significantly larger number of barriers [1,2]. The lower quantum level in a set of quantum wells (a fragment of a superlattice) cannot be lower than the bottom of the miniband of the superlattice itself. Therefore, to assess the possible influence of such processes, one needs to know the height of the bottom of the dimensional subband of the superlattice under consideration.

The dispersion equation for the Kronig–Penney potential (Fig. 1), which characterizes this structure, has been proposed long ago and is presented in numerous textbooks (e.g., [6,7]).

In the context of Bloch functions

$$\Psi(x) = u(x)\,\exp(iKx) \tag{1}$$

($u(x)$ is the amplitude of the Bloch function periodic with the superlattice period and K is the wave vector) with the condition that K is a real number and determines the allowed states in all possible cases, it is a rather complex transcendental equation in three variables of the following form:

$$\cos\big(K(a+b)\big) = \cos(ka)\,\mathrm{ch}(\gamma b) - 0.5\left[\frac{k}{\gamma} - \frac{\gamma}{k}\right]\sin(ka)\,\mathrm{sh}(\gamma b), \tag{2}$$

which, apparently, largely defies analysis without significant simplification. The situation is not helped much by the fact that two variables (wave vector k and damping decrement γ) are related:

$$\gamma = \sqrt{\frac{2m_2}{\hbar^2}(U_0 - E)}, \qquad k = \sqrt{\frac{2m_1}{\hbar^2}E}. \tag{3}$$

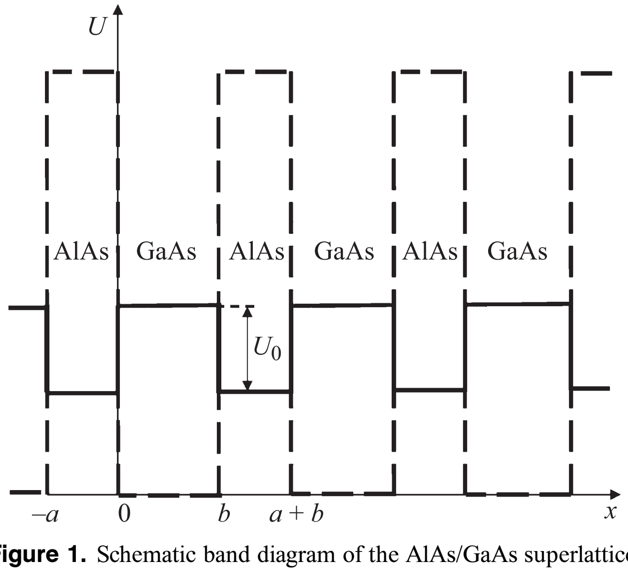

Figure 1. Schematic band diagram of the AlAs/GaAs superlattice: solid line — X valley; dashed line — Γ valley. The zero point is the bottom of the Γ valley of GaAs.

Here, U_0 is the barrier height, E is the electron energy (measured from the bottom of the X valley of AlAs), m_1 and m_2 are the effective electron masses in the well and in the barrier, and $\hbar$ is the Planck constant.

Therefore, various approaches (see, e. g., [7]), which revealed a number of general trends (specifically, sagging of the bottom of the conduction band relative to the quantum level in weakly coupled wells), have been devised. However, it seems that the issue of a superlattice with a set of small tightly coupled wells separated by thin barriers, similar to the one described above, has simply not arisen before.

Let us examine Eq. (2) at $K = 0$. In this case, it takes the form

$$k^2 \sin(ka)\mathrm{sh}(\gamma b) + 2k\gamma\big(1 - \cos(ka)\mathrm{ch}(\gamma b)\big) - \gamma^2 \sin(ka)\mathrm{sh}(\gamma b) = 0. \tag{4}$$

Expanding all the functions into a Taylor series under the assumption of smallness of their arguments, we obtain

$$\sin(ka) \approx ka, \qquad \cos(ka) \approx 1 - \frac{(ka)^2}{2},$$

$$\mathrm{sh}(\gamma b) \approx \gamma b, \qquad \mathrm{ch}(\gamma b) \approx 1 + \frac{(\gamma b)^2}{2}. \tag{5}$$

Naturally, this expansion is relevant only if the corresponding arguments are small enough. Both sine and cosine are characterized quite accurately by the first terms of the series with the argument

$$k\,a < \pi/4. \tag{6}$$

Thus, the height of the quantum level in the shallow well under consideration must be at least 15 times smaller than in an infinitely deep well with the same distance between the walls. In the examined case, this value for an infinitely deep well is ~ 1.2 eV with an AlAs barrier thickness of three monolayers (approximately 7.5 Å) [1] and an effective electron mass of $0.55m_0$ in the X valley [5]. The level height for a single well with a depth of 0.26 eV is 0.18 eV; therefore, its depth is 0.08 eV. Noted that different sources (see, e. g., [8,9]) provide varying data on effective masses and intervalley gaps.

