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PERIODIC SEMICONDUCTOR SUPERLATTICES—SOME ELECTRICAL, TRANSPORT AND OPTICAL PROPERTIES

DIMITRIJE TJAPKIN[a)], VITOMIR MILANOVIĆ[a,b)] and ZORAN IKONIĆ[a)]

a) *Faculty of Electrical Engineering, Bulevar Revolucije* 73, 11000 *Beograd, Yugoslavia*

b) *High PTT School, Zdravka Čelara* 16, 11000 *Beograd, Yugoslavia*

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Most important results of our investigation of semiconductor superlattices (*SL*) are presented in this article. Special attention is devoted to the influence of spatial variation of effective mass on *SL* electronic structure. We have derived the dispersion relation for the case of band nonparabolicity in constituent materials of *SL*, and proved it to be spin-independent. The transport and optical properties we studied are: the Einstein relation, envelope matrix elements for transitions between conduction and valance subbands, light absorbtion and gain coefficients. We also present some numerical results for GaAs-$Al_xGa_{1-x}As$ *SL* as an illustration for theoretical considerations.

1. Introduction

It is now widely accepted in literature to call superlattices those semiconductor structures in which the electrons are influenced not only by periodic atomic potential of crystal lattice, but by an additional potential having a considerably larger period as well. This additonal potential induces remarkable changes in the band structure of constituent material(s) of *SL*, a consequence of this being differences between optical, transport and other properties of *SL* and those of homogeneous semiconductors.

The article[1] by L. Esaki and R. Tsu (1970) is mainly taken to be the first one in this field. The so-called compositional *SL*, consisting of crystalline layers of alternating composition, has been proposed there. In 1973 such *SL*, composed of thin (in nm range) GaAs and $Al_xGa_{1+x}As$ layers was grown by molecular beam epitaxy (*MBE*) by L. L. Chang et al.[2]. Up to now this *SL* is the most extensively studied type, both theoretically and experimentally.

The other important type of *SL* is that proposed in 1972 by G. H. Dohler[3,4], with periodic potential obtained by alternating doping of otherwise homogeneous semiconductor with donors (*d*) and acceptors (*p*), possibly with intrinsic (*i*) layers separating the doped ones (*nipi*-structure). The first *SL* of this type was grown in 1981[5]. It is of interest to note that electrons and holes are spatially separated here, thus leading to an indirect band gap in real space.

The studies of transport properties of *SL* have been intensified since 1978, when R. Dingle et al.[6] proposed the modulation doping technique, that enables one to obtain considerable enlargement of carrier mobility in *SL* as compared to mobility in homogeneous semiconductors. New devices, such as high electron mobility transistor (*HEMT*)[7], and two-dimensional electron gas field effect transistor (*TEGFET*)[8], based on this effect that originates in spatial separation between ionized impurities (scatterers) and carriers, have been proposed. These structures have a number of advantages as compared to the corresponding structures based on homogeneous semiconductors (lower output resistance, higher gain, low noise level, and very low dissipation, being itself a limiting factors in *VLSI* technology[9]).

Not less interesting are optical properties of *SL*, studied extensively since 1974, particularly the intraband (intersubband) transitions, on of the effects not appearing in homogeneous semiconductors. The increased interest in their optical properties that arose recently is related with the possibility of making semiconductor lasers with *SL* active region. These lasers have larger photon energies then conventional semiconductor lasers, and this quantity can be tailored to a certain extent via design parameters variation. Also, the step-like density of states vs. energy dependence in *SL* results in lower values of threshold current and lower temperature sensitivity of these lasers as compared to their conventional counterparts.

All *SL* properties — band structure, mobility of carriers, conductance, light absorption coefficient etc. can be tailored in a wide range of several orders of magnitude by changing *SL* parameters, like layer width, material composition or imputrity concentration[10]. The possibility of making *SL* with desired properties implies their various applications in the near future.

In this article we present results of our research in this field, including some results of self-consistent treatment of *SL* properties, such as band structure, carrier concentration, potential, etc., particular attention being devoted to the influence of spatial variation*) of effective mass. Due attention will also be payed to the effects of nonparabolicity in constituent materials of *SL*, as well as to numerical aspect of self-consistent treatment. In the second part of this article we shall investigate the Einstein relation and some basic optical *SL* properties.

*) In case of band nonparabolicity the spatial variation of effective mass exists in *nipi SL* as well (for more details see Section 2b of this article).

2. *Self-consistent determination of basic SL properties*

The first point of the research is to determine the potential distribution. *SL* is composed of very thin layers, therefore it is clear that quantum effects will be rather prounonced here, and the potential can be found only by making use of self-consistent procedure. Self-consistent calculations of relevant parameters in semiconductor structures have been worked out in detail and applied to the *MOSFET* (see review article[10]), but, because of the peculiarities of *SL* structure, this method should undergo some modifications before its application to *SL*.

a) The case of parabolicty in constituent materials

In this section we shall investigate the compositional *I* type *SL* (same sign of band edge discontinuity), consisting of semiconductors *A* and *B*. We shall take the effective mass approximation to hold for both materials and that the band extrema are in Γ-point in $\vec{k}$-space. Therefore, carriers in both materials can be described by scalar effective masses m_A and m_B (which are different) and have rectangular dependence of effective mass on coordinate, $m^*(z)$. In this case, the kinetic energy operator has the form[11]

$$\hat{T} = \frac{1}{2} [\hat{p}_x \, \hat{p}_y \, \hat{p}_z] \cdot \begin{bmatrix} m^*(z)^{-1} & & 0 \\ & m^*(z)^{-1} & \\ 0 & & m^*(z)^{-1} \end{bmatrix} \cdot \begin{bmatrix} \hat{p}_x \\ \hat{p}_y \\ \hat{p}_z \end{bmatrix}, \tag{1}$$

where $\hat{p}_x$, $\hat{p}_y$, $\hat{p}_z$ are components of momentum operator*). This form of $\hat{T}$ satisfies both the Hermiticity and the probability current continuity at boundaries between two materials.

