ENERGY STATES AND TYPE OF $(GaAs)_n/(AlAs)_m$ SHORT-PERIOD SUPERLATTICES

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The possibility of the short-period $(GaAs)_n/(AlAs)_m$ superlattices properties description in the envelope function approximation with diagonal boundary conditions is considered. Within the framework of this model the explanation of experimentally observable influence of the superlattice layers thickness on its type is obtained. The influence of boundary conditions and the presence of the quantum well bottom defect on a minizone spectrum is analyzed.

As it is known, the composite superlattices (SLs) $(GaAs)_n/(AlAs)_m$ with layer thickness greater than 12 monolayers of bulk material, belong to direct gap or the 1-st type, while SLs with layers thickness less then 12 usually belong to indirect gap or the 2-nd type. Nevertheless as it was shown in the work [1], the reduction of barriers thickness in asymmetrical GaAs/AlAs SLs makes them direct-gap.

The main aim of the present work was an explanation of the reasons of the direct-gap character of the short-period asymmetrical GaAs/AlAs SLs, grown in a [100] direction. Photoluminescence spectra (PL) which ware obtained experimentally [1] show the presence of the phonon satellites for symmetrical samples and their absence for asymmetrical ones. This as well as consideration of the lux-intensity characteristics and intensity dependences on the excitation level depicted for SLs 10/10 and 10/5 in Fig. 1 [2,3], leads us to conclusion that asymmetrical SLs are direct-gap (or the 1-st type), and symmetrical ones are indirect-gap (or the 2-nd type). The presence of gain obtained for the sample 6/3 [2,3] (see Fig. 2) appears as an indirect confirmation of the above-stated.

To obtain a SL's minizone spectrum we have employed the envelope function approximation - one of the most convenient methods for superlattices description. The method is based on the effective mass approximation which was introduced by J.Luttinger and W.Kohn [4], that is why the consideration is conducted in continuum approximation and the bulk effective masses act as parameters of the materials. The validity of such short-period heterostructures description was theoretically proved by Foreman [5–7].

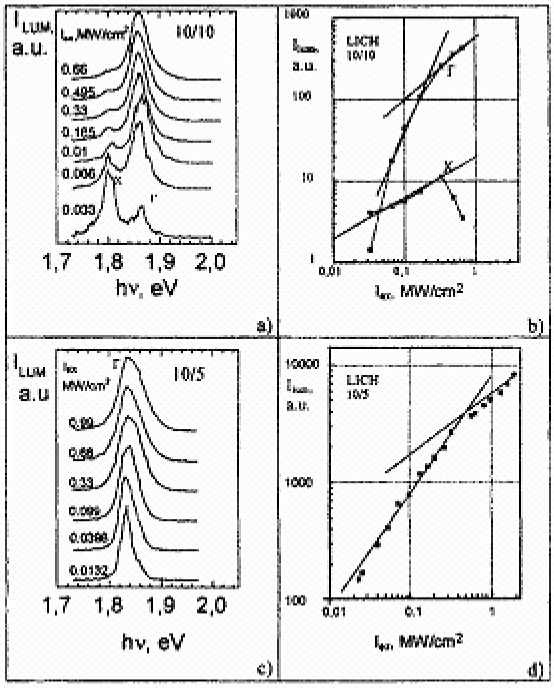

Fig. 1 Photoluminescence spectra of GaAs/AlAs for different excitation intensity [2,3].

For the mathematical description of SL in the method two functions are used: the envelope and its first derivative, which are connected on the interface by the certain boundary conditions. No matter of various possible kinds of boundary conditions existence from the phenomenological point of view, all of them should satisfy the requirement of the flux conservation through the interface.

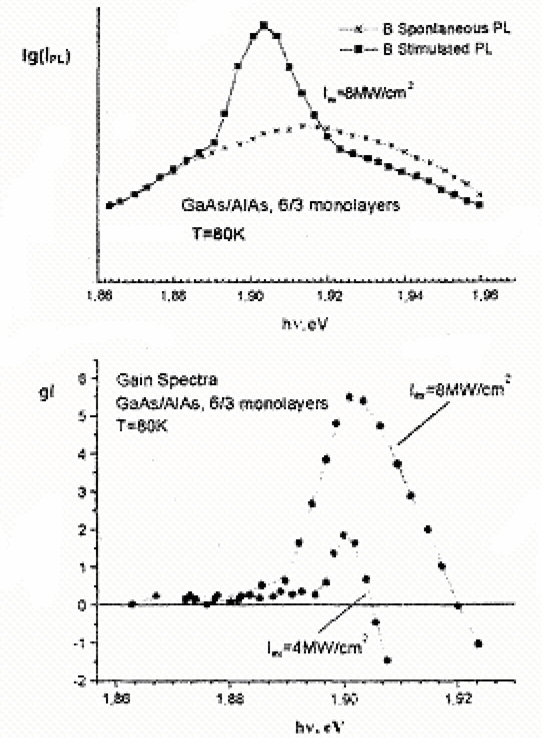

Fig. 2 Spectra of spontaneous and stimulated emission and optical gain in 6/3 SL.

