ELECTRONIC PROPERTIES OF SEMICONDUCTOR SUPERLATTICES

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KEY WORDS:superlattice, band structure, absorption, electronic properties, semiconductors

ABSTRACT: The paper presents the contemporary researches in the field of semiconductor superlattice, including the most important results of our investigations. The methods for determining the band structure in the envelope function approximation (parabolic and nonparabolic models) are presented, as well as a series of effects induced by position dependence of the effective mass. Furthermore, the first order optical process (single photon absorption) is analysed. Quasi-two-dimensionality of these structures causes the step-like dependence of absorption vs. photon energy, with pronounced exciton peaks, visible even at room temperatures. Finally, the most important potential of these structures are presented.

ELEKTRONSKE OSOBINE POLUPROVODNIČKE SUPER-REŠETKE

KLJUČNE REČI: super-rešetka, zonska struktura, apsorpcija, elektronske osobine, poluprovodnici

SADRŽAJ: U radu su izložena savremena istraživanja iz oblasti poluprovodničke super-rešetke, uključujući i najvažnije rezultate do kojih smo mi došli. U aproksimaciji anvelopnih talasnih funkcija (parabolični i neparabolični model) određivana je zonska struktura, s tim da je poseban akcenat dat na efekte koji su uslovljeni prostornom zavisnošću prividne mase. Dalje, analizirana je pojava apsorpcije; kvazi-dvodimenzionalnost ovih struktura uzrok je stepenastoj zavisnosti apsorpcije od energije fotona, sa izrazitim eksitonskim pikovima, vidljivim čak i na sobnoj temperaturi. Na kraju su izložene neke važne mogućnosti primene ovih struktura.

1. INTRODUCTION

The development of special technologies (e. g. molecular beam epitaxy, metalo-organic chemical vapor deposition[1]) makes possible the realization of very thin semiconductor layers (in the range from few to tens of nanometers), shorter than the electron mean free path but longer than lattice constant. The article[2]: "Superlattice and Negative Differential Conductivity in Semiconductors" by L. Esaki and R. Tsu (1970) is mainly taken to be the first one in this field. The so-called compositional superlattice (SL), has been proposed here. In 1973 such SL, composed of thin (in nm range) *GaAs* and $Al_xGa_{1-x}As$ layers was grown by molecular beam epitaxy by L. L. Chang et al.[3]. Up to now this SL is the most extensively studied, both theoretically and experimentally. The other type of SL is that proposed in 1972 by G. H. Döhler[4,5] with periodic potential obtained by alternating doping of otherwise homogeneous semiconductor with donors *(n)* and acceptors *(p)*, possibly with intrinsic *(i)* layers separating the doped ones (doping or *nipi* SL). The first SL of this type was grown in 1981[6].

For all types of SL the common feature is that its periodic potential is superposed on the local potential in host materials. The SL's potential period is in general considerably greater than the local potential period. This superposed potential induces the splitting of the conduction and the valence bands into the set of correspond minizones. The minizones spectrum has an essentially different structure than the zone spectrum of host materials, which causes that the SL's properties are entirely defferent from the correspond properties of bulk materials. The obvious example of this is the case of the *GaAs* SL, the thickness of *p*- and *n*- regions being 40 nm[7]. In this structure the recombination lifetime is about 10^{13} times greater than in bulk *GaAs*. If the layer thicknesses were decreased twice, the above ratio is about 10^3. This SL properties makes it one of the most propulsive structure nowadays, because by the simple change of parameters (the layer thickness, doping level and composition) we can tailor the desired characteristics.

