Mariusz MĄCZKA, Stanisław PAWŁOWSKI, Jolanta PLEWAKO

Rzeszow University of Technology

Comparative analysis of selected models of semiconductor superlattices

Abstract. *Electrical properties of semiconductor lasers may be described with the help of the numerical calculations performed for the superlattices with the infinite and finite dimensions. In the paper two models of superlattices are compared. In the first approach the finite length of the structure is considered and the Schrödinger equation for the nonpolarized and polarized structures is solved. In the second approach delocalized Bloch functions over the whole structure of the superlattice are considered.*

Streszczenie. *W pracy przedstawiono wybrane właściwości elektryczne laserów półprzewodnikowych, modelowanych za pomocą skończonych i nieskończonych półprzewodnikowych supersieci. Zamieszczono rozwiązania równań Schrödingera dla spolaryzowanej i niespolaryzowanej struktury supersieci. (**Wybrane właściwości elektryczne laserów półprzewodnikowych, modelowanych za pomocą skończonych i nieskończonych półprzewodnikowych supersieci**)*

Keywords: Schrödinger equation, Bloch functions, Wannier function, Wannier–Stark function.
Słowa kluczowe: równania Schrödingera, funkcje Blocha, funkcje Wannier'a, funkcje Wannier'a-Starka

Introduction

The methods for the superlattice simulations can be divided into two groups. The first one assumes finite dimensions of the model [1] and bases on the conventional solution of Schrödinger equation. The second one assumes infinite dimensions of the model and takes the advantage of the Bloch function periodicity [2].

In this work we present two simple models of the superlattice. One of them called Finite Model (FM) assumes finite dimensions of the structure. In the second one (called Infinite Model - IM) infinite dimensions of the structure are taken into account. In the result section we compare selected properties of both methods.

Model FM

We consider the superlattice as it is presented in Fig.1. The structure consists of N modules with L regions. In the region $z_j<z<z_j+1$ (with constant potential and uniform material composition) the envelope function can be written as:

$$\psi_j(z) = A_j e^{ik_j(E)(z-z_j)} + B_j e^{-ik_j(E)(z-z_j)} \tag{1}$$

The connection rules for the envelope functions in the structure may be defined as:

$$\psi_j\left(z_{j+1}\right) = \psi_{j+1}\left(z_{j+1}\right) \tag{2}$$

$$\frac{1}{m_{c,j}}\frac{\partial \psi_j}{\partial z}\bigg|_{z=z_{j+1}} = \frac{1}{m_{c,j+1}}\frac{\partial \psi_{j+1}}{\partial z}\bigg|_{z=z_{j+1}} \tag{3}$$

where m_{cj} and m_{cj+1} are the effective masses in the regions $z_j<z<z_{j+1}$ and $z_{j+1}<z<z_{j+2}$ of the model.

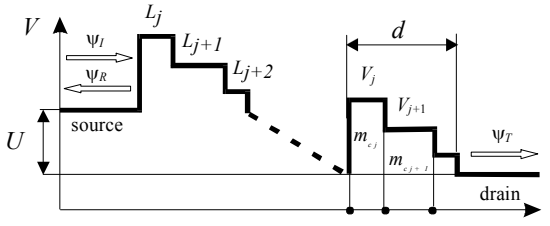

Fig. 1. Finite model of the superlattice

In the calculations the amplitude A_0 of the incident wave ψ_I level. The amplitude B_{L+1} of the propagating wave ψ_T is take as zero is assumed on the nonzero.

According to the Transfer Matrix Formulation (TMF) [2] we can write:

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = M_j(E)\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{4}$$

where:

$$M_j(E) = \frac{1}{2}\begin{pmatrix} (1+\alpha_j)\cdot e^{ik_j w_j} & (1-\alpha_j)\cdot e^{-ik_j w_j} \\ (1-\alpha_j)\cdot e^{ik_j w_j} & (1+\alpha_j)\cdot e^{-ik_j w_j} \end{pmatrix} \tag{5}$$

with $w_j = z_{j+1} - z_j$ and $\alpha_j = \dfrac{k_j m_{c,j+1}}{k_{j+1} m_{c,j}}$.