The Schrödinger equation for carrier motion (we observe electrons now) has the form

$$(\hat{T} + \hat{U})\psi = E\psi. \tag{2}$$

In (2) $\hat{U} = U(z)$ is the potential energy operator, E is the total electron energy, and $\psi(x, y, z)$ is the envelope wave function.

The *SL* structure varies along the z-direction only, therefore the potential energy also depends only on z, and motion in plane perpendicular to z can be described by a plane wave:

$$\psi(x, y, z) = \eta(z) \exp [\mathrm{i}(k_x x + k_y y)]. \tag{3}$$

Substituting (3) in (2) we get[11]

$$-\frac{\hbar^2}{2} \frac{\mathrm{d}}{\mathrm{d}z} \left(\frac{1}{m^*} \frac{\mathrm{d}\eta}{\mathrm{d}z} \right) + \left[U(z) + \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) \right] \eta = E\eta. \tag{4}$$

*) We put the z-axes to be perpendicular to *SL* layers.

Since it is the square absolute value of the wave function we are interested in now, it is enough to determine the function $\eta(z)$, i. e. to solve the Schrödinger eq. (4).

The expression in bracket [...] is the effective potential U_{eff} [11]. For different values of transversal component of wavevector $k_t = \sqrt{k_x^2 + k_y^2}$, U_{eff} has qualitatively different behaviour, where from we get two important conclusions:

1) The Schrödinger eq. has to be solved for each value of k_t particularly, and η is the explicite function of k_t.

2) The total electron energy is not a parabolic function of k_t.

These two effects disappear if the effective mass has no spatial variation (this is the case in doped *SL*).

Since the structure is periodic with period length d one has to apply periodic boundary conditions

$$\eta(z+d) = \eta(z)\,\lambda, \quad \eta'(z+d) = \eta'(z)\,\lambda, \quad \lambda \equiv \exp(ik_z d). \tag{5}$$

These boundary conditions have the same form as those in classical theory of band structure, where the Schrödinger eq. with free electron mass (no spatial variation) is used. However, one can show [12] that even in case of spatially variable effective mass conditions (5) hold. We take the effective mass has steplike changes at layer boundaries. Taking into account the continuity of the wavefunction one can, after performing integration around the boundary, show that $\frac{1}{m(z)} \cdot \frac{dn}{dz}$ is continuous as well. This condition is derived with the postulated form of Hamiltonian (1). Naturally, boundary conditions depend on microscopic structure of both materials. In Ref. 13 it was shown that boundary conditions can be written in the form (boundary at $z = 0$)

$$\begin{bmatrix} \eta_B(0) \\ a\eta_B'(0) \end{bmatrix} = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \cdot \begin{bmatrix} \eta_A(0) \\ a\eta_A'(0) \end{bmatrix}, \quad a = a(z) \text{ — lattice constant,} \tag{6}$$

where $[t_{ij}]$ is the transfer matrix, which contains information on microscopic structure of both materials, although in an implicite form. Calculations performed in Ref. 13 for GaAs-$Al_{0.2}Ga_{0.8}As$ *SL* showed that $t_{12} = t_{21} = 0$, $t_{11} = 1.021$ and $t_{22} = 1.101$, which agrees very well with boundary conditions we used.

With determined band structure and corresponding wavefunctions, electron concentration can be written in the form+)

$$n(z) = \sum_l n_l(z), \quad n_l(z) = \frac{d}{2\pi^3} \int_0^{\pi/d} dk_z \int_{-\infty}^{+\infty} \int_{-\infty}^{\infty} \frac{|n_l(\vec{k}, z)|^2 \, dk_x \, dk_y}{\exp\left[\frac{E_l(\vec{k}) - E_F}{kT}\right] + 1}. \tag{7}$$

In Eq. (7) $E_l(\vec{k})$ is the dispersion relation of l-th subband, and E_F the Fermi level, determined from the condition of global neutrality of *SL*. We should also note

+) The expression (7) appeared in our work [11], so far as we know, for the first time in the literature.

that $E_l(\vec{k})$ does not depend parabolically either on k_x or k_y or k_z in compositional *SL*. In doped *SL* $E_l(\vec{k}) = E_l^0(k_z) + (\hbar^2 k_t^2)/2m^*$, therefore integration over k_x and k_y can easily be performed, and (7) transforms into a more simple expression.

Making use of determined concentrations of electrons $n(z)$ and holes $p(z)$*), one can solve the Poisson's eq. taking into account the difference between dielectric constants of materials *A* and *B*. The boundary conditions for this eq. are periodic: assuming the potential to have zero value at $z = 0$ implies the same value at $z = d$.

The main part of this problem certainly is solving of Schrödinger equation. We shall present here two methods of solving it for symmetric *SL* (which are predominantly used both in theoretical and experimental research). Generalization of those methods for application to nonsymmetric cases is not a difficult problem qualitatively.