In approximation (5), Eq. (3) is reduced to the expression

$$k^2 a(a+b) - \gamma^2 b(a+b) + \frac{\gamma^2 k^2 a^2 b^2}{2} = 0, \tag{7}$$

and its solution with respect to the wave vector with account for the smallness of arguments of the functions included in it (which means that the last term in (7) is discarded) becomes very simple:

$$k^2 \approx \frac{b}{a}\gamma^2. \tag{8}$$

Taking (3) into account, one obtains the following for the corresponding energy:

$$E \approx \frac{m_2 b}{m_1 a + m_2 b} U. \tag{9}$$

If the effective masses are similar or equal,

$$E \approx \frac{b}{a+b} U. \tag{10}$$

We have examined the solution of the problem at $K = 0$ and, accordingly, $\cos\big(K(a+b)\big) = 1$. In this case, any small variation of K leads to an increase in wave vector k. Without loss of generality, we may write for convenience that $\cos\big((K+\Delta K)(a+b)\big) = 1 - \alpha\gamma^2 b^2$. Here, α is a small quantity. It is easy to demonstrate then that the wave vector magnitude in the examined system increases:

$$k^2 \approx \frac{b}{a}\gamma^2\left(1 + \frac{2b\alpha}{a+b}\right). \tag{11}$$

Thus, formula (10) characterizes in this case the allowed state in the lattice with minimum energy (the bottom of the dimensional subband). It should be noted that the condition of smallness of argument (6) is not satisfied even with (10) taken into account in the lattice of interest to us. However, the Taylor series expansion may then be expressed approximately as

$$\sin(ka) \approx ka - \frac{(k_0 a)^2 ka}{6},$$

$$\cos(ka) \approx 1 - \frac{(ka)^2}{2} + \frac{(k_0 a)^2 (ka)^2}{24},$$

$$\mathrm{sh}(\gamma b) \approx \gamma b + \frac{(\gamma_0 b)^2 \gamma b}{6},$$

$$\mathrm{ch}(\gamma b) \approx 1 + \frac{(\gamma b)^2}{2} + \frac{(\gamma_0 b)^2 (\gamma b)^2}{24}, \tag{12}$$

where k_0, γ_0 are solutions (8) of Eq. (7).

In the approximation of equality of the effective masses in the well and barrier ($0.55m_0$ and $0.5m_0$) [5], we introduce notation

$$G^2 = \gamma^2 + k^2 = \frac{2m^*}{\hbar^2} U \tag{13}$$

insert expansion (12) into Eq. (4), and, having performed elementary transformations, obtain

$$k^2 \approx \gamma^2 \frac{b}{a}\left(1 + \frac{ab(2b^2 + 2ab - 2a^2)G^2}{12(a+b)^2}\right) \times \left(1 + \frac{ab(2b^2 + 4ab - a^2)G^2}{12(a+b)^2}\right)^{-1}. \tag{14}$$

Solution (14) is valid at $k\,a < \pi/2$, which is quite sufficient for the given problem ($k(U_0)\,a = \pi/2.15$). Figure 2 shows the plot of function

$$f\left(\frac{b}{a}, aG\right) = \left(1 + \frac{b(b^2 + 2ab - 2a^2)a^2G^2}{12a(a+b)^2}\right) \times \left(1 + \frac{b(2b^2 + 4ab - a^2)a^2G^2}{12a(a+b)^2}\right)^{-1}. \tag{15}$$

