

## SEMICONDUCTOR SUPERLATTICE

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### *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 an envelope function approximation (parabolic and nonparabolic models) were presented, as well as a series of effects provoked by position dependence of the effective mass. Among transport processes the enormous increase of mobility in a modulation doped superlattice was shown, as well as the anomalous behaviour of the Einstein relation in them. Furthermore, the first order optical process (single photon absorption) is presented. Quasi-twodimensionality of these structures causes the step-like dependence of absorption vs. photon energy, with pronounced excitation peaks, visible even at room temperatures. The influence of electric field on quantum well light absorption is also discussed. Finally, the most important potential applications of these structures are presented.*

### 1. INTRODUCTION

The development of special technology, (e.g. molecular beam epitaxy, metallo-organic chemical vapor deposition<sup>1)</sup>) makes possible the realization of very thin semiconductor layers (in the range from few to tens nanometers), shorter than the electron mean free path but longer than lattice spacing. The article<sup>2)</sup>: "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  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  layers was grown by molecular beam epitaxy by L.L. Chang et al<sup>3)</sup>. 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<sup>4, 5)</sup> 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.<sup>6)</sup>

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 different 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<sup>7)</sup>. In this structure the recombination lifetime is about  $10^{13}$  times greater than in bulk GaAs. If the layer thicknesses were decreased by two times, 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.

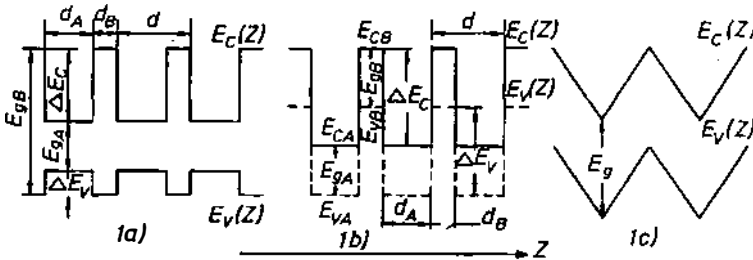


Fig. 1.

The idealized energy diagrams of the I type of compositional SL (Fig. 1a), II type (Fig. 1b) and the doping SL (Fig. 1c).

Figure 1 shows the idealised energy diagrams of compositional and doping SL. Nowadays in literature we distinguish the compositional SL of I type, with sum of discontinuities of the conduction  $\Delta E_C$  and the valence band  $\Delta E_V$  is equal to the difference of the energy gaps  $\Delta E_g$  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- $\text{Al}_x\text{Ga}_{1-x}\text{As}$  SL, while InAs-GaSb SL is most frequent mentioned as an example of II type SL. In the doping SL (Fig 1c) 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<sup>7)</sup>).

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.

In 1980 H. Sakaki<sup>8, 9)</sup> proposed a new structure: quantum wire, whose two dimensions are very small. The carriers in this structure form quasi-one-dimensional gas whose mobility, according to the predictions, is very large.

The paper<sup>10)</sup> considered the semiconductor tiny balls of small dimensions condensed in a glassy matrix. The carriers in a such structure were confined in a three-dimensional quantum well.

Esaki et al.<sup>11)</sup> proposed the introduction of a third constituent such as AlSb in the InAs–GaSb system. Such a triple-constituent system leads to a new concept of man-made polytype SL, which offers an additional degree of freedom.

## 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.

Primarily, let us suppose that all carriers are in  $\Gamma$ -minimum, as well as, that the surfaces of constant energy are spheres. Since the SL (certainly compositional) are made of two materials, Schrodinger's equation, due to the existence of the position dependence of effective mass cannot have the orthodox form (due to the probability current conservation). The form of the corresponding Hamiltonian, was the topic of a large number of paper<sup>12, 13)</sup>. However, we can consider that the recently accepted Schrodinger equation for envelope wavefunctions  $\psi$  is given by the expression (z-axis are assumed 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,  $U(z)$ —potential energy consisted the discontinuity  $U_0$  on interfaces, as well as the space charge potential, while  $k_t$  is the transversal wave vector. Expression in brackets [...] was called the effective potential energy  $U_{\text{eff}}$ <sup>14)</sup>. Fig. 2a shows  $U_{\text{eff}}(k_t^2)$  – dependence for GaAs– $\text{Al}_x\text{Ga}_{1-x}\text{As}$  SL. Since the effective mass  $m_1^*$  in GaAs is smaller than  $m_2^*$  in  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  for  $k_t < k_{t0}$ <sup>15)</sup> ( $k_{t0}^2 = 2U_0 m_1^* m_2^* / [\hbar^2 (m_2^* - m_1^*)]$ ) the wells exist in GaAs layers and barriers in  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  layers. If  $k_t = k_{t0}$ ,  $U_{\text{eff}}$  does not possess the spatial dependence, but even then, as was shown in the most general case by harmonic method<sup>16)</sup>, the energy spectrum is bandlike. In the case  $k_t > k_{t0}$ , the distribution of well and barriers is opposite. Therefore it ensues clearly that the dependence  $E(k_t^2)$  is distinctively nonlinear unlike the case of the position independent effective mass, where  $E$  is proportional to  $k_t^2$ . The expression for the concentration in the  $i$ -th minzone takes considerably complicated form<sup>14)</sup>:

$$n_i(z) = \frac{d}{\pi^2} \int_0^{\pi/d} dk_z \int_0^{+\infty} \frac{|\psi(k_z, k_t(z))|^2 k_t dk_t}{\exp(\eta) + 1}, \quad \eta \equiv (E_i(k_z, k_t^2) - E_F)/kT. \quad (2)$$

<sup>\*)</sup> The effects of  $E(k_t)$  nonparabolicity should be pronounced in effective mass SL<sup>21)</sup>,

In (2)  $\psi_{k_z, k_t}^i$  are the complex wavefunctions (explicitly dependent on  $k_t$ ) normalized to unity within the SL period. In the case of the quantum well, the electron concentration is the sum of "discrete" and "mobile" electrons<sup>17)</sup>:

$$n_d(z) = \frac{1}{\pi} \sum_{i=1}^p \int_0^{k_{ti}} \frac{\psi_{i, k_t}^2(z) k_t dk_t}{\exp(\eta_i) + 1}, \quad n_m(z) = \frac{1}{\pi^2} \int_0^{+\infty} dk_z \int_0^{+\infty}$$

$$\frac{[\psi_{e, k_z, k_t}^2(z) + \psi_{o, k_z, k_t}^2(z)] k_t dk_t}{\exp(\eta) + 1}, \quad \eta_i \equiv \frac{E_{i, k_t} - E_F}{kT}$$

$$\eta \equiv \frac{E_{k_z, k_t} - E_F}{kT} \quad (3)$$

where  $p$  is the number of discrete levels for  $k_t = 0$ ,  $k_{ti}$  is the transversal wave vector, for which the  $i$ -th discrete level vanishes, while  $\psi_e$  and  $\psi_o$  are even and the odd wavefunctions normalized in such a way that in the barrier material they have the form:  $\sin(k_z z + \phi_{e,o})$ <sup>17)</sup>.

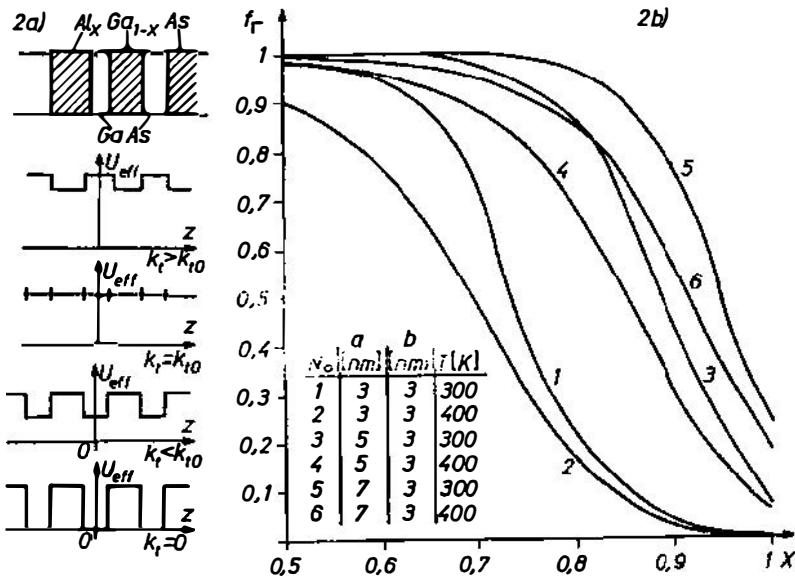


Fig. 2a.

The effective potential energy of the GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As SL for various values of the transversal wave vector  $k_t$ . Fig. 2b. The relative population of  $\Gamma$  minimum vs. the mole fraction  $x$  for GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As SL, (layer thicknesses are 3 nm, average electron concentration is  $3 \cdot 10^{17} \text{ cm}^{-3}$ )<sup>19)</sup>.