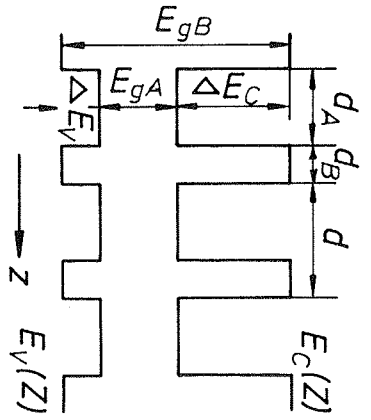

Fig. 1 *The idealized (rectangular) energy diagram of the I type of compositional SL*

Figure 1 shows the idealised energy diagrams of compositional SL. Nowdays in literature we distinguish the compositional SL of I type, with sum of discontinuities of the conduction ΔE_c and the valence band ΔE_v is equal to the difference of the energy gaps ΔE_g and SL of II type with $(\Delta E_c - \Delta E_v) = \Delta E_g$. The most frequent type of the I type is *GaAs-Al$_x$Ga$_{1-x}$As*, SL, while *InAs-GaSb* SL is commonly mentioned as an example of II type SL. In the doping SL the potential energy extrema are dislocated for a half period and thereby the maxima of the carriers concentrations ("indirect energy gap in real space" as pointed in[7]).

If barrier material thickness is quite large, then the interaction between wells vanishes. Such structures are called multiquantum wells (MQW) and the interest for their study has suddenly enhanced lately.

2. SUPERLATTICE BAND STRUCTURE

Due to the existence of the local and SL potentials, strictly taken, the band structure of the SL is determined in a quite complex way. However, in a majority of cases the wavefunctions of carriers can be represented as a linear combination of the local (Bloch) and the envelope functions (envelope function approximation - EFA), and the band structure can be determined by solving a one-dimensional Schrodinger equation.

First, let us suppose that all carriers are in Γ-minimum, as well as that the surfaces of constant energy are spheres. Since the SL (compositional) are made of two materials, Schrodinger's equation, due to the existence of the position dependence of effective mass cannot have the usual form (due to the probability current conservation). The form of the corresponding Hamiltonian was the topic of a large number of papers[8,9]. However, we can use the commonly accepted Schrodinger equation for envelope wavefunctions Ψ, as qiven by the expression (z-axis are asumed as SL axis):

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*}\frac{d\psi}{dz}\right)+\left\{U(z)+\frac{\hbar^2 k_t^2}{2m^*}\right\}\psi = E\psi \quad (1)$$

where E is the total electron (electrons assumed here) energy, $U(z)$ - the potential energy including the discontinuity U_o on interfaces, as well as the space charge potential, while k_t is the transversal wave vector. Expression in brackets (...) is the effective potential energy U_{eff}[10]. Fig. 2 shows $U_{eff}(k^2_t)$ - dependence for *GaAs-Al$_x$Ga$_{1-x}$As* SL. Since the effective mass m^*_1 in *GaAs* is smaller than m^*_2 in *Al$_x$Ga$_{1-x}$As* for $k_t < k_{to}$[11] ($k^2_{to} = 2U_o m^*_1 m^*_2/(\hbar^2(m^*_2 - m^*_1))$ the wells exist in *GaAs* layers and barriers in *Al$_x$Ga$_{1-x}$As* layers. If $k_t = k_{to}$, U_{eff} does not possess the spatial dependence, but even then, as was shown in the most general case by harmonic method[12], the energy spectrum is bandlike. In the case $k_t > k_{to}$, the distribution of wells and barriers is opposite. Thereform it ensues clearly that the dependence $E(k^2_t)$ is distinctly nonlinear unlike the case of the position independent effective mass, where E is proportional to k^2_t. The expression for the concentration in the i-th minzone takes considerably complicated form[10]:

$$n_i(z) = \frac{d}{\pi^2}\int_0^{\pi/d} dk_z \int_0^{+\infty} \frac{\left\{\psi^i_{k_z k_t}(z)\right\}^2 k_t dk_t}{\exp(\eta)+1} \quad (2)$$

$$\eta \equiv (E_i(k_z,k^2_t) - E_F)/kT \quad (3)$$

In (2) $\psi^i_{k_z,k_t}$ are the complex wavefunctions (explicitly dependent on k_t) normalized to unity within the SL period.

