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Electronic miniband formation in a two-dimensional semiconductor superlattice

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A system of periodically arranged uniform rods has been investigated, regarded as a two-dimensional superlattice. The assumed arrangement of rods within a supercell allows one to express the two-dimensional effective potential as a sum of two terms depending only on either x or y coordinate. The structure consists of two square lattices of square rods embedded in the matrix material. Rods in one lattice act as potential barriers for electrons, and those in the other as potential wells. The separation of the effective potential is shown not to imply Hamiltonian separation in the envelope function approximation. The energy spectra of the conduction band are computed for the numerical solution as well as for the analytical one, the latter wrongly assuming the separation of the Hamiltonian. The band structures computed in the two cases differ in band position and width.

Key words: *2D superlattice; electronic states; photovoltaic cell*

1. Introduction

Electronic superlattices are a sort of artificial materials that can be of use in designing third generation solar cells [1]. Special attention is paid to quantum dot superlattices, allowing increased efficiency of light to voltage conversion due to increased photovoltage as well as photocurrent [2]. Increased photovoltage is achieved thanks to the possibility of electron transitions between successive minibands in the superlattice structure, with multiple absorption of low-energy photons [3]. Moreover, in quantum dots, in which partial carrier binding occurs, thermalization time becomes significantly longer [4, 5]. This allows one to capture hot carriers before their relaxation to the miniband bottom with phonon emission [6]. The increased photocurrent in a superlattice solar cell is due to impact ionization (reverse Auger effect) consisting in the creation of an extra electron-hole pair at the cost of hot electron energy [7].

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Quantum dot superlattices were calculated in the envelope function approximation by Jiang [8] and Lazarenkova [9], who considered a system with an effective 3D potential that can be represented as a sum of three 1D square potentials, and assumed the separation of variables in the potential implying that of spatial coordinates in the envelope function Schrödinger equation. With these assumptions, the energy of a carrier in the considered 3D superlattice is a sum of terms determined independently by each of the three 1D Schrödinger equations for variables x, y and z. In this study, we show that separation of variables in the Hamiltonian is not legitimate in the envelope function approximation, even in the case of separable variables in the effective potential. The method used in [8] and [9] yields results with a small error for low energy minibands only, provided the quantum dot dimensions are comparable to the lattice constant. The reason of the illegitimacy of Hamiltonian separation is that separation of the variables x, y and z in the effective potential does not imply a similar separation in the inverse effective mass. The assumption of separable variables in the inverse effective mass results in altered curvature of the minibands, resulting in their altered width and position.

2. Model

We have performed calculations of a 2D semiconductor superlattice consisting of a system of periodically arranged rods embedded in a matrix of a different material. The results obtained from the 2D model can easily be expanded to the 3D case. Since we believe this will involve neither new effects nor qualitative changes in the model, we restrict our study to two dimensions in order to simplify the band structure analysis, and to reduce the amount of the time-consuming numerical calculations.

The system in question is studied in the envelope function approximation, implying the following form of the Schrödinger equation with spatially variable effective mass [10]:

$$-\frac{\hbar^2}{2}\nabla\frac{1}{m(x,y)}\nabla\psi(x,y)+V(x,y)\psi(x,y)=E\psi(x,y) \tag{1}$$

The effective potential was assumed to be representable as a sum of two 1D square potentials (of identical form):

$$V(x,y)=v(x)+v(y) \tag{2}$$

The addition of $v(x)$ and $v(y)$ results in a 2D potential, in which two square sublattices of square cross-section rods embedded in a homogeneous matrix material can be distinguished. The sublattices are shifted with respect to each other by the vector $\mathbf{R}=[1/2a,1/2a]$, where a is the superlattice constant. One sublattice represents a system of 2D wells (quantum wires), whereas the other consists of 2D barriers (quantum antiwires). Figure 1 shows the profiles of the 1D potentials $v(x)$ and $v(y)$, and the 2D potential $V(x,y)$ resulting from their addition.

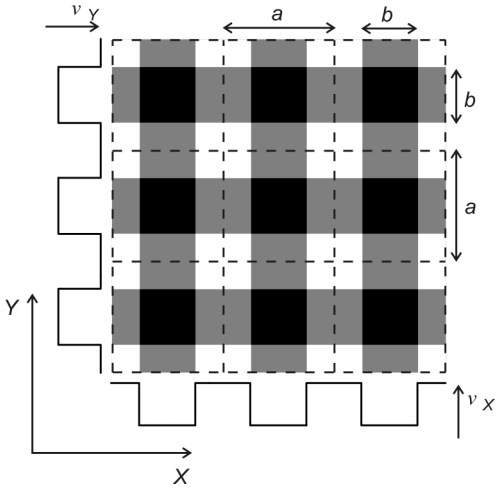

Fig.1. Two-dimensional superlattice potential presented as the resultant of two one-dimensional square potentials. The black, white and gray regions represent potential wells (quantum wires) V_w, barriers (quantum antiwires) V_b and the matrix, respectively

We have calculated electronic states in an $Al_dGa_{(1-d)}As$ superlattice, the assumed values of Al concentration in the three-component alloy being $d = 0.6$, 0.3 and 0 in the potential barriers, the matrix and the potential wells, respectively. The calculations are based on the following empirical formulae for the conduction band bottom level (the effective potential in eV) and the effective mass [11]:

$$V = 0.944d - 0.283, \qquad m = m_0\left(0.067 + 0.083d\right) \tag{3}$$

where m_0 is a free electron mass.