In our work we used boundary conditions introduced by Ivchenko and Pikus [8]:

$$m_1^{\alpha}\psi_1(z) = m_2^{\alpha}\psi_2(z)$$
$$m_1^{-1-\alpha}\frac{\partial}{\partial z}\psi_1(z) = m_2^{-1-\alpha}\frac{\partial}{\partial z}\psi_2(z), \qquad (1)$$

where α is variable adjusting parameter. As it was shown by Ando *et al.* [9], the value of α varies in the range [-1/2,0], that responds to continuous transition from boundary conditions introduced by Bastard [10] to Kronig-Penny model. In the present work we used the formalism of the transition matrices (or the interface matrices) offered by Ando *et al.* [11], that allows us to carry out calculations in more convenient form. In this notation the boundary conditions (1) take the form:

$$\begin{pmatrix}\psi_2\\ \varphi_2\end{pmatrix} = T_{21}\cdot\begin{pmatrix}\psi_1\\ \varphi_1\end{pmatrix};\quad T_{21} = \begin{pmatrix}\left(\frac{m_1}{m_2}\right)^{\alpha} & 0\\ 0 & \left(\frac{m_2}{m_1}\right)^{\alpha}\end{pmatrix}, \qquad (2)$$

where $\varphi_i = a_0\frac{m_0}{m_i}\frac{\partial}{\partial z}\psi_i$, and m_0, m_1, m_2 are free electron mass and the effective masses in the materials 1 and 2, respectively, a_0 is lattice constant. The condition of a flux conservation looks like:

$$\det T_{21} = 1\,. \qquad (3)$$

This takes place for the boundary conditions (1) with evidence.

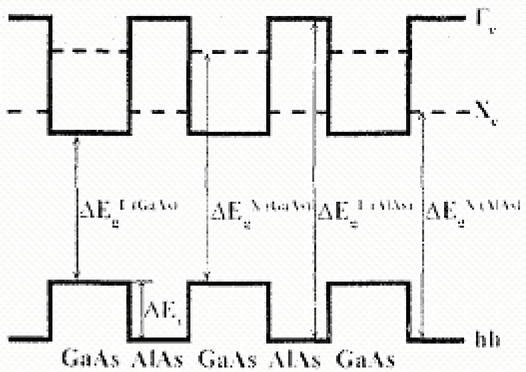

Fig. 3 Simple model of SL's bands edge profile

The change of the pair $\begin{pmatrix}\psi_i\\ \varphi_i\end{pmatrix}$ at transition through layers can be described [12] by matrices:

$$T_w(z) = \begin{pmatrix}\cos(k_w z) & -\frac{1}{k_w}\sin(k_w z)\\ k_w\sin(k_w z) & \cos(k_w z)\end{pmatrix},$$
$$T_b(z) = \begin{pmatrix}\mathrm{ch}(k_b z) & -\frac{1}{k_b}\mathrm{sh}(k_b z)\\ -k_b\,\mathrm{sh}(k_b z) & \mathrm{ch}(k_b z)\end{pmatrix} \qquad (4)$$

for wells and barriers, accordingly. Here k_w and k_b are wave vectors in well and barrier.

Using the Bloch theorem and taking into account the above considerations, for the simple structure shown in Fig. 3, we have the following:

$$\begin{pmatrix}\psi_2\\ \varphi_2\end{pmatrix}e^{ikd} = T_b(b)T_{21}T_w(a)T_{12}\begin{pmatrix}\psi_1\\ \varphi_1\end{pmatrix} \qquad (5)$$

or

$$e^{ikd}I = M,\quad M = T_b(b)T_{21}T_w(a)T_{12} \qquad (6)$$

Hence we obtain:

$$2\cos(kd) = Sp(M) \qquad (7)$$

After simplification this gives the equation, numerical solution of which allows the SL minizone spectrum to be obtained:

$$\cos(kd) = \cos(k_1 a)\mathrm{ch}(k_2 b) + \frac{1}{2}\left[R - R^{-1}\right]\sin(k_1 a)\mathrm{sh}(k_2 b)$$

$$R = \frac{k_2}{k_1}\left(\frac{m_1}{m_2}\right)^{2\alpha-1}, \quad k_1 = \frac{1}{\hbar}\sqrt{2m_1 E}, \quad k_2 = \frac{1}{\hbar}\sqrt{2m_2(U_0 - E)} \qquad (8)$$

