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A simple method for the determination of the superlattices band structure : formulation and applications

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Abstract : Assuming an approximated effective mass and using Bastard's boundary conditions, we introduce a simplified method which allows the determination of the energy levels forming the sub-band structure of non-symmetrical, non-periodical potential samples. The energy quantification condition allows the determination of the energy levels for electron and hole. The wave functions are easily deduced as well as the energy transition. We have applied this method to both theory and experimental data. Our finding shows a good agreement with previous experimental and theoretical results. The method is useful for any number of semiconductor layers arranged in any random way; thus making it more realistic, simpler and applicable to superlattice analysis and device designs.

Keywords : Superlattices, heterojunctions, multilayers, band structure

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1. Introduction

The superlattices that consist of many alternating semiconductor layers, have recently attracted attention of the researchers and attempts have been made to determinate their band structures. The Kronig-Penney model [1] was applied with the purpose to find out the nature of the band structure of massive semiconducting samples with periodically varying potentials [2,3]. It has also been applied to semiconductor superlattices [4–8] to investigate the qualitative nature of band structures and calculate quantum confined boundary energy sub-bands.

Mukherji and Nag [4] assumed that the wave function and its first derivative are continuous at the interface when they considered the effective-mass difference in formulation. Bastard [5] calculated the band structure of GaAs/GaAlAs and InAs/GaSb superlattices by matching propagating or evanescent envelope functions at the boundary of consecutive layers. In his model, Bastard [5] showed that the first derivative function divided by the effective mass is continuous at each interface when he used an envelope function approximation. In comparison to other boundary conditions [9–11], this proved to be the simplest. In addition, the results of particle energy calculation based on Bastard's boundary conditions were consistent with the experimental data obtained by Masselink *et al* [12]. Chomette *et al* [13] used the Kronig-Penney model [1] and the Bastard's boundary conditions and calculated the band offset of GaAs/GaAlAs superlattices. Cho and Prunal [14] developed a new formalism of the Kronig-Penney model [1], considerably simpler than the conventional one. Maiz *et al* [15] presented a simple method and applied it to study the GaAs/GaAlAs super-lattices their theoretical results showed a good agreement with those obtained by Cho and prunal [14]. Girault [16] has also prepared the InP/GaInAs superlattices and has carried out such study.

In this paper, assuming an approximated effective mass and using Bastard's boundary conditions, we introduce a further simplified method which allows the determination

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of the energy levels forming the sub-band structure of a non-periodical-potential multilayer sample.

We practice this method from both theoretical and experimental points of view. First, we apply it on the GaAs/GaAlAs superlattice and compare the findings with the previous ones. Secondly, we use this method to interpret the experimental data obtained by Girault [16] for the InP/GaInAs superlattice.

2. Formulation

To formulate our simple method, we have considered a general case where the sample consists of n semiconductor layers deposited on a substrate and limited by two media B and F, as shown in Figure 1.

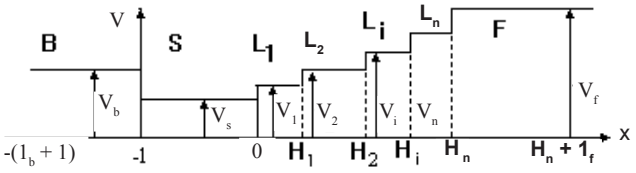

Figure 1. A schematic view of n layers .

Table 1. Characteristic of a heterostructure with n layers.

Layer	Index	Thickness	Barrier height difference	Electron effective mass
Backing	B	l_b	V_b	m_b^*
Substrate	S	l	V_s	m_s^*
Layer i	L_i	h_l	V_l	m_l^*
Medium F	F	l_f	V_f	m_f^*

The characteristics of the different layers are given by Table 1. The Schrödinger's equation may be described as :

For region B $\dfrac{\partial^2\psi_b}{\partial x^2} = k_b^2\psi_b$, $\quad -l-l_b \le x \le -l$

For region S $\dfrac{\partial^2\psi_s}{\partial x^2} = k_s^2\psi_s$, $\quad -l \le x \le 0$

For region L_i $\dfrac{\partial^2\psi_i}{\partial x^2} = k_i^2\psi_i$, $\quad H_{i-1} \le x \le H_i$

For region F $\dfrac{\partial^2\psi_f}{\partial x^2} = k_f^2\psi_f$, $\quad H_n \le x \le H_n + l_f$

where $k_i^2 = 2m_i^*(V_i - E)/\hbar^2$, $\quad i = b, s, 1, \ldots, n, f$

$$H_i = \sum_{j=1}^{j=i} h_j$$

and $H_i =$.

