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GREEN'S FUNCTION METHOD APPROACH TO ELECTRON CONFIGURATION OF SUPERLATTICES

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Abstract. As quantum low-dimensional structures are of current interest, we tried to study the basic microscopic behaviour of electron subsystem in superlattices. The microtheoretical method of two-time temperature dependent Green's functions was applied to calculate of electron energy spectra and spectral weights of electrons in superlattices (crystalline structures formed by alternating thin films with changed energy transfer between them). These analyses were performed combining the analytical (using the matrix representation of Chebishev's polynomials) and numerical (using the programme *Mathematica*) approach leading to interesting results for the explanation of some physical properties of these structures.

AMS Mathematics Subject Classification (1991): 82B24

Key words and phrases: superlattice, Green's functions, electron spectra.

1. Introduction

During the last few decades, superlattices have been the subject of intensive experimental and theoretical studies because of their potential applications in electronic devices and the large variety of transport and physical phenomena of these materials [1,2]. Consequently, much effort has been made to determine the electronic structure of these materials using the different methods of calculation [3-6].

A typical example of superlattices is multi-layered crystalline structures of the type $(AC)_m(BC)_n$, formed by alternating super-layers of m layers of the first two-component compound AC and n layers of the second compound BC, along the direction of crystal growth [4]. On the basis of our previous paper, related to crystalline thin film model [7,8], we apply Green's function method to calculate electron dispersion law and spectral weights of electrons in a superlattice. Influence of electron energy transfer between and inside the super-layers on electron spectra and states was analyzed.

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2. Dispersion law of electrons

Figure 1 represents the superlattice model formed by alternating super-layers (thin films) of n_a (thickness d_1) layers of constituent A and n_b layers (thickness d_2) of constituent B (model of periodical superlattice [3,4,6]) along the z direction, while infinite in the x and y directions. Crystal parameters along the x and y directions must be the same ($a_x^a = a_x^b = a_x$ and $a_y^a = a_y^b = a_y$), because the structure must not be stressed, while the parameters along the z direction may be different ($a_z^a = a^a \neq a_z^b = a^b$ and $a_z^{a-b} = a$).

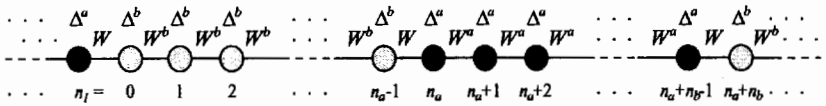

Figure 1: Position of electrons along the z-direction in the superlattice

Our analysis of the electronic subsystem is based on the standard tight-binding electron Hamiltonian (of modeled structure) in the harmonic and nearest-neighbour approximation [5-8]:

$$
\begin{aligned}
H = & \sum_{m_{x/y/z}=-N_{x/y/z}/2}^{N_{x/y/z}/2} \left\{ \sum_{m_l=0}^{n_a-1} \Delta^a a^+_{m_x m_y m_z m_l} a_{m_x m_y m_z m_l} + \right. \\
& + \sum_{m_l=n_a}^{n_a+n_b-1} \Delta^b a^+_{m_x m_y m_z m_l} a_{m_x m_y m_z m_l} - \\
& - \sum_{m_l=1}^{n_a-2} W^a a^+_{m_x m_y m_z m_l} \left(a_{m_x m_y m_z m_l-1} + a_{m_x m_y m_z m_l+1} \right) - \\
& - \sum_{m_l=n_a+1}^{n_a+n_b-2} W^b a^+_{m_x m_y m_z m_l} \left(a_{m_x m_y m_z m_l-1} + a_{m_x m_y m_z m_l+1} \right) - \\
& - a^+_{m_x m_y m_z,0} \left(W a_{m_x m_y m_z-1,n_a+n_b-1} + W^a a_{m_x m_y m_z,1} \right) - \\
& - a^+_{m_x m_y m_z,n_a-1} \left(W^a a_{m_x m_y m_z,n_a-2} + W a_{m_x m_y m_z,n_a} \right) - \\
& - a^+_{m_x m_y m_z,n_a} \left(W a_{m_x m_y m_z,n_a-1} + W^b a_{m_x m_y m_z,n_a+1} \right) - \\
& - a^+_{m_x m_y m_z,n_a+n_b-1} \left(W^b a_{m_x m_y m_z,n_a+n_b-2} + W a_{m_x m_y m_z+1,0} \right) - \\
& - \sum_{m_l} \left[W_x^{a/b} a^+_{m_x m_y m_z m_l} \left(a_{m_x-1,m_y m_z m_l} + a_{m_x+1,m_y m_z m_l} \right) + \right. \\
& \left. \left. + W_y^{a/b} a^+_{m_x m_y m_z m_l} \left(a_{m_x m_y-1,m_z m_l} + a_{m_x m_y+1,m_z m_l} \right) \right] \right\} ,
\end{aligned}
\tag{1}
$$