The cruical point of harmonic method is to represent all periodic variables (potential energy, effective mass, wave functions, ...) by complex Fourier series. It can be shown[14] that allowed values of energy are eigenvalues of an infinite symmetric square matrix $[S_{q,l}]$, elements of which are determined by

$$S_{q,l} = (U_{eff})_{q-l} + \frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{q-l}\left(k_z + \frac{2\pi}{d}q\right)\left(k_z + \frac{2\pi}{d}l\right) \quad q, l = 0, \pm 1, \pm 2, \ldots, \pm\infty. \tag{8}$$

Taking care of the fact that energy spectrum consists of bands if there is at least one nonzero off-diagonal element (which can easily be verified) we can after inspection of the matrix $S_{q,l}$ deduce some important and interesting conclusions about the existence of band character of energy spectrum. The energy spectrum is band-like if there exists:

1) Spatial variation of potential energy only (this case has been thoroughly studied in classical band theory).

2) Spatial variation of potential energy and effective mass (compositional *SL*).

3) Spatial variation of effective mass only.

It is interesting that even in case the potential energy is constant throught the structure, we get energy bands (this indeed happens in compositional *SL* for certain value of k_t).

The harmonic method, apart from displaying the physics of the problem very well, is a complex (although interesting by itself) numerical problem; its central part being the eigenvalue determination for an infinite full matrix.

Numerical solving can be more conveniently performed by using the method of even and odd functions, taken from the conventional band theory[15], with some modifications necessary for application to *SL*.

In symmetric *SL*, potential energy and effective mass are even functions. The wave function can be represented as a linear combination of even $\eta_e(z)$ and odd $\eta_0(z)$ functions[15]

$$\eta(z) = A\eta_0(z) + B\eta_e(z), \tag{9}$$

*) The Schrödinger eq. and concentration for electrons and holes have simmilar forms, so we shall not write the latter separately.

with fundamental boundary conditions for $\eta_0(z)$ and $\eta_l(z)$

$$\eta_0(0) = 1, \quad \eta_0'(0) = 0, \quad \eta_e(0) = 0 \quad \text{and} \quad \eta_e'(0) = 1. \tag{10}$$

Applying the periodic boundary conditions (5) we obtain the expression connecting energy and wavevector

$$\cos(k_z d) = 1 + \frac{2}{W}\eta_e\left(\frac{d}{2}\right)\eta_0'\left(\frac{d}{2}\right), \quad W = \eta_e\left(\frac{d}{2}\right)\eta_0'\left(\frac{d}{2}\right) - \eta_e'\left(\frac{d}{2}\right)\eta_0\left(\frac{d}{2}\right), \tag{11}$$

where constants A and B are to be determined from the first boundary condition (5) and the normalization condition

$$\int_{-d/2}^{d/2} |\eta|^2 \, \mathrm{d}z = 1. \tag{12}$$

Numeric calculations were performed for GaAs-$Al_xGa_{1-x}As$ $(A - B)$ *SL*, which is the most often studied type *I-SL* both theoretically and experimentally, using the method of even and odd functions. Rectangular variation of potential energy in the structure approximates the real situation (after neglecting the carriers), and is the first approximation in self-consistent solving. We also assume isoenergetic surface to be spherical for all energies of interest here (this will be more extensively discussed in the next section). We observed electrons belonging to the Γ-minimum, which is justified in the first iteration of self-consistent procedure, but in latter iterations one should not disregard electrons belonging to minimums at the edge of Brillouin zone (particularly for higher values of mole fraction x). One can deduce from a simple analysis that GaAs layers are quantum wells and $Al_xGa_{1-x}As$ layers barriers for k_t values smaller than a characteristic value k_{t0}, and vice versa for higher values of k_t (Fig. 1). For $k_t = k_{t0}$ the effective potential energy is constant throughout the structure. For assumed variations of $U(z)$ and $m^*(z)$, k_{t0} is determined by

$$k_{t0}^2 = \frac{2U_0 m_A m_B}{\hbar^2 (m_B - m_A)}, \quad U_{eff}^{(A)}(k_{t0}) = U_{eff}^{(B)}(k_{t0}), \quad (m_B > m_A), \tag{13}$$

where U_0 is the potential energy jump at the interface between layers, going in direction from GaAs to $Al_xGa_{1-x}As$. If $m_A > m_B$ positions of wells and barriers would not depend on k_t (this is never fulfilled in GaAs-$Al_xGa_{1-x}As$ *SL*). It is also worth noting that for energies lower than the barrier top we assumed the effective mass in material B to be unchanged, although these energies are in gap of B. Theoretical and experimental studies of tunneling in heterostructures confirmed this to hold[17].

Fig. 2 gives the band structure of GaAs-$Al_xGa_{1-x}As$ *SL*, with layer widths of 6 nm and 1,5 nm, respectively. The widths of bands and gaps depend appreci-

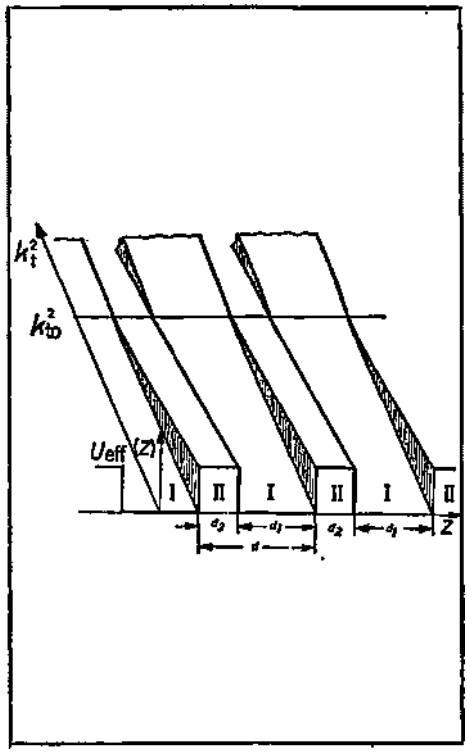

Fig. 1. The dependence of the *effective* potential energy on coordinate z and quantity k_t^2. The effective mass in material I is m_1 and in material II m_2 $(m_1 < m_2)$[16].