In band structure of host materials (such as: GaAs,  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ...) besides the direct  $\Gamma$  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<sup>18)</sup> it was shown that electrons in each of these minima create their independent minizone like spectra. Fig. 2b displays the dependence of the relative population of  $\Gamma$  minimum vs. mole fraction  $x$ , where from it is easily seen that for greater  $x$  and higher temperature almost all electrons are at indirect minima<sup>19)</sup>.

A very interesting structure is a semi-infinite SL, where beside minizone there exists the discrete spectrum, too. The number of discrete levels could be regulated by a simple change of thickness of materials<sup>20)</sup>.

Since a majority of materials composing the SL belong to III-V compounds, on 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<sup>22)</sup>, where the  $\Gamma_7$  spin-orbit split band was disregarded as well as (except for heavy holes) the coupling to other bands and free electron dispersion part.

Further this model developing, we have shown in<sup>23)</sup> that the Schrodinger equation could be written, only for electrons (analogously to (1)):

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

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<sup>23)</sup> as  $m_0^*(z) [1 + (E - E_c(z))/E_g(z)]$  ( $m_0^*$  is the band edge effective mass). The analysis of (1) shows that in nonsymmetric 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 reach even 10%.

The analysis of the SL band structure, taking into account the local potential is a very complicated problem, which has been treated lately in several paper. In paper<sup>24)</sup> it was shown by the application of the LCAO method that the EFA is a good approximation in  $\text{GaAs-Al}_x\text{Ga}_{1-x}\text{As}$  SL, while for the  $\text{GaSb-InAs}$  SL this could not by far be said. The paper<sup>25)</sup> 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<sup>26)</sup> starting from (1) are: 125 meV, 222 meV and 307 meV which is a very good agreement. As far as the holes are concerned the agreement is very weak.

### 3. TRANSPORT PROPERTIES OF SUPERLATTICE

The interest in studying the transport properties of SL increased suddenly in 1978, when the modulation doping method being proposed<sup>27)</sup>. The essence of the method is in the following: the barrier material is doped by donors, while the well material

\*) Let us mention that in the most recent paper<sup>29)</sup> the mobility of  $2 \cdot 10^6 \text{ cm}^2/\text{Vs}$  was not experimentally exceeded.

is undoped (more exactly it is weakly doped by acceptors). Due to the existence of the barrier, almost all electrons are in the well. In such a way the carriers are spatially separated from the impurities. At higher temperatures, the optical phonon scattering is dominant, while at lower temperature the impurity scattering is dominant, so that the mobility in modulation doped SL at higher temperatures is approximately equal to the bulk mobility. For lower temperatures it can be shown that  $\mu \sim N_S^{3/2} / N_I^{2/3}$  ( $N_S$  – the surface density of electrons,  $N_I$  – concentration of ionized impurities) and since  $N_I$  is very small in GaAs layer, the mobility increases enormously. Fig. 3a displays mobility vs temperature dependence (reported from 1978 to 1982), wherefrom it is seen that low temperature mobility exceeds even by two orders the mobility of the bulk\*). In a quantum wire, by theoretical predictions the mobility could be increased even to  $10^8 \text{ cm}^2 / \text{Vs}$ ).

Only few papers were published on the Einstein relation (the diffusion constant  $D$  and mobility  $\mu$  ratio) hitherto, though, in our opinion, this problem is of interest especially in the analysis of devices operation. In<sup>31)</sup> it was shown that  $D/\mu$  in the SL depends on the scattering mechanisms. However, if we assume the unique chemical potential and if we average the diffusion constant and mobility, then  $D/\mu$  ratio does not depend on the scattering mechanisms, but on the band structure, only<sup>31)</sup>. Fig. 3b presents  $D/\mu$  vs  $N_S$  dependence. At smaller  $N_S$ ,  $D/\mu$  tends towards  $kT/e$  which is the  $D/\mu$  ratio in bulk nondegenerate semiconductors. At the increase  $N_S$ ,  $D/\mu$  passes through the maximum, then through the minimum. The pronouncement of these extreme decreases with increasing temperature. This behaviour, that we have not met in the literature until now, can probably be explained by peculiarities of SL band structure.