For the whole structure equation (4) can be written as:

$$\begin{pmatrix} A_{L+1} \\ B_{L+1} \end{pmatrix} = S\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{6}$$

where:

$$S = M_{L+1}M_L \ldots M_0 \equiv \prod_{j=L+1}^{0} M_j \tag{7}$$

Inversion of the relation (6) with the assumption $B_{L+1}=0$ gives:

$$B_0 = -\frac{S_{2,1}}{S_{2,2}}A_0 \qquad A_{L+1} = -\frac{\det S}{S_{2,2}}A_0 \tag{8}$$

Relations (8) allow to obtain the transmission coefficients (T):

$$T \equiv \left|\frac{k_{L+1}}{k_0}\left(\frac{A_{L+1}}{A_0}\right)^2\right| = \left|\frac{k_{L+1}}{k_0}\left(\frac{\det S}{S_{2,2}}\right)^2\right| \tag{9}$$

and to calculate the current of drain on the basis of:

$$I_d = \frac{2e}{h}\int_{E_c}^{\infty} T(E)\left[f(E) - f(E+eU)\right]dE \tag{10}$$

where $f(E)$ denotes the Fermi-Dirac distribution.

Model IM

Superlattices are the periodic structures in which the eigenstates of the Hamiltonian may be described with the help of the Bloch states $\varphi_q^{\nu}(z)$, where ν is the index of the miniband and q is the Bloch vector which spans the interval $\left\langle -\pi/d, \pi/d \right\rangle$. The eigenstates can be constructed with the help of TMF method. For the investigated superlattice

structure we assumed the envelope function in the form (1) and the connection rules (2) and (3). If a single period consists of L regions with the uniform material composition, the Bloch condition in the form:

(11) $$\varphi_q(z+d) = e^{iqd}\varphi_q(z)$$

implies the relation [2]:

(12) $$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = \prod_{j=1}^{N} M_j(E) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = e^{iqd} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

Values of the energy E, which define the allowed minibands $E^{\nu}(q)$, are obtained due to the numerical solution of the Eq. (12) for the given values of q. These functions can be written as:

(13) $$E^{\nu}(q) = E^{\nu} + \sum_{h=1}^{\infty} 2T_h^{\nu} \cos(hdq)$$

where T_h^{ν} is the h^{th} harmonic coefficient for the ν miniband and $E^{\nu} = {}^{d}\!/_{2\pi} \int_{-\pi/d}^{\pi/d} E^{\nu}(q)dq$.

The Bloch functions in the form (1) are delocalized over the whole superlattice. This is the reason for which the difficulties appear when the electric field is applied. In such case the set of Wannier functions [2]:

(14) $$W^{\nu}(z-nd) = \sqrt{\frac{d}{2\pi}} \int_{-\pi/d}^{\pi/d} \varphi_q^{\nu}(z) \cdot e^{-inqd} dq$$

may be very helpful because of they are localized. These functions are constructed from the normalized Bloch states :

(15) $$\int \left[\varphi_q^{\nu'}(z)\right]^* \left[\varphi_q^{\nu}(z)\right] dz = \delta_{\nu\nu'}\delta(q-q')$$

In the creation of Wannier function we must take care of Bloch functions phases choosing. Furthermore, the phases must be chosen arbitrarily for each value of q.
If an electric field is applied the Hamiltonian includes the scalar potential V:

(16) $$eV(z) = -eFz$$

Thus, eigenstates may be written as [2]

(17) $$\left|\Phi_j^{\nu}\right\rangle = \sqrt{\frac{d}{2\pi}} \int_{-\pi/d}^{\pi/d} \exp\left(E_{jq}\right) \left|\varphi_q^{\nu}\right\rangle dq$$

with

(18) $$E_{jq} = \frac{i}{eF} \int_0^q \left[E_j^{\nu} - E^{\nu}(q')\right] dq$$

where Φ_j^{ν} are the Wannier-Stark states of band ν localized around well j. The function Φ_j^{ν}(z) gives the information about the influence of the electric field on the wave function.

Results

The modeling structure is made of $Al_xGa_{1-x}As$ with x=0,3 [2]. Effective mass is assumed to be: $m_c = (0{,}067 + 0{,}083x)$ and conduction band energy is $E_c = 0{,}8x$ eV . The energy dispersion $E(\vec{k}) = E_c\hbar^2k^2 / 2m_c$ is used and non-parabolic effect for $GaAs/AlAs$ is included using the energy-dependent effective mass: $m_c(E) = m_c(E - E_v)/(E_c - E_v)$, where $m_c = 0{,}067m_0$, E_c = 0 eV, E_v = 1,52 eV for $GaAs$ and $m_c = 0{,}152m_0$, E_c = 1,06 eV, E_v = -2,07 eV for $AlAs$.