ably on transversal component of wave vector. As one can immediatelly see from Fig. 2 we should also note that for certain values of energy and wavevector the energy gap disappears. Conditions for zero energy gap (*ZEG*) existence are extensively discussed in Ref. 16; at this place we shall only mention that there are two conditions, one of them being a direct consequence of spatial variation of effective mass.

b) *The case of nonparabolic bands in constituent materials*

One of lack of the above theory is that it relies on parabolic energy vs. wavevector dependence in constituent materials of *SL*. These are III—V semiconductors with the dispersion relation given more precisely by Kane expression[18]

$$\frac{2\Pi^2}{3E_g}\hbar^2k^2 = \frac{\hbar^2k^2}{2m_0^*} = E\left(1+\frac{E}{E_g}\right). \tag{14}$$

Equation (14) is valid in each host materials. In (14) Π is Kane's matrix element (usually in literature[20] taken to have the same value for all materials), E_g is the

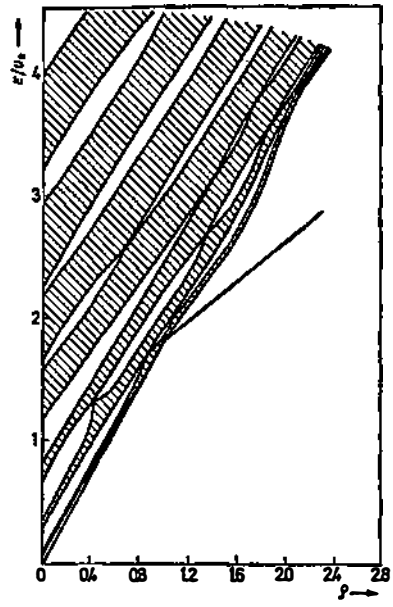

Fig. 2. Configuration of the energy spectrum for the $Al_xGa_{1-x}As$-GaAs superlattice structure ($x = 1$); $d_1 = 6 \cdot 10^{-7}$ m, $d_2 = 0.25\ d_1$ ($\varrho = E_{t1}/E_{t0}$)[16].

energy gap, m_0^* — the effective electron mass at $k = 0$[+], and E energy measured from the bottom of conduction band. This dependence is given in Fig. 3. Parabolic approximation is given by broken line: evidently, this is a better approximation if energies are closer to bottom of conduction or top of valence band. Eq. (14) holds for electrons and light holes. Actually, in III—V semiconductors heavy holes and holes from band lying under the valence band top cannot be disregarded. However, disregarding these holes leads to the Schrödinger eq. in the form[*]

$$([T_{ij}] + [U_{ij}]) \cdot [f_j] = E\,[f_j], \quad i, j = 1, \ldots, 6, \tag{15}$$

where non-zero elements of matrix $[T_{ij}]$ are:

$$t_{13} = t_{62} = -\sqrt{3}\,t_{51} = \sqrt{3}\,t_{24} = a = \frac{\Pi}{\sqrt{2}}(\hat{p}_x - \mathrm{i}\hat{p}_y),$$

$$t_{31} = t_{26} = \sqrt{3}\,t_{42} = -\sqrt{3}\,t_{15} = a^*, \tag{15a}$$

$$t_{41} = t_{14} = t_{25} = t_{52} = \left(\frac{2}{3}\right)^{1/2} \Pi\,\hat{p}_z.$$

[+] Within this model light hole mass is equal to electron mass (at $k = 0$), except for opposite sign.

[*] The first matrix element on the left side is taken from[19], and refers to homogeneous III—V semiconductors.

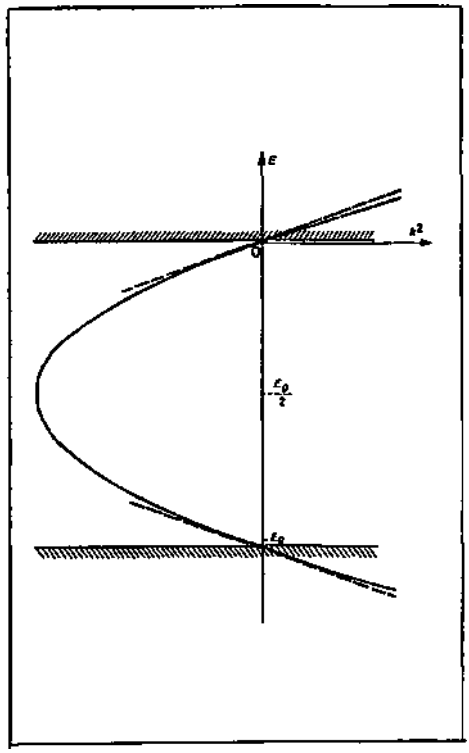

Fig. 3. Energy E vs. wavevector squared absolute value k^2 dependence by Kane model[18]. Broken line gives this dependence in effective mass approximation (for electrons and holes).

Matrix $[U]$ is diagonal matrix with nonzero elements $U_{ii} = E_c(z)$ for $i = 1, 2$, and $U_{ii}(z) = E_v(z)$ for $i = 3, 4, 5$ and 6, where $E_c(z)$ and $E_v(z)$ are energies of the bottom of conduction and top of valence band, respectively, along the SL.