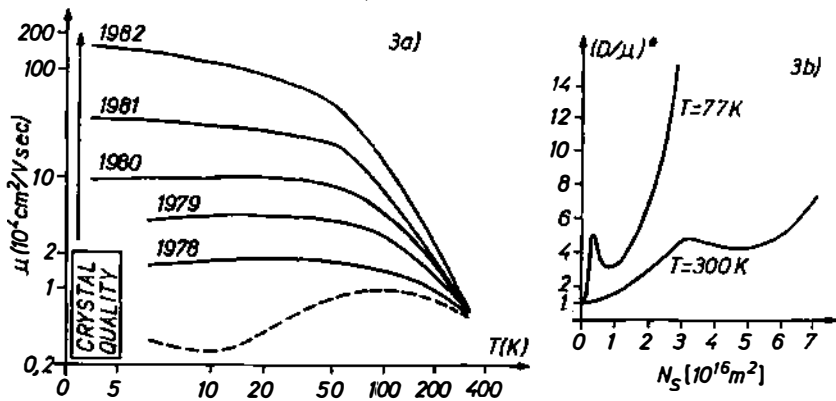


Fig. 3

Highest electron mobilities from 1978 to 1982 in modulation doped GaAs. The lowest curve (dashed lines), marked bulk GaAs. Structures vary, but all contain about  $10^{17}$  carriers/cm<sup>3</sup> in their conduction regions (From<sup>30)</sup>). Fig. 3b dependence of the ratio  $(D/\mu)^* \equiv (D/\mu)/(kT/e)$  vs. the surface density  $N_S$  for GaAs–Al<sub>0.3</sub>Ga<sub>0.7</sub>As SL with layer thickness 6 nm and 15 nm, respectively (From<sup>31)</sup>).

#### 4. OPTICAL PROPERTIES OF SUPERLATTICE

In the SL and in quantum wells, apart from interband (the transition 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 last ones do not appear in bulk semiconductors. We can show that the absorption coefficient for the interband transition is given by the expression<sup>32)</sup>:

$$\alpha_{ij} = \frac{e^2 P_1^2}{2(2\pi)^2 \epsilon_0 c \bar{n} m_0^2 \omega} \int |M_{ij}|^2 \delta [E_{ei}(\vec{k}) + E_{hj}(\vec{k}) + E_{g1} - \hbar\omega] \cdot FD \cdot d^3 k, \quad (5)$$

where  $P_1$  is Kane's matrix element in GaAs,  $\bar{n}$  the average refraction index,  $\hbar\omega$  photon energy, while  $E_{ei}$  and  $E_{hj}$  energies of electrons and holes, measured from the extrema of the respective bands. FD factor is equal to the difference of Fermi-Dirac distribution for  $E_{ei}$  and  $E_{hj}$  as well as in the case of interband absorption it is very near to unity. The envelope matrix element  $M_{ij}$  is given by:

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

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 eq (5) modifies:  $P_1^2/\bar{n}^2$  being substituted by unity. The argument of the  $\delta$ -function is now  $(E_{ei} - E_{hj} - \hbar\omega)$ , while the envelope matrix element is:

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

In the intraband transition FD factor is to be taken into account, and in a majority of cases it amounts to  $f_{FD}(E_{hj})$ . In symmetric SL the wavefunctions have the definite parity, only at the minizone boundaries, and for  $k_z = 0, \pi/d$  there are selection rules. In GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As SL, the matrix elements corresponding to the interband transition ( $i = j$ ) are near to unity, especially for the electron-heavy hole transitions<sup>32)</sup>. 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 than in the case  $i = j$ . In the doped SL, interband matrix elements are very small, so that it is possible to obtain the recombination lifetime of several tens of minutes<sup>6)</sup>. In nonsymmetric SL there are no any selection rules. The dependence  $\alpha(\omega) \cdot \omega$  vs.  $\omega$  has a quasi step-like character, with the pronounced jumps of absorption with the 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 in SL more bounded than in bulk, so that they can be observed even at room temperatures.

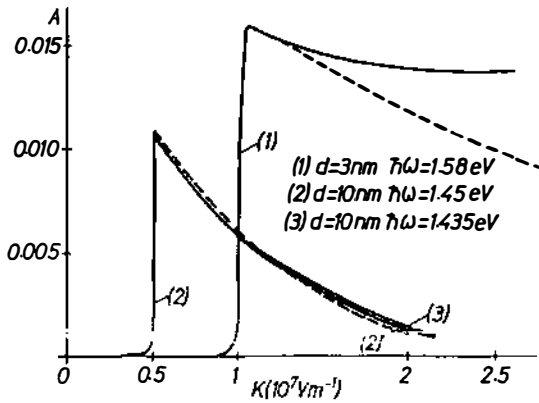


Fig. 4.