where $\Delta^{a/b}$ denotes the energy of electron localization on crystal sites, while $W_x^{a/b}$, $W_y^{a/b}$ and $W^{a/b}$ represent energy transfer between electrons inside the super-layers along the x, y and z directions, respectively; W is electron energy transfer between the super-layers along the z direction; $m_{x/y}$ is the site index along the x or y direction; m_z is the super-layer index (along the z direction), while $m_l \in [0, n_a + n_b - 1]$ is the site index inside the super-layer. Using the cycling conditions for x and y coordinates: $f_{m_x m_y m_z m_l + N_{x/y}} = f_{m_x m_y m_z m_l} \Rightarrow e^{iN_{x/y}k_{x/y}a_{x/y}} = e^{2\pi\nu_{x/y}i}$, we can write the cycling condition for super-layer along the z-direction:

$$(2) \qquad f_{m_x m_y m_z m_l + (n_a+n_b)N_z} = f_{m_x m_y m_z m_l} \; ; \Rightarrow \; e^{i(n_a+n_b)N_z k_z \tilde{a}} = e^{2\pi\nu_z i} \, .$$

Allowed values of k_z can be the counted by counter $\nu_z \in 0, \pm 1, \pm 2, ..., \pm N_z/2$. In that way, we can define the bounds of the first Brillouin zone (BZ) along the z direction [9,10]:

$$(3) k_z \in \left[-\frac{\pi}{(n_a+n_b)\tilde{a}}, +\frac{\pi}{(n_a+n_b)\tilde{a}} \right] \; ; \quad \tilde{a} = \frac{(n_a-1)a^a + (n_b-1)a^b + 2a}{n_a+n_b} \, ,$$

where $\tilde{a}$ is the mean value of interlayer distance along the z direction.

In order to find electron dispersion law of superlattice we shall calculate single-particle anti-commutator Green's function, using the Hamiltonian (1):

$$(4) \qquad G_{\vec{n}n_l;\vec{m}m_l} = \Theta(t)\langle\left\{ a_{n_x n_y n_z n_l}, a^+_{m_x m_y m_z m_l} \right\}\rangle \, .$$

After applying the time Fourier transform we get equation of motion for Green's function:

$$\begin{aligned} (5) \quad & \hbar\omega G_{\vec{n};\vec{m}} = \frac{i\hbar}{2\pi}\delta_{\vec{n};\vec{m}} + \Delta_{\vec{n}} G_{\vec{n};\vec{m}} - \\ & - W_x^{\vec{n}} \left(G_{n_x-1,n_y n_z n_l;\vec{m}} + G_{n_x+1,n_y n_z n_l;\vec{m}} \right) - \\ & - W_y^{\vec{n}} \left(G_{n_x n_y-1,n_z n_l;\vec{m}} + G_{n_x n_y+1,n_z n_l;\vec{m}} \right) - \\ & - W_{\vec{n};n_x n_y n_z n_l-1} G_{n_x n_y n_z n_l-1;\vec{m}} - W_{\vec{n};n_x n_y n_z n_l+1} G_{n_x n_y n_z n_l+1;\vec{m}} \, , \end{aligned}$$

where $\Delta \in \{\Delta_a, \Delta_b\}$, $W_{x/y}^{\vec{n}} \in \{W_{x/y}^a, W_{x/y}^b\}$ and $W_{\vec{n};n_x n_y n_z n_l \pm 1} \in \{W^a, W^b, W\}$, depending on the position in the super-layer.