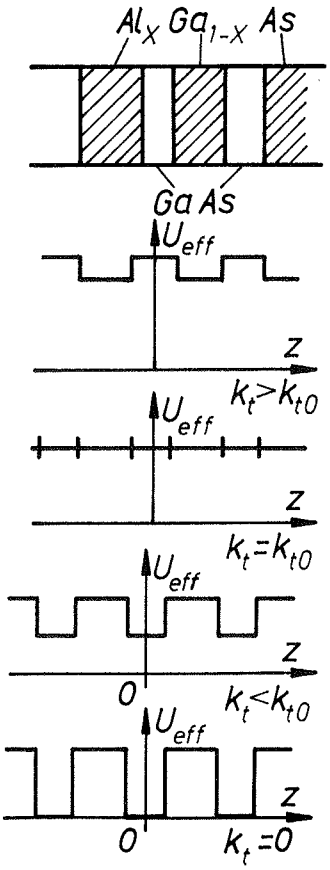

Fig. 2 *The effective potential energy of the GaAs-Al$_k$Ga$_{1-x}$As SL for various values of the transversal wave vector k_t.*

The effects of $E(k_t)$ nonparabolicity are more pronounced in the effective-mass superlattice (EMSL), which can be considered as a new type of compositional SL, with positional dependence of the potential induced only by the effective mass positional dependence. The constituent semiconductors are chosen so that the conduction (or valence) band discontinuity is missing. A number of candidate semiconductors for EMSL are given in[13]. Applying the usual Bloch boundary conditions to eqn (1) in this case, we may derive the $E(k_z, k^2_t)$ dependence for EMSL, and it is given in[14].

For numerical illustration, in Fig. 3 we give the $E(E_{t1})$ band diagram for a hypothetical, but roughly realistic EMSL, with $m_1 = 2m_2 = 0.2m_0$ (m_0 is the free-electron mass), with layers each 10 nm thick. What can immedi-