The dependence of QW absorption (in absolute units) on electric field  $K$  for several values of photon energy  $\hbar\omega$  and well thickness  $d$  (Al mole fraction in bulk  $x = 0.3$ ). The broken lines correspond to envelope matrix elements vs. field dependence calculated from discrete levels model.

Of interest is the problem of high absorption of quantum well in the presence of electric field. The optical properties of bulk in the electric field were very intensively studied at the beginning of the 1960<sup>33)</sup>. It may be shown<sup>34)</sup> that the absorption of the whole structure (quantum well and two semi-infinite semiconductors) is infinite and the absorption coefficient is equal to that of barrier material. The quantum well absorption is introduced as a difference of absorption of structure with and without quantum well. The energy spectrum, in this case, for both types of carrier is continuous. At weak fields, the widths of resonance levels are very small, the spectrum is quasi-discrete, so that the absorption is proportional to the matrix element (the dotted lines in Fig. 4). If photon energy  $\hbar\omega$  is fixed, for small field values, the absorption is negligible, because  $\hbar\omega$  is smaller than the difference of electron and hole resonant levels. For some definite field value,  $\hbar\omega$  becomes equal to this difference and the absorption increases abruptly, reaches the maximum and then decreases weakly, because the matrix elements decrease (the maxima of the envelope functions of electrons and hole go apart). This is clearly seen from Fig. 4<sup>34)</sup> where the absorption vs. field dependence is depicted for 3 nm and 10 nm quantum well and photon energies of 1.58 meV, 1.45 meV, 1.435 meV.

## 5. APPLICATION OF SUPERLATTICE

In our opinion, the most important effect for the SL application is the enormous increase of mobility, on the basis of which FET\* were constructed<sup>35)</sup>. All these devices are similar: under the gate electrode is  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  layer doped by donors. Next to it there is an undoped GaAs layer. The mobility of the electrons in GaAs layer, as already explained, is very large, due to which these transistors are devices with very small switching time (of order ps) and very large bandwidth (of order GHz<sup>35)</sup>). 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 de-

fine  $\Delta F$  as product of the dissipation of energy  $\Delta W$  and switching time  $\Delta t$ <sup>36)</sup>.  $\Delta F$  should be the fundamental parameter indicating the overall performance of a quantum mechanical standpoint. As can be seen from Fig. 5 in present realization only Josephson Fluxon devices have better characteristics than HEMT's but only with respect to  $\Delta W$  (naturally, the smallest value  $\Delta F$  which can be reached is bounded by the uncertainty relation and it is equal to Planck'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 electric field; in order to get higher absorption a multi quantum well is used.

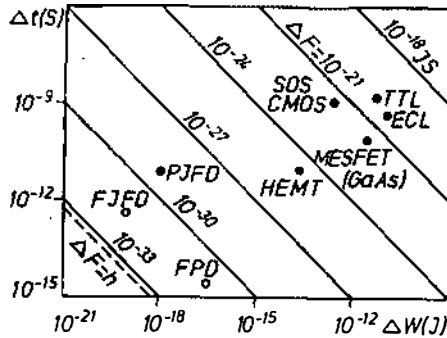


Fig. 5.

The switching time and dissipation of energy for different logical devices. PJFD means present Josephson Fluxon devices, FJFD future JFD and FPD—future photon devices (from<sup>36)</sup>)

Already in<sup>1)</sup> the possibility of a SL was analysed as a structure with the negative differential conductivity. This possibility did not get the respective experimental confirmation until today.

## 6. 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, which 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

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

energy spectrum, such as: the pronounced nonparabolicity energy vs square of transversal wave vector  $k_{\perp}$  dependence, explicit envelope wavefunctions vs.  $k_{\perp}$  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 non-symmetric SL, corresponding to various orientation of the spin. The comparative analysis with "local" methods provides a good agreement only for the electrons. Among transport properties we dealt with the enormous increase of mobility in modulation doped SL and Einstein relation, where the effect specific for SL are encountered. Out of optical properties single photon absorption (interband and intraband transitions) was analysed. The quantum well in the electric field is also discussed. As far as, the application is concerned, we stressed particularly the transistors with very high electron mobility, which were already realized in laboratories and which will find their place especially in superfast computers.

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