Performing partial spatial (xyz) Fourier transform (because translational symmetry is broken for index l):

$$f_{\vec{n};\vec{m}} = \frac{1}{N_x N_y N_z} \sum_{k_x k_y k_z} f_{n_l;m_l} \, e^{i[a_x k_x (n_x - m_x) + a_y k_y (n_y - m_y) + \tilde{a}(n_a+n_b)k_z(n_z-m_z) + J]} \, ,$$

(6)

$$J = \begin{cases} 1. \; a^a k_z (n_l - m_l) & , \; n_l - m_l < n_a \\ 2. \; a^a k_z (n_a - 1) + a k_z & , \; n_l - m_l = n_a \\ 3. \; a^a k_z (n_a - 1) + a k_z + a^b k_z (n_l - m_l - n_a) & , \; n_a < n_l - m_l < n_a + n_b \\ 4. \; a^a k_z (n_a - 1) + a^b k_z (n_b - 1) + 2a k_z & , \; n_l - m_l = n_a + n_b \end{cases}$$

(7)

we obtain the system of $n_a + n_b$ nonhomogenious algebraic-difference equations for Green's functions [6,9,10]:

$$
\begin{aligned}
&[\hbar\omega - \Delta^a + 2\left(W_x^a \cos a_x k_x + W_y^a \cos a_y k_y\right)] G_0 + \\
&+ W G_{n_a+n_b-1} e^{-iak_z} + W^a G_1 e^{ia^a k_z} = \frac{i\hbar}{2\pi}\delta_0 \\
&[\hbar\omega - \Delta^a + 2\left(W_x^a \cos a_x k_x + W_y^a \cos a_y k_y\right)] G_1 + \\
&+ W^a \left(G_0 e^{-ia^a k_z} + G_2 e^{ia^a k_z}\right) = \frac{i\hbar}{2\pi}\delta_1 \\
&\qquad\qquad * \quad * \quad * \quad * \\
&[\hbar\omega - \Delta^a + 2\left(W_x^a \cos a_x k_x + W_y^a \cos a_y k_y\right)] G_{n_a-2} + \\
&+ W^a \left(G_{n_a-3} e^{-ia^a k_z} + G_{n_a-1} e^{ia^a k_z}\right) = \frac{i\hbar}{2\pi}\delta_{n_a-2} \\
&[\hbar\omega - \Delta^a + 2\left(W_x^a \cos a_x k_x + W_y^a \cos a_y k_y\right)] G_{n_a-1} + \\
&+ W^a G_{n_a-2} e^{-ia^a k_z} + W G_{n_a} e^{iak_z} = \frac{i\hbar}{2\pi}\delta_{n_a-1} \\
(8)\quad &[\hbar\omega - \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a} + \\
&+ W G_{n_a-1} e^{-iak_z} + W^b G_{n_a+1} e^{ia^b k_z} = \frac{i\hbar}{2\pi}\delta_{n_a} \\
&[\hbar\omega - \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a+1} + \\
&+ W^b \left(G_{n_a} e^{-ia^b k_z} + G_{n_a+2} e^{ia^b k_z}\right) = \frac{i\hbar}{2\pi}\delta_{n_a+1} \\
&\qquad\qquad * \quad * \quad * \quad * \\
&[\hbar\omega - \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a+n_b-2} + \\
&+ W^b \left(G_{n_a+n_b-3} e^{-ia^b k_z} + G_{n_a+n_b-1} e^{ia^b k_z}\right) = \frac{i\hbar}{2\pi}\delta_{n_a+n_b-2} \\
&[\hbar\omega - \Delta^b + 2\left(W_x^b \cos a_x k_x + W_y^b \cos a_y k_y\right)] G_{n_a+n_b-1} + \\
&+ W^b G_{n_a+n_b-2} e^{-ia^b k_z} + W + G_0 e^{iak_z} = \frac{i\hbar}{2\pi}\delta_{n_a+n_b-1} .
\end{aligned}
$$

There are only $n_a + n_b$ different Green's functions, because the super-layers are formed of $n_a + n_b$ nonequivalent crystal layers (count by index l). Therefore, we write the above system using the relation: $G_{n_x n_y n_z n_l + (n_a+n_b)} = G_{n_x n_y n_z n_l}$.