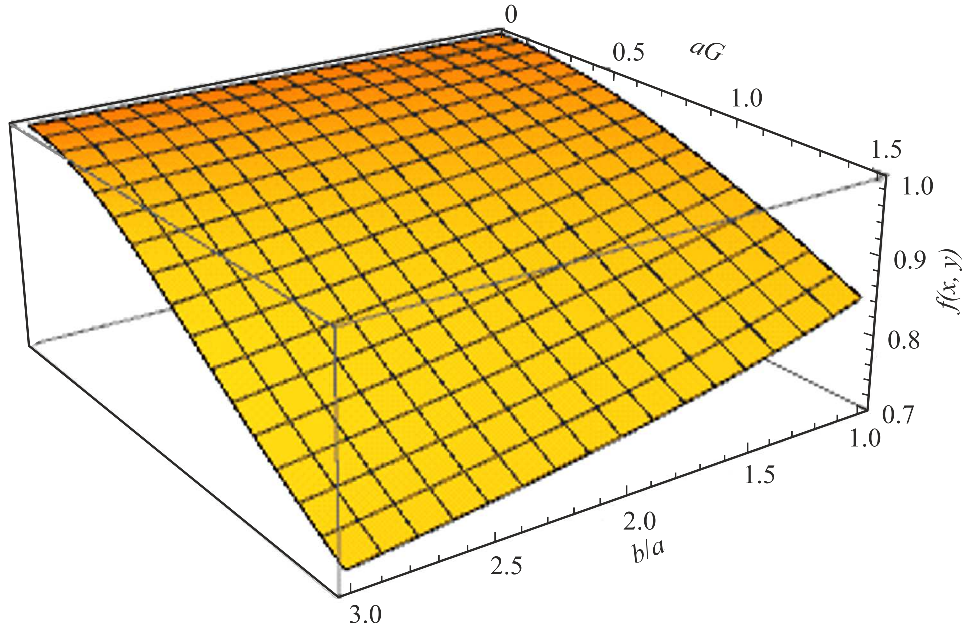

Figure 2. Variation of correction function (15) with ratio of barrier thickness b to quantum well size a and product $aG = a\sqrt{\gamma^2 + k^2}$.

This plot, which represents the correction coefficient to (7), makes it is clear that the value of correction function (15) is 0.75−0.85 within the range of parameters of interest to us.

It should be noted that the correction to (8) in (14) differs fundamentally from what could be derived from (7):

$$k^2 \approx \frac{\gamma^2 b}{a}\left(1 - \frac{a\gamma^2 b^2}{2(a+b)}\right), \tag{16}$$

if the last term in (7) is not discarded due to smallness. This is attributable to the fact that all terms of the corresponding order of smallness are taken into account in (14), but the same is not true of (7) if the last term is not discarded.

Expansion (12) may be refined further by adding terms of the next order of smallness:

$$\sin(ka) \approx ka - \frac{(k_0a)^2 ka}{6} + \frac{(k_0a)^4 ka}{120},$$

$$\cos(ka) \approx 1 - \frac{(ka)^2}{2} + \frac{(k_0a)^2(ka)^2}{24} - \frac{(k_0a)^4(ka)^2}{720},$$

$$\mathrm{sh}(\gamma b) \approx \gamma b + \frac{(\gamma_0 b)^2 \gamma b}{6} + \frac{(\gamma_0 b)^4 \gamma b}{120},$$

$$\mathrm{ch}(\gamma b) \approx 1 + \frac{(\gamma b)^2}{2} + \frac{(\gamma_0 b)^2(\gamma b)^2}{24} + \frac{(\gamma_0 b)^4(\gamma b)^2}{720}. \tag{17}$$

Inserting it into Eq. (3), one may refine formula (13):

$$k^2 \approx \frac{\gamma^2 b}{a}\left(1 + \frac{ab(b^2+2ab-2a^2)G^2}{12(a+b)^2} + \frac{a^2b^2(b^3+3ab^2-10a^2b+3a^3)G^4}{360(a+b)^3}\right) \times \left(1 + \frac{ab(2b^2+4ab-a^2)G^2}{12(a+b)^2} + \frac{a^2b^2(3b^3+5ab^2-12a^2b+a^3)G^4}{360(a+b)^3}\right)^{-1}. \tag{18}$$