Functions f_1 and f_2 in matrix $[f_j]$ are electron wavefunctions corresponding to opposite spins, f_3 and f_4 are heavy hole, f_5 and f_6 light hole wavefunctions. It is important to note that potential energy $-e\varphi(z)$ is included in $E_c(z)$ and $E_v(z)$, $\varphi(z)$ being the potential in the structure. The reference energy level is the bottom of conduction band in materijal having smaller energy gap (we label this one with »A«).

The matrix equation (15) represents a system of six equations, that can be separated into pairs of equations for electrons, light and heavy holes. Carrier motion in the $x - y$ plane is quasifree, and wavefunctions $f_1, \ldots, f_6$ can be written in a similar form as (3), with envelope wavefunctions $\eta_1, \ldots, \eta_6$. We shall continue solving the equation for electrons, consisting of two coupled equations in η-representation

$$-\frac{1}{2}\hbar^2 \frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{M^*}\frac{\mathrm{d}\eta_{1,2}}{\mathrm{d}z}\right] + U_{eff}\,\eta_{1,2} + \frac{\hbar^2}{4}(k_y \pm \mathrm{i}k_x)\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{M^*}\right]\eta_{2,1} = E\eta_{1,2}, \tag{16}$$

where $M^*(z)$ is generalized effective mass determined by

$$M^*(z) \equiv m_0^* \left(1 + \frac{E - E_c(z)}{E_g(z)}\right) = \begin{cases} m_{01}^* \left(1 + \dfrac{E + e\varphi}{E_{g1}}\right) & \text{in material } A, \\ m_{02}^* \left(1 + \dfrac{E + e\varphi - U_0}{E_{g2}}\right) & \text{in material } B. \end{cases} \tag{17}$$

Generalized effective mass is a function of electron energy and potential. Assuming a constant potential (e. g. equal to zero), $\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{M^*}\right]$ turns to zero everywhere except at layer boundaries, and (16) separates into two equations coupled only through boundary conditions[21]. However, if nonconstant $\varphi(z)$ exists, and it does in all iterations of selfconsistent procedure except the first one, equations (16) are coupled. After changing variables

$$\eta_1 = \eta_1^* \exp\left(\frac{\mathrm{i}\Theta}{2}\right), \quad \eta_2 = \eta_2^* \exp\left(-\frac{\mathrm{i}\Theta}{2}\right) \tag{18}$$

where Θ is the argument of $k_y - \mathrm{i}k_x$, (16) becomes

$$-\frac{1}{2}\hbar^2 \frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{M^*}\frac{\mathrm{d}\eta_{1,2}^*}{\mathrm{d}z}\right] + U_{eff}\,\eta_{1,2}^* + \frac{\hbar^2}{4}k_t \frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{M^*}\right]\eta_{2,1}^* = E\eta_{1,2}^*. \tag{19}$$

Equations (19) can simply be decoupled by introduction of new functions g_1 and g_2 being sum and difference of η_1^* and η_2^*. Now (19) can be be written as

$$-\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{M^*}\frac{\mathrm{d}g_{1,2}}{\mathrm{d}z}\right) + \left(U_{eff} \pm \frac{\hbar^2}{4}k_t \frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{M^*}\right]\right) g_{1,2} = E g_{1,2}. \tag{20}$$

In symmetric SL potential and effective mass are even functions, but the expression in bracket in (20) has no definite parity. In this case wavefunctions generated through fundamental boundary conditions (10) have no definite parity as well. Now, wavefunctions g_1 and g_2 can be written as

$$\begin{gathered} g_1 = A_1 F_1(z) + B_1 F_2(z) \quad F_1(0) = 1, \quad F_1'(0) = 0, \\ F_2(0) = 0 \quad \text{and} \quad F_2'(0) = 1 \end{gathered} \tag{21}$$

and similarly for g_2. We note again that $F_1(z)$ and $F_2(z)$ are neither even nor odd. These functions can be represented in the form

$$F_1(z) = y_0(z) + u_e(z) \quad \text{and} \quad F_2(z) = y_e(z) + u_0(z), \tag{22}$$

where $y_e(z)$ and $u_e(z)$ are even and $y_0(z)$ and $u_0(z)$ odd functions. Applying the periodic boundary conditions (5) we get the dispersion relation $E(\vec{k})$

$$\cos(k_z d) = \frac{y_e y_0' + y_0 y_e' - (u_0 u_e' + u_e u_0')}{y_0 y_e' - y_e y_0' + (u_e u_0' - u_0 u_e')}. \tag{23}$$

The same expression can be derived from the second Eq. of (20); however, if we observed nonsymmetric *SL* we would get two different dispersion relations. Disregard of coupling of opposite spin wavefunctions turns $u_0(z)$ and $u_e(z)$ identically to zero, and (23) turns to (11).

At the end of this section we shall derive the boundary conditions at the interface of two materials. Using the continuity of wavefunctions g_1 and g_2, after integration of (20) in the vicinity of interface, one concludes that expressions

$$\frac{1}{M^*}\left(\frac{dg_1}{dz} - \frac{k_t}{2} g_1\right) \quad \text{and} \quad \frac{1}{M^*}\left(\frac{dg_2}{dz} + \frac{k_t}{2} g_2\right), \tag{24}$$

have to be continuous at the boundary. For $k_t = 0$ (24) transforms to boundary conditions we used in Section 2a. At the time this article is written we are about to complete numerical calculations for doping *SL*, having linear potential in zero-order approximation, where spatial variation of effective mass has to be taken into account.

c) *Numerical aspects of self-consistent procedure*

The central problem in self-consistent procedure, from both theoretical and numerical point of view, certainly is solving of Schrödinger equation; Poissons equation should just be integrated twice (numerically). We gave two methods of solving the Schrödinger eq. in Section 2a. The first one, based on *harmonic method*, is still a subject of our research and we shall describe here the procedure based on the method of even and odd functions. We shall assume the parabolic approximation holds.