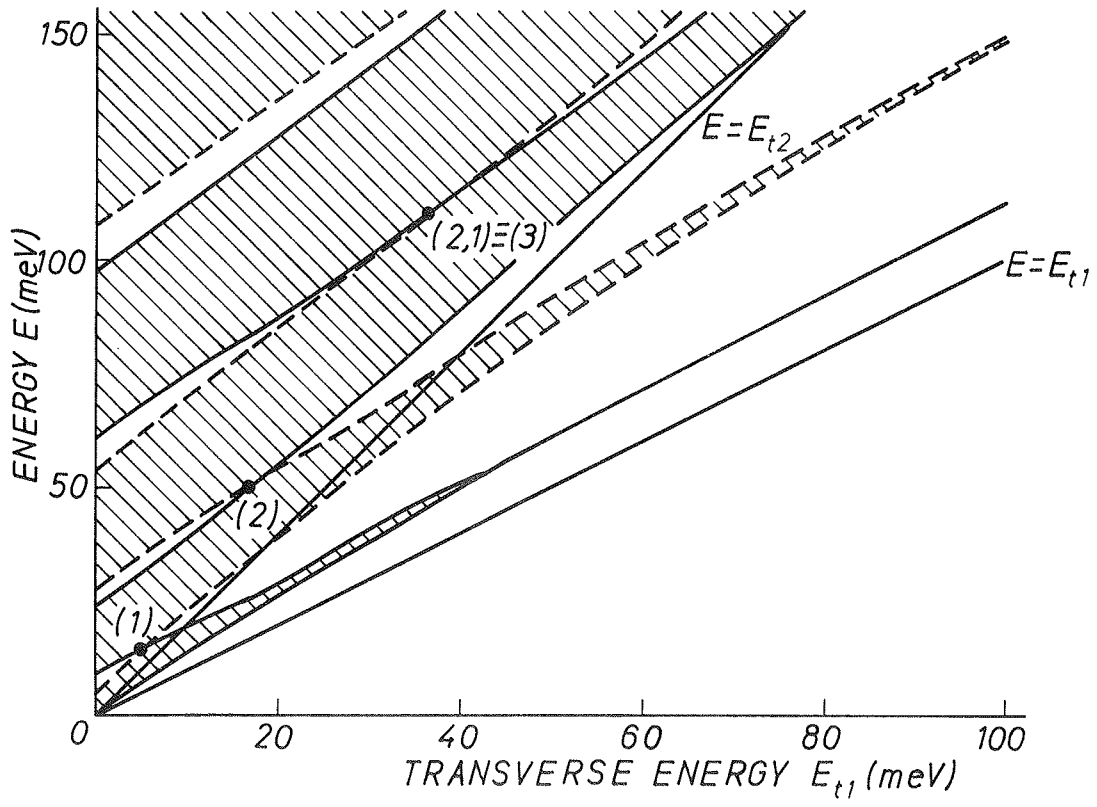

Fig. 3 *Energy band-diagram for an EMSL with $d_1 = d_2 = 10$ nm and $m_1 = 2m_2 = 0.2m_0$. The crosshatched areas denote the allowed bands. The solid (dashed) band-edge lines corespond to even (odd) wave functions. Points of line intersection are labeled with (l,n) where l and n are integers or with (s) the integer, too. Note that points (2,1) and (3) coincide ($E_{tl} = \pi^2\hbar^2/h^2_{t}/m_l$).*

ately be seen from Fig. 3 is that the zero energy gap conditions (ZEG) in the EMSL occur for much lower energies E and E_{t1} than is the case in conventional (e.g., $GaAs$-$Al_xGa_{1-x}As$) superlattices, where ZEG points may be calculated to be in the eV range and are therefore hardly of any significance for most of macroscopic properties. In the EMSL ZEG points fall in a thermically populated energy range, and thus do influence the EMSL properties, e.g., carrier concentration, absorption, etc. Excluding the band-edge discontinuities, $E(k^2_t)$ dependence in an EMSL is pronouncedly nonlinear (Fig. 3).

Furthermore, a very interesting point is the inversion of parity of band-edge wave function when crossing ZEG points; e.g., for small k_t top of thr first miniband possesses the odd wave functions, and not the even one, as does its bottom. Only after crossing thr ZEG's point does the wave function parity at both bottom and top become the same (even for odd minibands and vice versa, for high enough transverse wave vector k_t). This fact may be important when evaluating optical transition matrix elements because their values may turn from finite ones to zero for small change of k_t.

We also note that no ZEG's may appear for energies $E < E_{t2}$. With increasing k_t the effective barriers (layers II) get higher, which makes the allowed bands progressively narrower and eventually nearly discrete (this happens at realistic values of E_{t1}, a couple of kT at $T = 300$ K).

In conduction band structure of host materials (such as: $GaAs$, $Al_xGa_{1-x}As$...) besides the direct Γ minimum, there are a indirect X and L minima. For smaller $x(x \leq 0.3)$ the indirect minima are above the direct minimum and are weakly populated by carriers. At the increase of x, the indirect minima approach the central minima, and at further increase of x they come below it. In[15] it was shown that electrons in each of these minima create their independent minizone like spectra. Fig. 4 displays the dependence of the relative population of Γ minimum vs. mole fraction x, where from it is easily seen that for larger x and higher temperature almost all electrons are at indirect minima[16].

A very interesting structure is a semi-infinite SL, where besides the minizonal there exists the discrete spectrum, too. The number of discrete levels could be regulated by a simple change of thickness of materials[17].

Since a majority of meterials used for SL belong to III-V compounds in a more accurate analysis of the band structure, the nonparabolic effect (Kane's type) is to be taken into account. G. Bastard modified Kane's model in[18], where the Γ_7 spin-orbit split band was disregarded as well as (except for heavy holes) the coupling to other bands and free electron dispersion part.