For values of the energy less than the potential limits V_b and V_f, the acceptable solutions of these equations are $(1 \le i \le n)$:

$\psi_b = W\exp(k_b(x-l))$ For $-l-l_b \le x \le -l$

$\psi_s = U\exp(k_f x) + V\exp(k_f x)$ For $-l \le x \le 0$

$\psi_i = X_i\exp(-k_i(H_i - x)) + Y_i\exp(+k_i(H_i - x))$ For $H_{i-1} \le x \le H_i$

$\psi_f = A\exp(-k_f(x - H_n))$ For $H_n \le x \le H_n + l_f$

The use of Bastard's boundary conditions at each interface and the elimination of W, U, V, X_i, and Y_i $(1 \le i \le n)$ lead to the following equality :

$a_n P_n X_n + b_n Q_n Y_n = 0,$

where

$a_i = \exp(-k_i h_i)$, $\quad b_i = \exp(k_i h_i)$, $\quad c_{i,j} = c_j = \dfrac{k_i m_j^*}{k_j m_i^*}$,

$P_0 = (1 - c_{b,s})$, $\quad Q_0 = -(1 + c_{b,s})$

$P_i = (c_{i-1,i} + 1)a_{i-1}P_{i-1} + (c_{i-1,i} - 1)b_{i-1}Q_{i-1}$,

$Q_i = (c_{i-1,i} - 1)a_{i-1}P_{i-1} + (c_{i-1,i} + 1)b_{i-1}Q_{i-1}$.

The substitution of X_n and Y_n by their expressions as a function of A gives :

$A\,B_n = 0$,

where $B_n = (c_{n,f} - 1)a_n P_n + (c_{n,f} + 1)b_n Q_n$

The demonstration of this expression in general, was done by the recurrence method [14]. Since A is the amplitude of the function in the medium F, it must be different from zero and then $B_n = 0$ is the energy quantification condition. The energy levels are obtained by the energy values for which the curve of the B_n meets the energy axis.

When we consider the function $F(E)$ definite as: $F(E) = \text{signum}(B_n(E))$ where the signum function computes the sign of the leading coefficient of expression [if $x \neq 0$ then signum $(x) = x/\text{abs}(x)$ and signum(0) = 0]. The energy levels are indicated by a vertical segments perpendicular to the energy axis which constitute the curve of the function $F(E)$. In this case, the energy values are determined with a great precision.

3. Study of the GaAs/AlGaAs superlattice

In order to verify our method, we use the application of Maiz *et al* [15]. We have calculated the electron energy values of the GaAs/$Al_xGa_{1-x}As$ superlattice sub-bands, with x = 0.5, a = 100Å, and b = 10 Å, the barrier of potential V is 375 meV [12,17–19], the electron effective mass is $0.067m_o$ inside the well and $0.1085m_o$ [20] at the

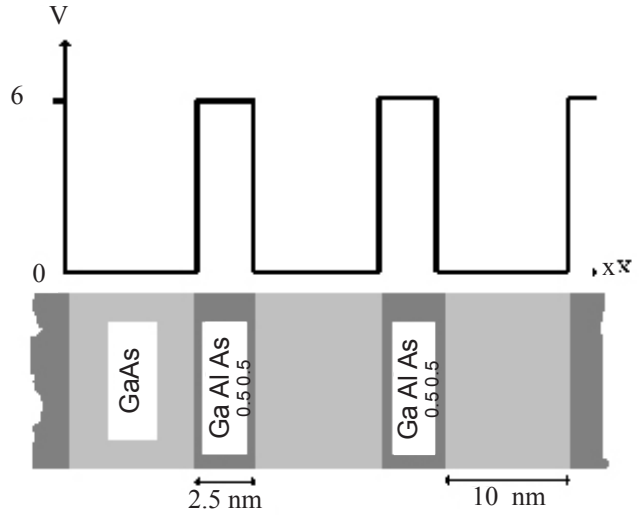

Figure 2. A schematic view of the GaAs/AlGaAs superlattice.

the number of wells and that all the picks are located in the sub-band predicted elsewhere [1,14,15]. The exact wave function associated with each energy is calculated by inse

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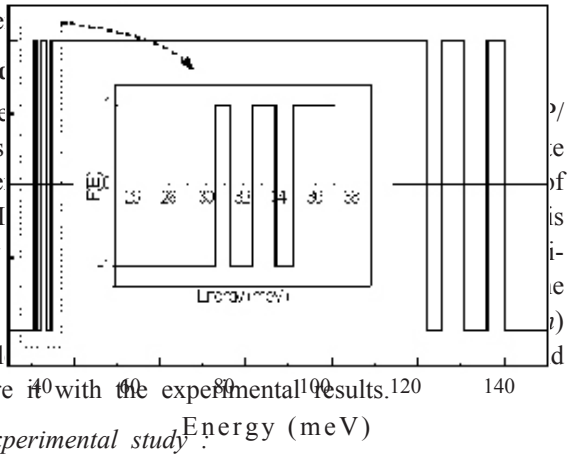

Figure 3. curve of $A(E)$ for $n = 8$ and $10 < E$ (meV) < 150.