We simplified model by studying simple cubic lattice, where: $a^a = a^b = \tilde{a} = a = a_z$ and $a_x^{a/b} = a_y^{a/b} = a_z = a$. Introducing the following shortnotes: $W_{x/y}^a/W = W^a/W = \alpha$, $W_{x/y}^b/W = W^b/W = \beta$, $F = 2\left(\cos ak_x + \cos ak_y\right)$ we

can write the determinant of the system in the form:

$$(9)\quad \begin{bmatrix} \varrho_\alpha & \alpha\,e^{+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-} \\ \alpha\,e^{-} & \varrho_\alpha & \alpha\,e^{+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \alpha\,e^{-} & \varrho_\alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ - & - & - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & \varrho_\alpha & \alpha\,e^{+} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-} & \varrho_\alpha & e^{+} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-} & \varrho_\beta & e^{+} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \beta\,e^{-} & \varrho_\beta & 0 & 0 & 0 \\ - & - & - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \varrho_\beta & \beta\,e^{+} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta\,e^{-} & \varrho_\beta & \beta\,e^{+} \\ e^{+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta\,e^{-} & \varrho_\beta \end{bmatrix}_{n_a+n_b}$$

where: $\varrho_\alpha = \dfrac{\hbar\omega - \Delta}{W} + \alpha F$, $\varrho_\beta = \dfrac{\hbar\omega - \varepsilon\Delta}{W} + \beta F$, $e^{+} = e^{iak_z}$, $e^{-} = e^{-iak_z}$.

The unknown $n_a + n_b$ Green's functions can be found as $G_{n_l;m_l} = \dfrac{D_{n_l;m_l}}{D}$, where $D_{n_l;m_l}$ is the variable determinant, while D is the system determinant. The calculation of Green's function poles, which define the spectrum of possible electron energies, turns into calculation of the roots of the system determinant, i.e.:

$$(10)\quad D = \alpha^{(n_a+n_b)}\mathcal{P}_{n_a}\left(\frac{\varrho}{\alpha}\right)\mathcal{P}_{n_b}\left(\frac{\varrho}{\alpha}\right) - 2\alpha^{(n_a+n_b-2)}\mathcal{P}_{n_a-1}\left(\frac{\varrho}{\alpha}\right)\mathcal{P}_{n_b-1}\left(\frac{\varrho}{\alpha}\right) +$$

$$(11)\quad + \alpha^{(n_a+n_b-4)}\mathcal{P}_{n_a-2}\left(\frac{\varrho}{\alpha}\right)\mathcal{P}_{n_b-2}\left(\frac{\varrho}{\alpha}\right) +$$

$$+ (-1)^{(n_a+n_b+1)}\alpha^{(n_a+n_b-2)}\,2\cos\left[(n_a+n_b)ak_z\right] = 0\,,$$

where $\mathcal{P}_n$ are Chebishev's type polynomials [8]. Condition (10) is written for a simple superlattice formed of super-layers of the identical atoms ($\Delta^a = \Delta^b = \Delta$ and $W^a = W^b = W$), while energy transfer between the super-layers is different ($W \neq \tilde{W}$). In general case, this condition can be solved only numerically. Various combinations of super-layers numbers (n_a and n_b) and electron transfer energies (W and $\tilde{W}$) were analyzed. The numerical results for $k_x = k_y = 0$ are graphically presented in Figs 2 and 3.

Due to the new periodicity along the z-direction electron dispersion curve of superlattice splits into several ($n_a + n_b = d$) quasi-continual dispersion branches separated by forbidden bands. If energy transfer between the super-layers is weaker than inside them ($W < \tilde{W}$) all allowed energy bands lie inside the bulk energy limits ($\hbar\omega/\tilde{W} \in [0,4]$), i.e. the superlattice energy zone becomes narrower (Fig. 2). By analogy with thin film model [7,8], we can say that the bottom and top energy gap appear. That is involving direct consequence of lowering electron transfer between the super-layers. Superlattice energy zone spreads outside the bulk energy boundaries when the energy transfer $W > \tilde{W}$. Then, energy mini-bands of localized electron states appear (Fig. 3). In variance to the crystalline film [7], involving discrete localized states, mini-bands of localized states in the superlattice are quasi-continual, due to infinity of the superlattice.