Recalling the theoretical considerations of Section 2a, particularly relations (9)—(12), the numerical procedure would consist of following steps:

— determination of $\eta_e(z)$ and $\eta_0(z)$ for a number of values of energy E and absolute value of the transversal component of wavevector, making use of standard methods for second-order differential equations integration (see Ref. 21);

— calculation of the right side of (11) for each value of E and k_t. If absolute value of the result exceeds one, this energy level lies in band gap, and in the opposite case it belongs to allowed band, and the corresponding value of k_z can be determined;

— constants A and B are to be determined from one of periodic boundary conditions (15) and normalizing condition (12).

Here we present numerical calculations for two *SL*:

a) with layer widths 4 nm for both GaAs and $Al_{0.3}Ga_{0.7}As$, and b) with GaAs and $Al_{0.2}Ga_{0.8}As$ layer widths 10 nm and 4 nm, respectively. We assumed rectan-

gular variation of potential energy, given numerically. $\eta_0(z)$ and $\eta_e(z)$ were determined by fourth order Runge-Kutta method*), taking into account the continuity of $\frac{1}{m}\frac{d\eta_{0,e}}{dz}$ at boundaries. Calculated values of widths of bands and gaps were compared with »exact« values. For rectangular potential energy and effective mass variation, wavefunctions η_0 and η_e can be represented through trigonometric or hyperbolic functions, and energy vs. wavevector dependence can be determined by solving the corresponding transcedent equations using standard methods (e. g. bisection). Band widths obtained in this way can be taken as *exact*. Relative error of band widths vs. k_t^* dependence is given in Fig. 4 (results for *SL* a) only are given; those for b) can be found in Ref. 22). Inspection of Fig. 4 immediately reveals that error decreases with decreasing step, and for step length of 0.025 nm it never exceeds 1%. Calculations using even smaller steps (not presented here) show that error does not decrease any more, but suprisingly enough increases, probably because of increasing number of points. Error is very weakly dependent on k_t, at least for smaller k_t-values (yet covering the whole area of interest for concentra-

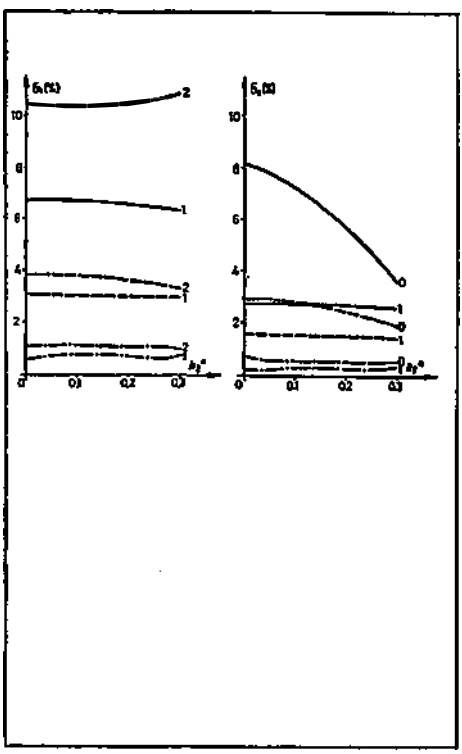

Fig. 4. Relative error made in bands (δ_b) and gaps (δ_g) widths determination vs. transversal component of wavevector $k_t^* = k_t/k_{t0}$. GaAs-$Al_{0.3}Ga_{0.7}As$ layer thicknesses are 4 nm both. Full line corresponds to 0.1 nm step, broken line to 0.05 nm, and dotted line to 0.025 nm step. Numbers 0, 1, 2 denote the zeroth, first and second band[22].

*) Fourth order Runge-Kutta methods for equations of type $y'' = f(x, y)$, are described e. g. in Ref. 21.

tion evaluation). It is also evident from Fig. 4 that the higher the energy, less exactly it is determined. This is not a too unfavourable feature of self-consistent procedure, since the number of carriers decreases with increasing band index.

Obviously, the proposed method gives good results for rectangular potential energy variation. There is no reason it would not give results of similar quality if this variation does not depart too much from rectangular. This really is the case in second, third, and higher iterations of self-consistent procedure, (where potential energy distribution is given numerically, and where numerical methods are the only useable) by usual doping levels.

3. *Some transport and optical properties*

a) *The Einstein relation*

As already noted in the introduction, transport properties of *SL* are quite different from the corresponding properties of homogeneous semiconductors. At the first place we think of great mobility enhancement. In this part we shall present our results concerning the Einstein relation.

Electrons (and holes) of *SL* subbands form two-dimensional electron (hole) gas in the planes of layers, with surface density given by

$$N_s = \int_0^d n(z)\,\mathrm{d}z = \sum_l N_l, \quad N_l = \int_0^d n_l(z)\,\mathrm{d}z. \tag{25}$$

Assuming the electric field in z-direction is much higher than in plane perpendicular to z, unique gradient of chemical potential W_F can be used for all energies in the subband we observe (for more details see Ref. 23). Now, the diffusion constant D_l and mobility μ_l ratio is given by[23]

$$\frac{D_l}{\mu_l} = \frac{kT}{e}\frac{N_l}{M_l}, \quad M_l \equiv \frac{d}{(2\pi)^3}\int_0^{\pi/d}\mathrm{d}k_z \int_{-\infty}^{+\infty}\!\!\int \frac{\eta_l}{(\eta_l - 1)^2}\,\mathrm{d}k_x\mathrm{d}k_y, \quad \eta_l \equiv \exp\left(\frac{E_l(\vec{k}) - E_F}{kT}\right). \tag{26}$$

The values of D_l and μ_l refer to the l-th subband, and are determined as average values of $D_l(k_z)$ and $\mu_l(k_z)$ (averaged over the k_z component of wavevector)[23]. If more than one subband is populated the Einstein relation reads[22]

$$D/\mu = \frac{kT\sum M_l}{e\sum N_l}, \tag{27}$$

where summation is to be performed over all populated subbands. Without the assumption on uniqueness of chemical potential one would get the ratio D_l/μ_l (and D/μ) depends on scattering mechanisms.