The magnitude of this refinement is less than 10% even at $ka = \pi$ (Fig. 3). This figure presents the plot of function

$$f\left(\frac{b}{a}, aG\right) = \left(1 + \frac{b(b^2+2ab-2a^2)a^2G^2}{12a(a+b)^2} + \frac{b^2(b^3+3ab^2-10a^2b+3a^3)a^4G^4}{360a^2(a+b)^3}\right) \times \left(1 + \frac{b(2b^2+4ab-a^2)a^2G^2}{12a(a+b)^2} + \frac{b^2(3b^3+5ab^2-12a^2b+a^3)a^4G^4}{360a^2(a+b)^3}\right)^{-1} - \left(1 + \frac{b(b^2+2ab-2a^2)a^2G^2}{12a(a+b)^2}\right) \times \left(1 + \frac{b(2b^2+4ab-a^2)a^2G^2}{12a(a+b)^2}\right)^{-1}. \tag{19}$$

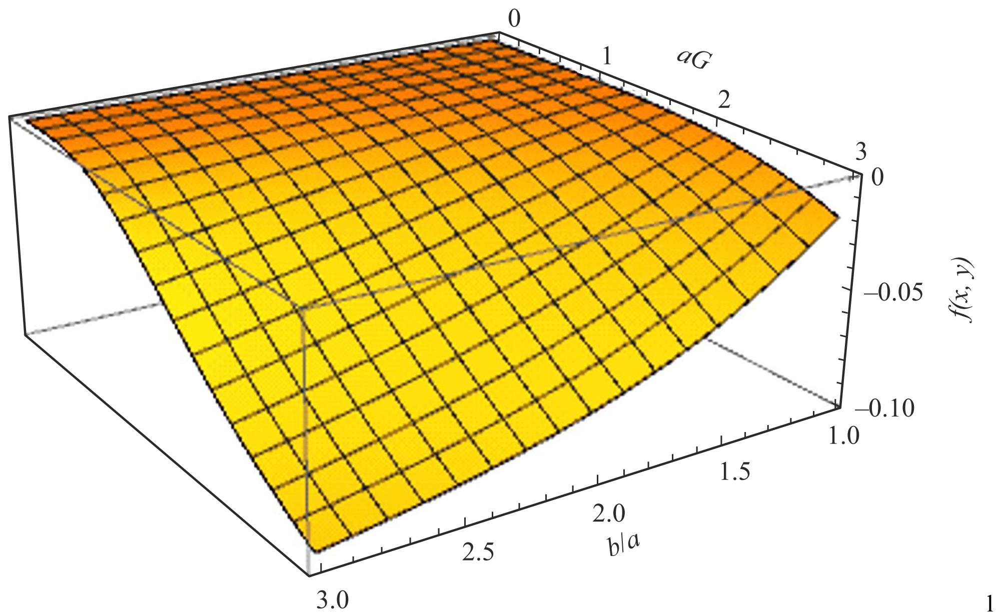

Figure 3. Variation of correction function (19) with ratio of barrier thickness b to quantum well size a and product $aG = a\sqrt{\gamma^2 + k^2}$.

With (8), (12), and (19) taken into account, the bottom of the dimensional subband in the system under consideration is located at a depth (distance from the top of the barrier to the bottom of the subband) of 0.11−0.13 eV. On the one hand, this is significantly (3−3.5 times) greater than the electron energy at crystal lattice temperatures up to 450 K (the maximum allowed temperature in the channel of a GaAs-based transistor). On the other hand, the upper valleys usually contain fairly hot electrons, and such a potential barrier is not very effective for them. However, additional donor-acceptor doping is apparently needed to eliminate possible relaxation effects and increase the efficiency of the barrier system on the substrate side in such structures [2]. On the gate side, the potential associated with surface states is likely to be sufficient (especially in very thin structures).

As the thickness of AlAs layers increases, the bottom of the subband will sink toward the bottom of the quantum well, while the height of the barrier to be overcome by an electron escaping from the well will increase. Even with a layer width of 10 atomic monolayers, the level height in the corresponding single quantum well is just 0.05 eV; when the width exceeds 12 monolayers, a second quantum level appears.

The obtained results suggest that the depth of the bottom of the dimensional subband relative to the top of the corresponding barrier is at the level of 0.11−0.13 eV for the upper valleys of GaAs/AlAs superlattices used in heterostructures of field-effect transistors; i. e., the effective barrier height is almost two times lower than the one in a structure with AlAs layers thicker than 10 atomic monolayers.

Conflict of interest

The author declares that he has no conflict of interest.

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