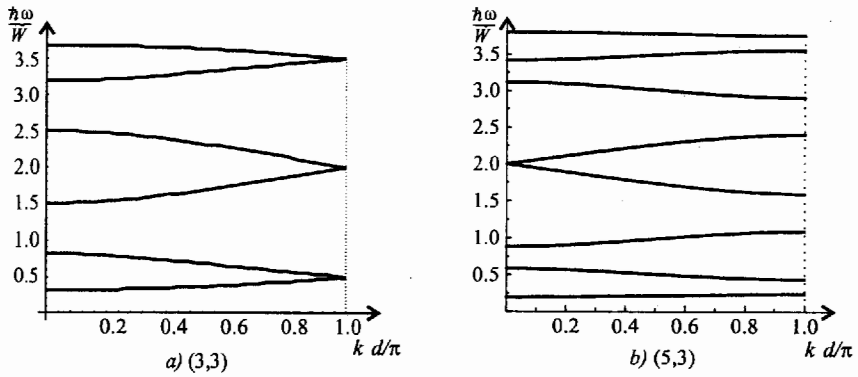

Figure 2: Electron dispersion law for $W = 0.5\tilde{W}$

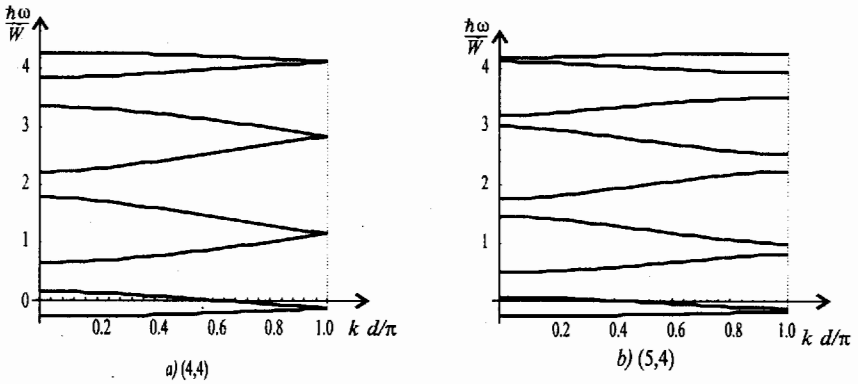

Figure 3: Electron dispersion law for $W = 1.5\tilde{W}$

Position, as well as distribution, of energy mini-bands depend on the number of layers and electron energy transfer. In the case of symmetrical superlattices ($n_a = n_b$), with identical atoms ($a = b$), energy mini-bands join at the end of the first Brillouin zone. The change of electronic transfer between the identical symmetrical super-layers does not lead to opening of the forbidden zones for $k_z = \pi/(n_a + n_b)\tilde{a}$ [6,10]. The superlattice parameter is: $(n_a + n_b)/2 = n_a$, because both of the super-layers have the same length. If central mini-bands join at the edge or at centre of the Brillouin zone, electron dispersion law has a symmetry around the line $\hbar\omega/\tilde{W} = 2$ (Fig 2b). The symmetry at the point $k_z = \dfrac{\pi}{2\tilde{a}(n_a + n_b)}, \dfrac{\hbar\omega}{\tilde{W}} = 2$ (Fig. 3b) appears when the mini-bands are not joined [6].

3. Spectral weights and spatial distribution

Space distribution of electrons can be found by the layer's spectral weights of Green's functions [9,11]. The starting point is the system of equations for Green's functions (8), written in matrix form: $\hat{\mathcal{D}}\tilde{\mathcal{G}} = \tilde{\mathcal{K}}$, where $\hat{\mathcal{D}}$ is the $(n_a + n_b)$ order system matrix, while $\tilde{\mathcal{G}}$ and $\tilde{\mathcal{K}}$ are Green's functions and the "right-hand side" vectors [11]. Applying the inverse matrix $\hat{\mathcal{D}}^{-1}$ we get: $\tilde{\mathcal{G}} = \hat{\mathcal{D}}^{-1}\tilde{\mathcal{K}}$, i.e:

$$G_{n_l;m_l} = \frac{1}{D}\sum_q D_{n_l;q_l}\mathcal{K}_{q_l;m_l} = \frac{1}{D}\frac{i\hbar}{2\pi W}\sum_q D_{n_l;q_l}\delta_{q_l;m_l} \,. \tag{12}$$