Having these equations numerically solved, we obtained minizone spectra of the SLs. In Fig. 4 the results and their comparison with experimental data are submitted. One can see, that the obtained results demonstrate both qualitative and quantitative agreement with experimental data: so for symmetrical SLs, it is possible to adjust such values of α, that the X-states appear to be lower than the Γ-states, this means that such SLs are indirect-gap, what corresponds to the experiment. At the same time asymmetrical SLs for all values of α remain the direct-gap ones. Not only qualitative, but also quantitative conformity is present here, so for SL 10/10 it was possible to adjust two parameters simultaneously: they are positions of intensity maxima for Γ_e-Γ_{hh} and X_e-Γ_{hh} transitions.

Despite the good agreement, the validity of such approach, when only diagonal elements of the interface matrix are taken into account, remains unclear. So the question arises: is it possible to reach the same results by introducing in the transition matrix an off-diagonal element t_{21}? In this case the transition matrix is written as

$$T_{21} = \begin{pmatrix} \left(\frac{m_1}{m_2}\right)^{\alpha} & 0 \\ t_{21} & \left(\frac{m_2}{m_1}\right)^{\alpha} \end{pmatrix} \qquad (9)$$

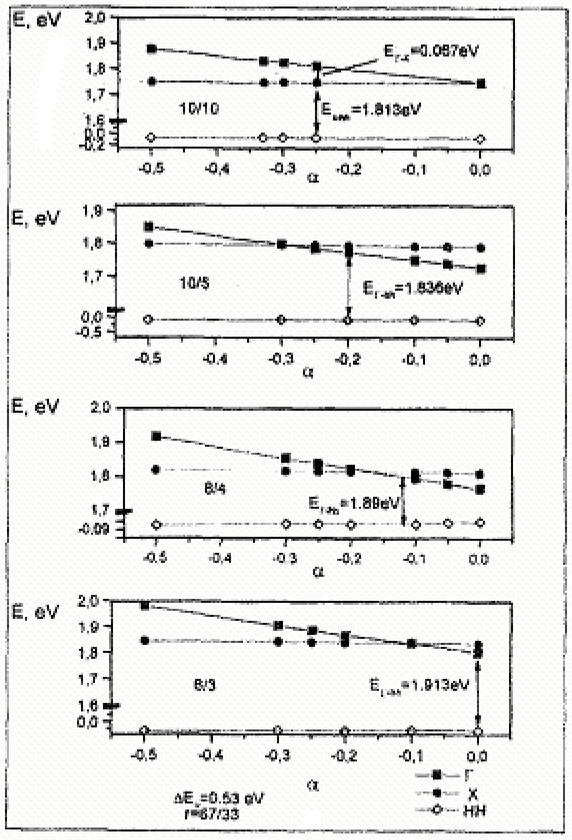

Fig. 4 Calculated minizone energy states dependences on the boundary conditions.

Having carried out calculations, similar to those as in the previous case, we shall come to following dispersion equation:

$$\cos(kd) = \cos(k_1 a)\mathrm{ch}(k_2 b) + \left(\frac{m_2}{m_1}\right)^{\alpha+1}\frac{t_{21}}{k_2}\cos(k_1 a)\mathrm{sh}(k_2 b) +$$
$$+\frac{1}{2}\left\{\left(\frac{m_1}{m_2}\right)^{\alpha}\frac{t_{21}}{k_1}\sin(k_1 a)\mathrm{ch}(k_2 b) + \frac{m_2}{m_1}\frac{t_{21}^2}{k_1 k_2}\sin(k_1 a)\mathrm{sh}(k_2 b) + \right. \qquad (10)$$
$$\left. +\left[R - R^{-1}\right]\sin(k_1 a)\mathrm{sh}(k_2 b)\right\}$$

Minizones edge dependences on t_{21} at various α for SLs 10/10 and 10/5 obtained from (10) demonstrate that the qualitative agreement is preserved and the quantitative deviations grow with t_{21} increase. Hence, at any α the quantitative agreement of the obtained energy intervals for transitions between Γ_e, X_e and Γ_{hh} states with experimental values is worsened, though in the certain range of t_{21} variation the qualitative conformity concerning the SL type is preserved. From here it follows that the above described method with the *diagonal* boundary conditions (1) *can be used* for the short-period SLs description.