Developing this model further, we have shown in[19] that the Schrodinger equation could be written, only for electrons (analogously to (1)):

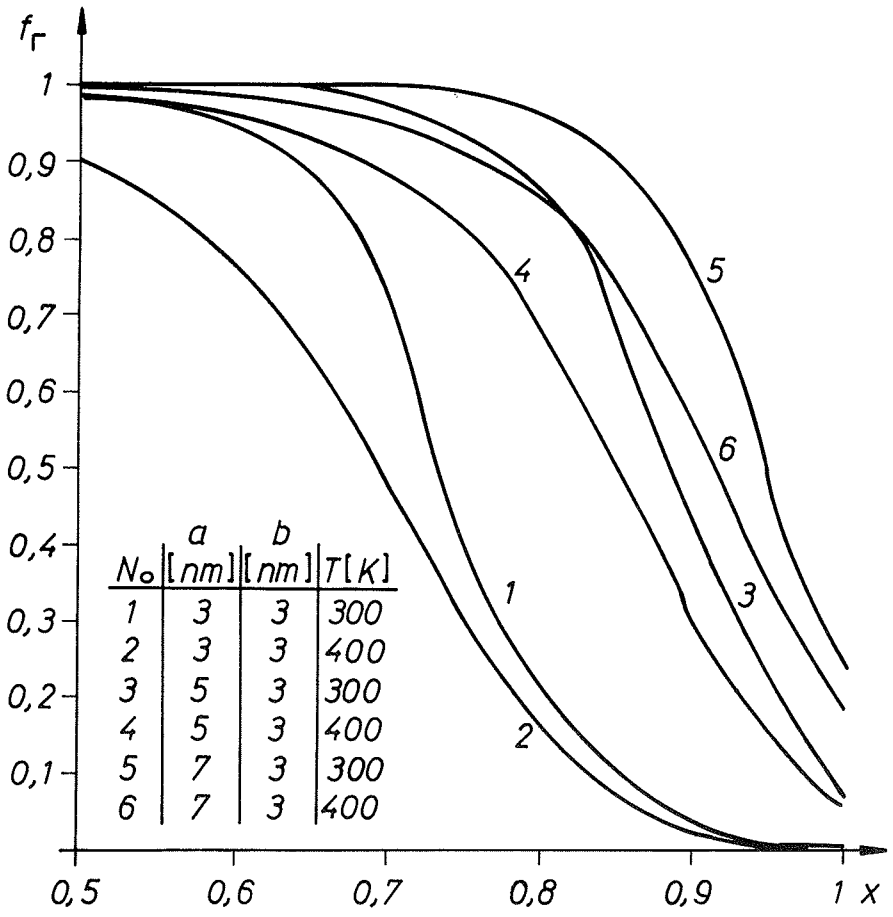

Fig. 4 *The relative population of Γ minimum vs. the mole fraction x for GaAs-$Al_xGa_{1-x}As$ SL, (layer thicknesses are 3 nm, average electron concentraation is $3.10^{17} cm^{-3}$)[16].*

$$-\frac{\hbar^2}{2}\left(\frac{d}{dz}\frac{1}{M^*}\frac{d\psi_{1,2}}{dz}\right)+\left(U_{eff}\pm\frac{\hbar^2}{4}k_t\frac{d}{dz}\left(\frac{1}{M^*}\right)\right)\psi_{1,2}$$

$$=E\psi_{1,2} \qquad (4)$$

where $\psi_{1,2}$ are the envelope wavefunctions of electrons corresponding to the "up" and "down" spin, while M^* *is the extended effective mass defined in*[19] as $m_o^*(z)(1+(E-E_c(z))/Eg(z))$ (m^*_o is the band edge effective mass). The analysis of (4) shows that in non-symmetric SL (e.g. saw-tooth SL) we have for $k_t \neq 0$ two different energy spectra, while in symmetrical SL the energy spectrum is unique. Our calculations for *GaAs* doping SL show that the agreement of the parabolic and the nonparabolic models is better for lower minizones; for higher ones the deviation may reach even 10%.

The analysis of the SL band structure, taking into account the local potential is a very complicated problem, whish has been treated recently in several papers. In[20] it was shown by the application of the LCAO method that the EFA is a good approximation in *GaAs-$Al_xGa_{1-x}As$* SL, while for the *GaSb-InAs* SL this is not the case. The paper[21] provides the calculation of the band structure of the saw-tooth SL by the pseudopotential method. For this SL (period of 14 nm) the bottoms of first three minizones are: 140 meV, 270 meV and 310 meV. Our results[22] starting from (1) are: 125 meV, 222 meV and 207 meV which is a very good agreement. As far as the holes are concerned the agreement is somewhat less favourable.