In doped SL the spatial variation of effective mass is absent (within the parabolic approximation), energy depends parabolically on k_x and k_y, therefore integration over k_x and k_y can be performed immediatelly, and the Einstein relation (26) reduces to a rather simple expression.

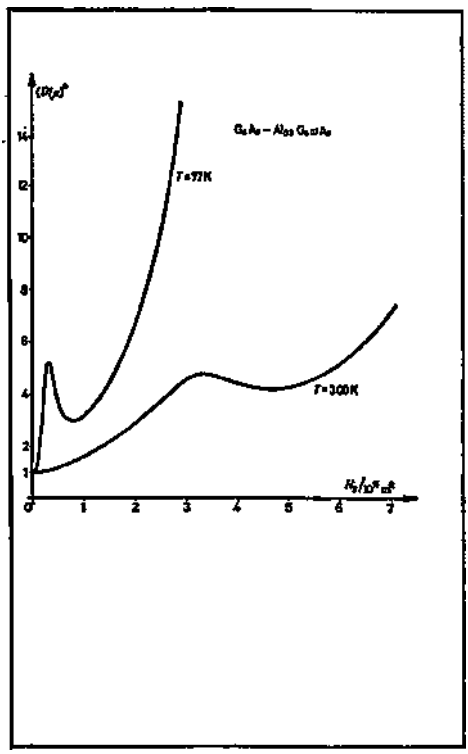

Fig. 5. The dependence of the ratio $(D/\mu)^* \equiv (D/\mu)\ (kT/e)$ versus the surface density N_s for GaAs-$Al_{0.3}Ga_{0.7}$As superlattice with layer thickness 6 nm and 1.5 nm, respectively. The rectangular distribution of the potential energy (and effective mass as well) was assumed[23].

Here we present numerical results for SL with GaAs and $Al_{0.3}Ga_{0.7}As$ layers 6 nm and 1.5 nm wide, respectively. Dependence of normalized ratio $\left(\frac{D}{\mu}\right)^* = \frac{D/\mu}{kT/e}$ on surface electron density N_S, at temperatures $T = 300$ K and $T = 77$ K is given in Fig. 5. For low values of N_s (it decrcases with decreasing temperature) D/μ approaches kT/e, indicating that the Einstein relation has the same form as in nondegenerate three-dimensional electron gas. With increasing N_s, $(D/\mu)^*$ goes through two local extrema — a maximum and a minimum, and then increases permanently. This behaviour, that we have not met in the literature unitil now, can probably be explained by peculiarities of SL band structure.

b) *Optical properties*

We shall briefly discuss some properties of dipole matrix elements for transitions between conduction and valence subbands. Taking account of variable value of momentum matrix element and dielectric constant in constituent materials of *SL*, we derived the expression for envelope matrix elements (ratio of matrix element in *SL* and that in GaAs)[24]. Their values in *rectangular SL* were calculated analitically, and, as an illustration, we give here the dependence of $|M_{env}|^2$ on k_z for GaAs-$Al_{0.4}Ga_{0.6}As$ *SL* with laver widths 10 nm and 4 nm. Matrix elements for transitions between subbands with same indices are given in Fig. 6a ('denotes light holes), and those for different indices in Fig. 6b. Broken lines show the effect of neglect of spatial variation of momentum matrix eement in *SL* (for a few cases only).

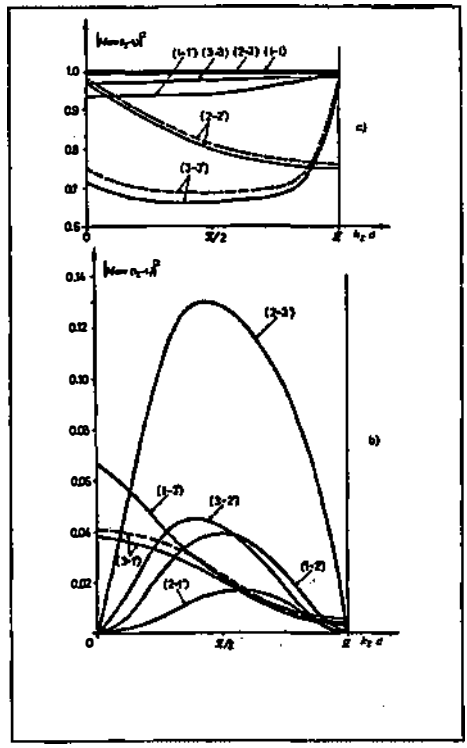

Fig. 6. Square moduls of envelope matrix elements of interband transitions for GaAs-$Al_xGa_{1-x}As$ superlattice thicknesses of layer 10 nm and 4 nm, respectively. In Fig. 6a are given matrix elements for transitions between mizones with same indexes, and in Fig. 6b with different index ($x = 0.4$).