Taking into account that experimental data are obtained in real samples, which can contain defects and internal strains, we have considered an opportunity of quantum well bottom defect influence (the model is depicted in Fig. 5) on a minizone spectrum. Having constructed complete transition matrix through such structure with subsequent its simplification, we come to the dispersion equation:

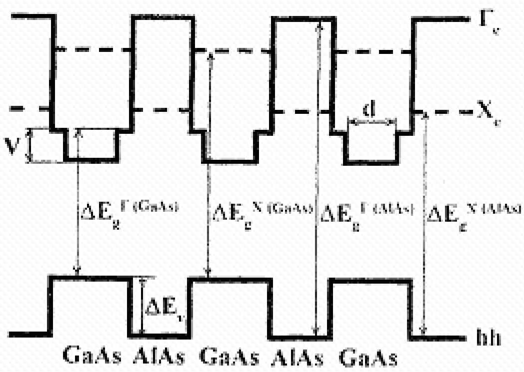

Fig. 5 Bands edge profile of SL in the model with defect in a quantum well bottom.

$$\cos(ks) = F(E)$$

$$F(E) = \frac{1}{2}\{[R_1 - R_1^{-1}]\sin(2\zeta d)\sin^2(k(l-d)) + [R_2 - R_2^{-1}]\cos(2\zeta d)\sin(2k(l-d)) +$$

$$+[R_3 - R_3^{-1}]\sin(2\zeta d)\cos^2(2k(l-d))\}\mathrm{sh}(qb) + \frac{1}{2}[R_4 - R_4^{-1}]\sin(2\zeta d)\sin(2k(l-d))\mathrm{ch}(qb) +$$

$$+\cos(2\zeta d)\cos(2k(l-d))\mathrm{ch}(qb)$$

$$R_1 = \frac{m_l k^2 m_d}{\zeta m^2 q}, \quad R_2 = \frac{mq}{m_l k}, \quad R_3 = \frac{q m_d}{\zeta m_l}, \quad R_4 = \frac{\zeta m}{k m_d} \qquad (11)$$

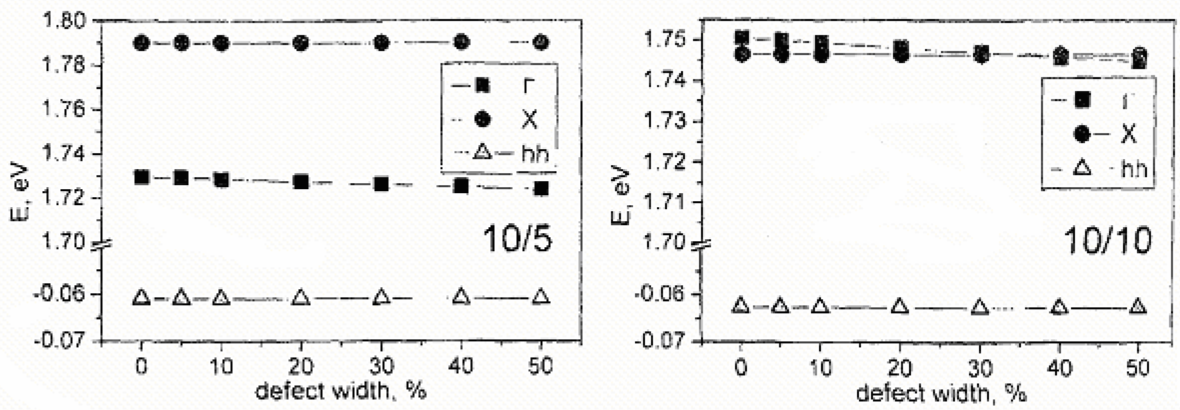

Fig. 6 Minizone energy dependence on defect width when its depth is ~1% of barrier's height for 10/5 and 10/10. SLs

Dependences shown in Fig. 6. were obtained by variation of the defect parameters. From their analysis it follows that for essential influence on the spectrum the defect depth should be about 0.5 eV, what seems to be excessive. Nevertheless qualitative conformity takes place within the framework of this model as well.

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ЕНЕРГЕТИЧНІ СТАНИ І ТИП КОРОТКОПЕРІОДИЧНИХ НАДГРАТОК $(GaAs)_n/(AlAs)_m$

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Розглянуто можливість опису властивостей короткоперіодичних надграток $(GaAs)_n/(AlAs)_m$ методом обвідної функції з діагональними граничними умовами. В рамках цієї моделі отримано пояснення впливу товщини шарів надгратки на її тип, що спостерігається експериментально. Проаналізовано вплив граничних умов і наявності дефекту дна квантової ями на мінізонний спектр.