3. OPTICAL PROPERTIES OF SUPERLATTICE

In the SL and in quantum wells, apart from interband (the transitions between the *i*-th minizone of valence band and the *j*-th minizone of conduction band), the interband transitions are also allowed (between the minizones within either of the bands). The later ones do not appear in bulk seniconductors. We can show that the absorption coefficient for the interband transitions is given by the expression[23]:

$$\alpha_{ij}=\frac{e^2|P_1|^2}{2(2\pi)^2\varepsilon_o c\bar{n}m_o^2\omega}\int|M_{ij}|^2\delta$$

$$\left(E_{ei}(\vec{k})+E_{nj}(\vec{k})+E_{g1}-\hbar\omega\right)\cdot FD\cdot d^3\vec{k}, \qquad (5)$$

where P_1 is Kane's matrix element in *GaAs*, $\bar{n}$ the average refraction index, $\hbar\omega$ the photon energy, while E_{ei} and E_{hj} are energies of electrons and holes, measured from the extrema of the respective bands. *FD* factor is equal to the difference of Fermi- Dirac distribu-

tion E_{ei} and E_{hj}: in case of interband absorption it is very near to unity. The envelope matrix element M_{ij} is given by:

$$M_{ij} = \int_0^d \psi_i^* (z)\, \psi_j (z)\, P^* (z)\, dz, \qquad (6)$$

where $P^*(z)$ is the ratio of Kane's matrix element at point z and P_1. This dependence is very weak $(0.85 \leq P^* \leq 1)$. In the case of intraband transition eqn (5) modifies: $|P_1|/\hbar^2$ being substituted by unity. The argument of the δ-function is now $(E_{ei} - E_{ej} - \hbar\omega)$, while the envelope matrix element is:

$$M_{ij} = \int_0^d \psi_i^* (z)\, \frac{d\psi_j (z)}{dz} \cdot dz. \qquad (7)$$

For the intraband transitions the FD factor is to be taken into account, and in a majority of cases it amounts to $f_{FD}(E_{ej})$. In symmetric SL the wavefunctions have the definite parity only at the minizone boundaries, and for $k_z \in (0, \pi/d)$ there are no selectrion rules. In $GaAs$-$Al_xGa_{1-x}As$ SL, the matrix elements corresponding to the interband transitions $(i = j)$ are near to unity, especially for the electron-heavy hole transitions[32]. In the case $i \neq j$, if i and j are of different parity, the matrix elements are zero at the minizone edge, while their maximum value is smaller by an order of magnitude than in the cese $i = j$. In the doping SL, interband matrix elements are very small, so that it is possible to obtain the recombination lifetime of several tens of minutes[6]. In nonsymmetric SL there are no selection rules. The dependence $\alpha(\omega) \cdot \omega$ vs. ω has a quasi step-like character, with the pronounced jumps of absorption with finite widths, equal to the sum of widths of the corresponding minizones. The experimental dependences have very pronounced peaks of absorption. This is the consequence of the existence of excitons, which are more bounded in SL than in bulk, so that they can be observed even at room temperatures.

We have performed a calculation of envelope matrix elements for an $Al_xGa_{1-x}As$ sowtooth SL (interband transitions), and analysed their dependence on Q_e, the ratio of the conduction band discontinuity ΔE_c and the band gap difference ΔE_g at the $GaAs/Al_xGa_{1-x}As$ interface.