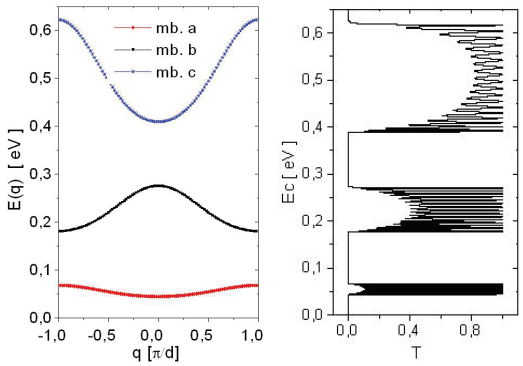

Fig.2. The calculated minibands with model IM (A) and FM (B) models

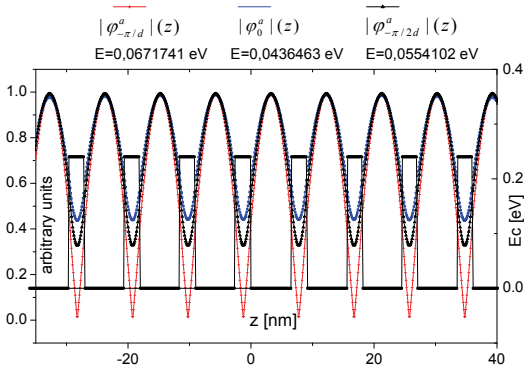

Fig.3. The modules of selected Bloch functions calculated with IM model

In both described models simulations started with computation of allowed minibands in nonpolarized structure. Results are illustrated in Fig. 2. For IM model (Fig. 2A) the widths of minibands Δ^a, Δ^b, Δ^c, are 23,6 meV, 98 meV, 233 meV, respectively whereas the energies of these miniband centers are E^a = 55,41 meV, E^b = 223,1 meV, E^c = 490,5 meV, what corresponds to results in ref. [2].

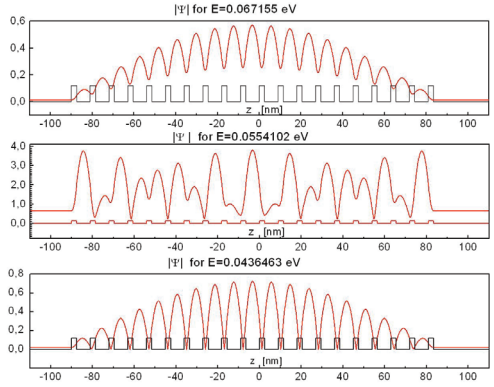

Fig.4. The modules of selected Bloch functions calculated with IM model

Transmission coefficient (T) vs. energy, obtained by the use of FM model, is presented in Fig. 2B. The highest

values of T (near 1) are localized in the same ranges of energy as the minibands illustrated in Fig.2A.

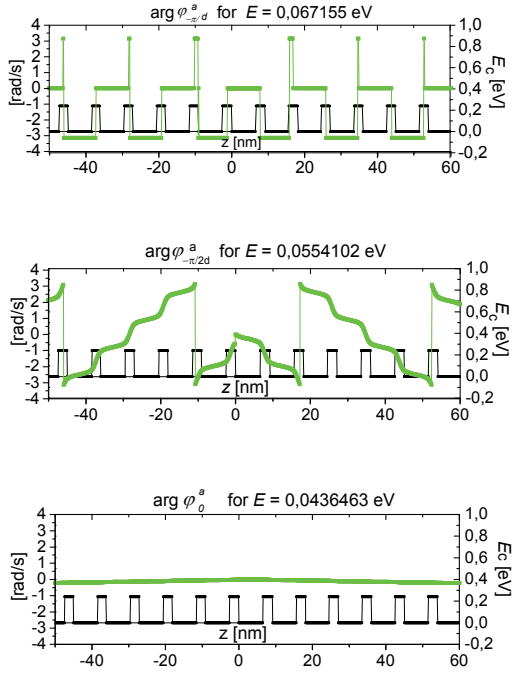

Fig.5. The phases of selected Bloch functions calcu lated with IM model

The Bloch states for three selected energies are presented in Fig. 3. The figure is split in order to show the functions for the energies: bottom (E = 0,0436463 eV), center (E = 0,0554102 eV) and top (E = 0,067155 eV) of lowest miniband, signed as a). One can observe that the modules of all Bloch functions have the same values of maxima (localized in centers of wells) throughout the whole structure.