Equations (3) imply a linear dependence between the effective mass and the conduction band bottom level. Therefore, Eq. (2) allows separation of variables in the effective mass. It can easily be proved, however, that a similar dependence does not apply in the case of the inverse effective mass. The approximate formula:

$$\frac{1}{m(x,y)} \approx \frac{1}{2m(x)} + \frac{1}{2m(y)} \tag{4}$$

reproduces the inverse effective mass in the rods (i.e., in the barriers and wells: $1/m_b$, $1/m_w$), but leads to incorrect values in the matrix. The approximation (4) allows one to separate the x and y variables in the Hamiltonian and to write the dispersion relation in the form:

$$\cos\left(k_\alpha a\right) = \cos\left(k_w^\alpha b\right)\cos\left(k_b^\alpha\left(a-b\right)\right) - \frac{1}{2}\left(\frac{k_b^\alpha m_w}{k_w^\alpha m_b} + \frac{k_w^\alpha m_b}{k_b^\alpha m_w}\right)\sin\left(k_w^\alpha b\right)\sin\left(k_b^\alpha\left(a-b\right)\right)$$

where

$$k_b^\alpha = \frac{1}{\hbar}\sqrt{2m_b\left(E_\alpha - \frac{V_b}{2}\right)}, \qquad k_w^\alpha = \frac{1}{\hbar}\sqrt{2m_w\left(E_\alpha - \frac{V_w}{2}\right)}, \qquad \alpha = x, y; \qquad E_x + E_y = E \tag{5}$$

The first two equations in (5), having the form of dispersion relation for 1D potentials $v(x)$ and $v(y)$, determine the E_x and E_y terms contributing to the total electron energy E.

In this study, we compare the band structure calculated from the approximate analytical Equation (5) to that resulting from numerical calculations not involving the approximation (4). The numerical calculations are based on the plane wave method. With the envelope function expanded in the plane wave basis:

$$\psi(x,y) = \frac{1}{a^2}\sum_{\mathbf{G}} \phi_{\mathbf{G}} \mathrm{e}^{j\mathbf{r}\cdot(\mathbf{G}+\mathbf{k})} \tag{6}$$

the Schrödinger equation (1) becomes the following system of algebraic equations:

$$\sum_{\mathbf{G}'}\left(\frac{\hbar^2}{2}(\mathbf{G}+\mathbf{k})\cdot(\mathbf{G}'+\mathbf{k})W_{\mathbf{G}'-\mathbf{G}} + V_{\mathbf{G}'-\mathbf{G}}\right)\varphi_{\mathbf{G}'} = E\varphi_{\mathbf{G}} \tag{7}$$

representing the eigenproblem for energy of an electron with fixed wavenumber $\mathbf{k} = [k_x, k_y]$. Parameters $V_{\mathbf{G}}$ and $W_{\mathbf{G}}$ are the Fourier coefficients of the potential and of the inverse effective mass, respectively. It is easy to see that the only non-zero Fourier coefficients of a function of the form of Eq. (2) are:

$$V_{[G_x,0]} = v_{G_x}, \qquad V_{[0,G_y]} = v_{G_y}, \qquad V_{[0,0]} = \overline{V}(x,y) \tag{8}$$

where v_{G_x} and v_{G_y} are the coefficients in 1D Fourier series expansion of functions $v(x)$ and $v(y)$. As regards the coefficients $W_{\mathbf{G}}$, they all have non-zero values in general. The assumption of separable x and y variables in the inverse effective mass implies:

$$W_{[G_x,G_y]} \approx 0 \qquad \text{for} \qquad G_x \neq 0 \qquad \text{and} \qquad G_y \neq 0 \tag{9}$$

Approximation (9) takes into account only the largest Fourier coefficients $W_{\mathbf{G}}$, for which $G_x = 0$ or $G_y = 0$.

3. Results

In Figure 2, the dispersion has been plotted along the path Γ–X–M–Γ connecting the respective critical points in the Brillouin zone. Figures 2a–d show the miniband structure for the following values of superlattice constant a: b, 1.5b, 2b, 4b, where b, fixed at 40 Å, represents the side length of the square potential well in a supercell centre (cf. Fig. 1). The reference energy level ($E = 0$) corresponds to the conduction band bottom within the matrix. Solid lines represent the dispersion relation for the model assuming separation of variables in the inverse effective mass; results of numerical solution of Eq. (1) with no approximation are represented by the dotted lines.

The energy minibands above the matrix potential visibly sag with increasing superlattice constant (Fig.2a-d). This is a consequence of growing size of barriers and the matrix area between them. The first miniband is not significantly affected, though.

This can be explained by its position within the energy range corresponding to the central well associated with a single rod of fixed dimensions (see Fig. 1).