By comparing the envelope wave functions obtained via the effective-mass model[22] and the pseudopotential method[21], we found the agreement is approximately as good for energies, so we believe that the former may be fairly reliably used in calculation of optical-transition matrix elements. The dependence of $|M_{c,v}|^2$ for $k = 0$ on Q_e is given in Fig. 5 for $(e\text{-}hh)$ transitions. For higher values of Q_e ($\approx$ 0.85) the transition matrix elements between minizones with the same indices are nearly equal to unity, because electron hole wave functions have very similar forms. With decreasing Q_e these matrix elements also decrease, e. g., $|M_{c,v}|^2 = 0.18$ $(Q_e = 0.6)$ for the (3-3) transition. In case of transitions between minizones having different indices, however, the opposite is true: $|M_{c,v}|^2$ increase with decreasing Q_e. The transition matrix element between the third electron and

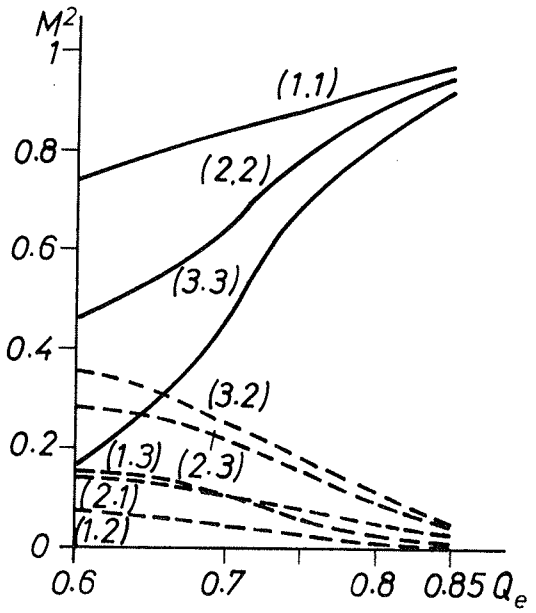

Fig. 5 *The electron-heavy-hole transition envelope-matrix elements at k=0 for sawtooth superlattice with period d=14 nm and maximal Al mole fraction $x_{max} = 0.3$. The first number in parentheses is the electron minizone index, and the second is the hole minizone index.*

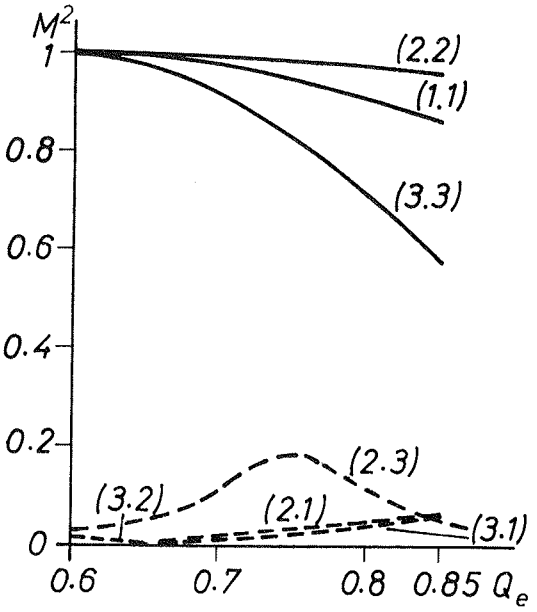

Fig. 6 *The electron-light-hole transition envelope-matrix elements at k=0 for sawtooth superlattice with parameters as in Fig. 5.*

the first heavy-hole minizone is considerably less than the others ($|M_{c,v}|^2 \leq 0.04$ for all Q_e).

For the electron-light-hole transitions (Fig. 6), the matrix elements connecting minizones of the same index increase with decreasing Q_e, and for $Q_e \leq 0.65$ they are very close to unity, while those for minizones having different indices follow no simple rules. Certainly, because of the lack of inversion symmetry in sawtooth superlattices, there are no parity- forbidden transitions here, as can be seen from Figs. 5 and 6.