$D_{n_l;q_l}$ being co-factors of the system matrix. We calculated only the diagonal Green's functions $G_{n_l;n_l}$, due to their importance in equilibrium processes. Factorizing the multi-pole functions [9,11] we obtain:

$$G_{n_l;n_l} = \frac{i\hbar}{2\pi W}\sum_{\nu=1}^{n_a+n_b}\frac{g_{n_l;n_l}(\varrho_\nu)}{\varrho - \varrho_\nu} \,. \tag{13}$$

The spectral weights $g_{n_l;n_l}(\varrho)$ are given by:

$$g_{n_l;n_l}(\varrho) = \frac{D_{n_l;n_l}(\varrho_\nu)}{\frac{d}{d\varrho}D(\varrho)|_{\varrho=\varrho(\nu)}} \tag{14}$$

Spectral weights represent squared moduli of the wave function and enable us to analyze spatial distribution of finding electrons along the superlattice layers (z direction). By numerical analyses we calculate the spectral weights of electrons for the above simple superlattices (Fig. 4).

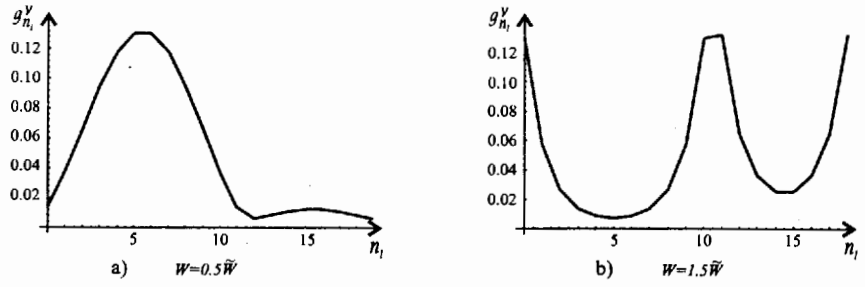

Figure 4: Space distribution of electron in superlattice

If $W < \tilde{W}$, all states are bulk (Fig. 4a), while for $W > \tilde{W}$ localized states can appear (Fig. 4b). Some bulk states are distributed equally in both of the materials, but the states of lowest and highest energies are distributed only

in one of them. Space distribution depends on the number of layers in the superlattice. For an even number of layers (dispersion law has symmetry about the line $\hbar\omega/\tilde{W} = 2$) there is the symmetry of space distribution (for lowest and highest energies, etc.) Localized states appear in the centre of the Brillouin zone if $W > \tilde{W}$, but at edge just for a sufficient value of $W/\tilde{W}$. For an odd number of layers (symmetry of the dispersion law about the point $(k_z = \pi/(2a(n_a + n_b)), \hbar\omega/\tilde{W} = 2)$) there is symmetry between the centre and the edge of the Brillouin zone and localized states appear always when $W > \tilde{W}$ [11]. Localized states appear, mostly, on higher energies. By increasing the ratio $W/\tilde{W}$ the number of these states increases.

4. Conclusion

We applied Green's function method to study electron configuration of superlattices. Apart from electron dispersion law and spectral weights, calculated here, this approach enables the consistent derivation of some other statistical characteristics values of superlattices (thermodynamics, transport, dielectric and other physical properties). By analyzing electron spectra and states of electrons in the superlattice we obtain the following results:

1. An infinite superlattice separates the free electron continuum onto the allowed extended states and forbidden bands, as a results of a new periodicity of the superlattice, as well as changed electron transfer between the super-layers.
2. All mini-bands lie inside the bulk energy bounds when the energy transfer of electrons between the super-layers is weaker than inside them, so the bottom and top energy gaps appear. These typical bulk states can be distributed only in one of the films, what is shown by the analysis of spatial distribution of electrons.
3. Superlattice energy zone spreads outside the bulk energy bounds when electron energy transfer between the super-layers stronger than inside them. Energy mini-bands of localized states appear. Probability of finding an electron in these states is maximal in the boundary layers with sharp decrease inside layers.

The interest to described nanostructures in material science is based on the possibility of manipulation of the physical properties of materials and devices by changing mentioned characteristic parameters (number of layers and electron energy transfer). On the basis of this model and applied method it is possible to investigate some other models of superlattice, such as aperiodic (Fibonacci) superlattice with novel physical properties [12].

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