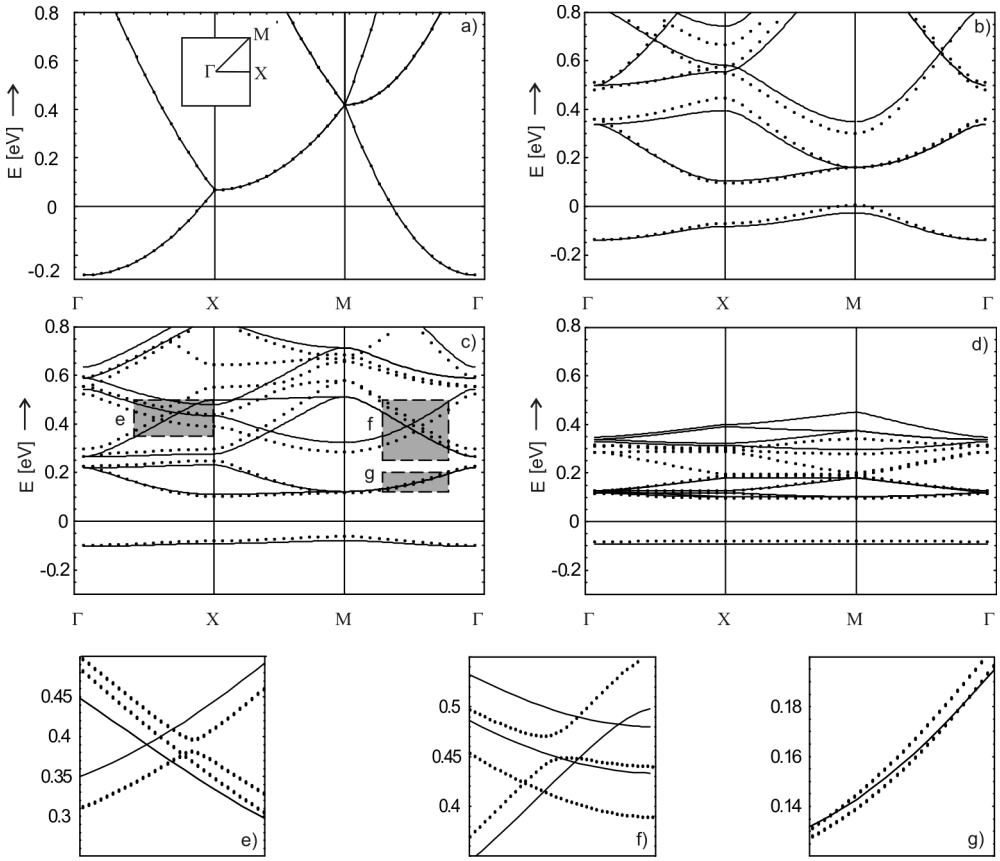

Fig. 2. The dispersion relation along the high-symmetry lines connecting critical points *Γ-X-M-Γ* (see the inset in (a)). The solid lines represent bands in the approximate model assuming separability of variables in $1/m(x,y)$; the dotted lines represent the band structure resulting from numerical calculations (i.e., without the assumption of separability of variables in $1/m(x,y)$). The plots correspond to the well width $b = 40$ Å and four values of the superlattice constant: $a = b$ (a), $a = 1.5b$ (b), $a = 2b$ (c), and $a = 4b$ (d). The results of numerical calculations reveal eliminated accidental degeneration along high-symmetry lines (e), (f), (g) and in some miniband intersection points (e), (f); see the close-ups of (c)

Figure 2a shows the dispersion relation for an empty superlattice, with electrons moving in the homogeneous GaAs. The effective mass being homogeneous, congruent results are obtained by both methods. Figures 2b–d clearly indicate that for high superlattice constant values, the approximation assuming separability of variables in $1/m(x,y)$ yields results substantially different from those obtained without the approximation. The reason of this discrepancy are incorrect values of the matrix $1/m(x,y)$ obtained with the approximation (4).

The approximation (4) results in overestimation of the effective mass value. In Figures 2b–d, the width of the minibands calculated by the approximate method is visibly lower. The overestimation of the effective mass value can be deduced from the reduced miniband curvature.

A supercell in the superlattice under investigation has the symmetry of a square, which involves a significant degeneration of energy bands in the system. Figures 2e–g indicate that additional accidental degeneration along some high symmetry lines occurs in the model assuming separability of variables in $1/m(x,y)$. However, the results of the precise plane wave method calculations prove that in fact the degeneration does not occur. Accidental degeneration in some miniband intersection points is eliminated as well (Figs. 2e–f).

4. Conclusion

Separation of variables in the envelope function Schrödinger equation (i.e., the Schrödinger equation with spatially variable effective mass) proves illegitimate even in the case of effective potential having the form $V(x,y) = v(x)+v(y)$.

Assumed in [8, 9], the approximation (4) yields results close to the precise ones only for the superlattice constant values small with respect to the quantum well dimensions. Therefore, in this range of model parameters, the analytical solutions (5) can be used for theoretical investigation of electronic states in 2D superlattices.

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