4.1. Experimental study :

Girault [16] experimented three various samples S1, S2, and S3 of the InP/GaInAs superlattice. Table 3 shows the thickness of the GaInAs layers. He proved that many transitions can be seen and calculated. He noticed that the transition energy changes according to the thickness of the constituting wells. Girault observed about ten transitions between the levels of electrons and holes but he could detect only two transitions for the sample S1 and four for each of the other ones. Table 4 summarizes the energy of the observed transitions for each sample.

Table 3. Wells thickness.

Sample	S1	S2	S3
GaInAs layer thickness	1.8 nm	18 nm	30 nm

Table 4. Observed transitions energies.

Transition energies (meV)	S1	S2	S3
$hh_1 \rightarrow e_1$	1050	740	730
$hh_2 \rightarrow e_2$	*	800	760
$hh_3 \rightarrow e_3$	*	885	800
$hh_4 \rightarrow e_4$	*	990	850
$lh_1 \rightarrow e_1$	1160	*	*

4.2. Theoretical study :

The energy quantification condition is written assuming that the media *B* and *F* represent the same medium which is the InP layer where the barrier potential is adjusted to *Ve* = 360 meV for electron and *Vh* = 260 meV for holes. As the conduction band of GaInAs is not parabolic, we write the effective mass for the electron in the well as :

$$m(E) = m_o[1 + \acute{a}(E - Eg)] .$$

Eg represents the energy gap. Palik *et al* [21] proposed the value 1.3 meV^{-1} for α and later Sarkar *et al* [22] assigned it to 2 meV^{-1} but we find it to be 1.8 meV^{-1}. Table 5 gives the characteristics of the InP/GaInAs superlattice.

(*a*) *Electron energy levels :*

Using our method, we calculate the electron energy levels and we find only one level for the sample S1 because of the smallness of the GaInAs thickness. We also noted four other energy levels for each of the other samples. We observe that the first energy level decreases when the well thickness increases. Table 6 describes our theoretical results.

Table 5. InP/GaInAs superlattice characteristics.

Layer	V_e	V_t	m_e	m_h	m_l
InP	360 meV	260 meV	0.079 m_o	0.45 m_o	0.12 m_o
GaInAs	0	0	0.04 m_o	0.6 m_o	0.05 m_o

Table 6. Electron energy levels.

Samples	Energy levels (meV)							
	S1		S2			S3		
Electron	965	743	794	869	957	733	756	790
835								

(*b*) *Hole energy levels :*

To calculate the energy levels of the hole, we assume that an electron is inside a well instead of a hole. The barrier potential is *Vh* and the effective masses are the ones of holes. For the sample S2, the exact high hole energy values are indicated by vertical segments as shown in Figure 4. Table 7 summarizes the hole energy levels.

Table 7. Hole energy levels.

Hole and samples	Energy levels (meV)								
	S1			S2			S3		
High	83	1.46	7	15	28	3	6	11	16
Low	173	13	56	129	230	5.8	24	54	99

Figure 4. curve of $F(E)$ for $n = 0$ and $0 < E(\text{meV}) < 40$.

(*c*) *Discussion :*

To compare the experimental results with the theoretical ones, we find the energy of the transitions as observed by Girault. We note that the difference is small and does not exceed 2%. This justifies the success of our method. Table 8 displays transition energies both theoretical and experimental transition energies.

Table 8. Comparison of theoretical results with experimental data.

Superlattice	S1		S2		S3	
Transition energies (meV)	Theor.	Exper.	Theor.	Exper.	Theor.	Exper.
$hh_1 \rightarrow e_1$	1048	1050	744	740	736	730
$hh_2 \rightarrow e_2$	*	*	801	800	762	760
$hh_3 \rightarrow e_3$	*	*	884	885	801	800
$hh_4 \rightarrow e_4$	*	*	985	990	851	850
$lh_1 \rightarrow e_1$	1138	1160	*	*	*	*

5. Conclusion

We have introduced a more simplified method which allows the determination of the band structure of non-symmetrical, non-periodical potentials samples. The energy quantification condition allows the determination of the energy levels for electron and hole by a simple look at the energy axis, and are indicated directly by vertical segments. The wave functions are easily deduced as well as the energy transitions. We have applied this method on both theoritical and experimental levels. Our finding shows a good agreement with previous experimental [16] and th

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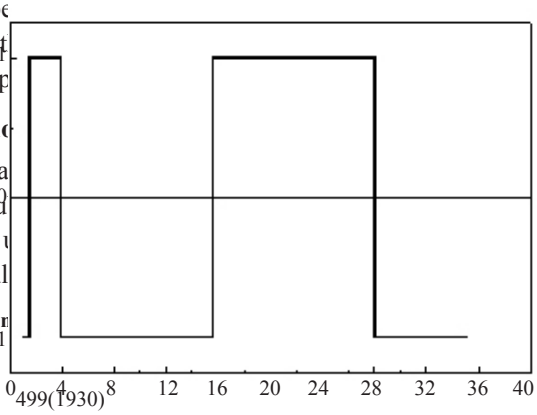

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