Due to the effective-masses position dependence, the wave functions and envelope-matrix elements depend on the transverse wave vector k_t (of electron and hole to be generated by photon absorption). However, for $k_t << k_{to}$ corresponding to photon energies not too far from the absorption threshold, this dependence is only slight, e. g., for (2,2) *e-hh* transition ($x_{max} = 0.4$, $d = 14$ nm) the matrix element is constant within 2% for a photon energy range of 50 meV. The matrix elements vary as k_z varies over the first Brillouin minizone as well. This dependence is very pronounced only for transitions between levels with different indices (matrix elements may change up to 2 orders of magnitude in such cases). Furthermore, we note that the matrix elements for dominant transitions - (1,1), (2,2), etc. in sawtooth superlattices are rather sensitive functions of Q_e contrary to the case of the conventional "rectangular" superlattices.

4. APPLICATIONS OF SUPERLATTICES

The most important property for the SL appliccation is the enormous increase of mobility, on the basis of which FET's*) were constructed[24]. All these devices are similar: under the gate electrode there is a $Al_xGa_{1-x}As$ layer doped by donors. Next to it there is an undoped *GaAs* layer. The mobility of the electrons in *GaAs* layer, is very large, due to witch these transitions are devices with very small switching time (of order *ps*) and very large bandwidth (of order *GHz*[24]). These performances provide to use HEMT's (and other SL based transistors) as logical circuits in superfast computers of the fifth generation and in microwave technics, too. Let us define ΔF as product of the dissipation of energy ΔW and switching time Δt[25]. ΔF should be the fundamental parametar indicating the overall performance of the device for switching logical applications. As can be seen from Fig. 7 in present realization only Josephson Fluxon devices have better characteristics than HEMT's but only with respect to ΔW (naturally, the smallest value ΔF which can be reached is bounded by uncertainty relation and it is equal to Plank's constant h).

The SL based lasers, due to the two dimensionality of carriers have considerably smaller temperature sensitivity of the threshold current and of the gain than the conventional lasers. Apart from that the gain in lasers, for the same inversion is independent of the temperature and pumping intensity.

The electronic modulator of light is being intensively worked on, based on the quantum well in the electronic field; in order to get higher absorption a multi quantum well is used.

*)such as: HEMT (High Electron Mobility Transistor), TEGFET (Two Dimensional (FET) and MODFET (Modulation Doped (FET).

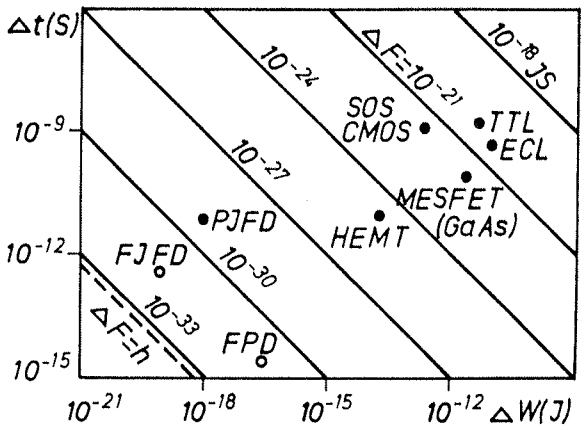

Fig. 7 *The switching time and dissipation of energy for different logical devices. PJFD means present Josephson Flixon devices, FJFD future JFD and FPD-future photon devices (from (25)).*

The possibility of a SL was also analysed as a structure with the negative differential conductivity, which has been experimentally observed recently, and opens new possibilities for SL applications.

5. CONCLUSION

In the introductory part of the paper, apart from the historical survey, the basic property of the SL was pointed out as a new material, where the desired characteristics can be tailored by a simple change of SL parameters. In the part of the paper devoted to the SL band structure, the emphasize was laid on the influence of the spatial dependence of the effective mass. This dependence implies a series of new properties of the energy spectrum, such as: the pronounced nonparabolicity energy vs square of transversal wave vector k_t dependence,explicit envelope wavefunctions vs. k_t dependence. These effects require considerably more complicated expression for carrier concentration (3). If the nonparabolicity in host materials is assumed two branches of spectrum appear in nonsymmetric SL, corresponding to various orientation of the spin. Out of optical properties single photon absorption (interband and intraband transitions) was analysed. As far as, SL applications are concerned we stressed particularly the transistors with very high electron mobility, which were already realized in laboratories and which will their place especially in superfast computers.

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