However, the values of minima (localized in centers of barriers) increase, when the energies decrease.

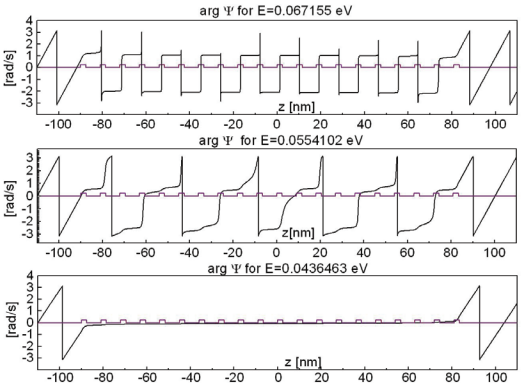

Fig.6. The phases of selected Bloch functions calculated with FM model

The calculations performed with the FM model (see Fig. 4) show that the maxima values of |Ψ| functions create envelope, which is strongly dependent on energies.

In the Fig. 5 we can see the changes of the phases of Bloch functions, presented in Fig.3., however Fig. 6 illustrates the phases of functions showed in Fig. 4.

These results suggest that the behavior of the phases calculated by the use of FM and IM models, despite some insignificant differences, is similar.

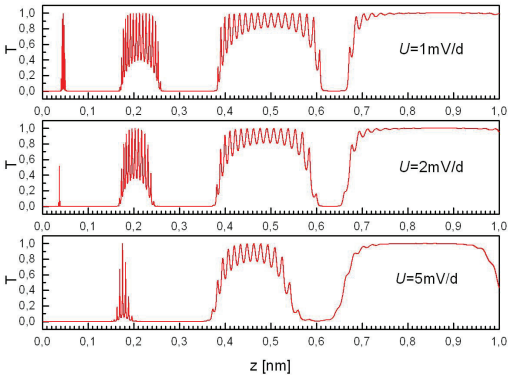

Fig.7. Transmission coefficients (T) calculated with FM model for polarized structure

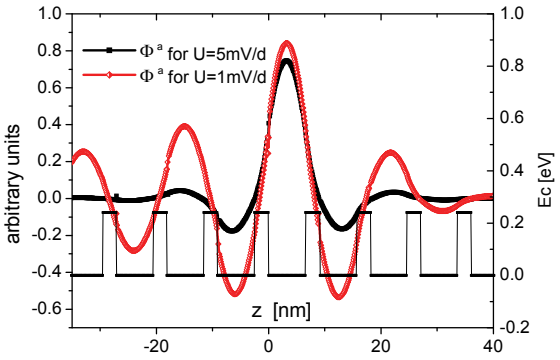

Fig.8. The Wannier-Stark functions calculated with IM model

The very interesting results are obtained when the structure is polarized. Fig.7. presents the transmission coefficients (T) for three values of voltages. These calculations show, that the electric field shifted minibands and decreased their widths. When the voltage is set to higher values than 5 mV/d, the first miniband (a) vanishes, and electrons in this miniband are localized. This case is illustrated in the Fig. 8. There are the Wannier-Stark functions for two values of voltages. We can notice, that for U = 1 mV/d the Wannier-Stark function for first miniband (a) is not localized, however, for U = 5 mV/d it is clearly localized.

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***Authors**: dr inż. Mariusz Mączka, Politechnika Rzeszowska, Katedra Podstaw Elektroniki, ul. W. Pola 2, 35-959 Rzeszów, E-mail: mmaczka@prz.edu.pl dr Stanisław Pawłowski, Politechnika Rzeszowska, Katedra Elektrodynamiki i Układów Elektromaszynowych, ul. W. Pola 2, 35-959 Rzeszów, E-mail: spawlo@prz.edu.pl; dr inż. Jolanta Plewako, Politechnika Rzeszowska, Katedra Energoelektroniki i Elektroenergetyki, ul. W. Pola 2, 35-959 Rzeszów, E-mail: jplewako@prz.edu.pl*