Evidently, error is not too great, at least in these examples; however, it can sometimes get much greater values, approaching 100%, but these elements have very small values anyway, so it is not too important. Also, one can see that no pair of indices turns the matrix element identically to zero, unlike the case of opposite parity indices in quantum wells, and also that elements with different indices have smaller values than those with same indices, same as in quantum wells.

Having determined the values of matrix elements and the band structure, one can proceed to find the dependence of light absorption or gain on frequency[24]. Assuming the absorption process does not change appreciably the equilibrium in undoped or weakly doped *SL*, its dependence on frequency is to be determined from

$$\alpha_{t_1,t_2}\,\omega \sim \int |M_{env(t_1-t_2)}|^2\,\delta\,[E_{c,t_1}(\vec{k}) - E_{v,t_2}(\vec{k}) - \hbar\omega]\,\mathrm{d}^3\vec{k}. \tag{28}$$

Numerical results indicate that, as we have expected, the standard tight-binding method and neglect of M_{env} dependence on $\vec{k}$ give good results for lower values of quantum energy, whereas one must calculate (28) numerically to get the exact apsorption at higer energies.

If there exist nonnegligible concentrations of electrons and holes in *SL* (e. g. in lasers), assuming the carrier distribution within each band is equilibrium Fermi-Dirac, gain in this structure can be found from an expression same as (28), except for a factor $(f_e + f_h - 1)$ inside the integral, where f_e and f_h are distribution functions for electrons and holes, respectively.

4. *Conclusion*

This article presents a review of results of our investigation of semiconductor *SL*. Some of results are from other articles, and are presented in a review form, while Sections 2b, 2c and 3 contain results presented here for the first time.

The first section is devoted to the self-consistent procedure for finding potential and other relevant parameters. Proposed methods (method of even and odd functions, *harmonic method*) take account of the fact that constituent materials of *SL* have different carrier effective masses, the fact that complicates the procedure, particularly for Schrödinger equation. However, taking this into account, one can get more adequate picture of processes in *SL*.

A very important and interesting problem, according to our opinion, is the influence of nonparabolicity of dispersion relation in constituent materials of *SL*. Starting from a general form of Schrödinger eq. (15) that describes electrons, light and heavy holes, we derived the dispersion relation for electrons in *SL* (23), and showed that is spin-independent in symmetric *SL*. However, in nonsymmetric *SL* two different relations exist. Besides, we proved that, if nonconstant potential exists in the structure, effective mass varies inside each material, the fact not noticed up to now.

The numerical procedure for solving the Schrödinger eq. is proposed in Section 2c. An analysis of error in finding subband widths (for rectangular potential distribution) indicates that error will not exceed 1% for carefully chosen step. This leads to conclusion that this method is efficient enough in cases where potential energy distribution does not depart too much from rectangular (this happens in self-consistent procedure).

We have also studied some transport and optical properties of *SL*. Among transport properties it was the Einstein relation we investigated and derived some general relations. The dependence of diffusion constant-mobility ratio on surface density of carriers has an unusual form with two local extrema.

Some optical properties: (envelope) transition matrix elements, absorption, and gain coefficients were also studied: we found that these important parameters can be determined more exactly if one takes account of spatial variation of effective mass and momentum matrix element.

Finally we shall give a list of problems that would, according to our opinion, be interesting to work on:

— to analyse the self-consistent problem, starting with microscopic potential in each material. It may be that one can derive some criterium that would justify the application of effective mass approximation, and find error made by using it;

— to do the numerical realization of harmonic method. The central problem here is to find eigenvalues of an infinite full matrix;

— to complete the self-consistent procedure, assuming the dispersion relations of *SL* constituent materials to be given by Kane expression;

— to analyse the anomalous mobility enhancement, making use of the band structure we have here, and to compare results of this analysis with existing results for the Einstein relation;

— to calculate transition matrix elements for *SL* with arbitrary potential distribution, and possibly to tailor the *SL* to get some desired optical parameters, e. g. gain-frequency dependence;

— to make a carefull study of properties of half-infinite *SL*. This structure was not a subject of the present atricle, but was investigated in Ref. 25. One should also point out their possible advantages (in the applicative sence) over »real« *SL*;

— to investigate the possibility of application of *SL* as a »new« material, i. e. to find the range of change of global *new* parameters that can be obtained by varying layer widths, and material composition. This happens to be the central problem in the applicative sence.

Acknowledgments

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PERIODIČNE POLUPROVODNIČKE SUPER-REŠETKE — NEKE ELEKTRIČNE, TRANSPORTNE I OPTIČKE OSOBINE

DIMITRIJE TJAPKIN[a], VITOMIR MILANOVIĆ[a,b] i ZORAN IKONIĆ[a]

[a] *Elektrotehnički fakultet, Bulevar Revolucije* 73, 11000 *Beograd, Jugoslavija*

[b] *Viša PTT škola, Zdravka Čelara* 16, 11000 *Beograd, Jugoslavija*

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U radu smo izložili važnije rezultate naših istraživanja iz oblasti poluprovodničke super-rešetke. Posebna pažnja posvećena je uticaju prostorne zavisnosti prividne mase na energetski spektar strukture. U slučaju postojanja neparaboličnosti zona u polaznim materijama izveli smo disperzionu relaciju i pokazali da je ona jedinstvena za obe orijentacije spina. U okviru transportnih i optičkih osobina analizirani su: Ajnštajnova relacija, anvelopni matrični elementi, koeficijent apsorpcije i pojačanja. Izložena teorija ilustrovana je numeričkim rezultatima na GaAs-Al_xGa_{1-x}As super-rešetci.