



ATHEORETICAL INVESTIGATION OF AlGa_N/Ga_N SUPERLATTICE NANOSTRUCTURES USING TRANSFER MATRIC METHOD

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Abstract

In this work a theoretical investigation for studying the resonant tunneling in multibarrier semiconductor heterostructures (AlGa_N/Ga_N) superlattice nanostructure has been presented. The behavior of wave function intensity has been studied for superlattice structures, by solving Schrödinger time independent equation using Transfer Matrix Method (TMM). TMM was used to find the eigen states. The transmission coefficient was estimated in the case of resonant tunneling of electrons through the barriers in heterostructures. From the obtained results it was found that the factors that affecting on the eigen states are barrier effective mass, barrier height and number of wells. The results of the wave function intensity obtained in the present work are compared with Ref.[1].

تم في هذا البحث تقديم دراسة نظرية لمميزات الشبكة الفائقة (AlGa_N/Ga_N) النانوية المصفاة من وصلات غير متجانسة وذلك من خلال حل معادلة شرودنجر غير المعتمدة على الزمن بطريقة مصفوفة النقل. ان من اهم المميزات التي درست في هذا البحث هي مميزات النفق الرنيني وذلك من خلال حساب معاملات النفاذ. حُسبت القيم الذاتية المقيدة لحالات النظام وتم التعرف على شكل الدوال الموجية المقابلة لها. درست هذه المميزات تحت تأثير عوامل مختلفة مثل الكتلة المؤثرة وارتفاع حاجز الجهد وعدد الآبار التي تكون الشبكة الفائقة.

1. Introduction

In the Semiconductor materials the electrical properties are directly related to the behavior of electrons in the crystal lattice. The behavior and characteristics of these electrons can be described by the formulation of Schrödinger's wave equation which will be applied to particular potential functions.

Heterojunction is a junction of different semiconductor materials having different band-gaps[2] as a result of the difference in the refraction index and the difference in band-gap energies of the materials used. The heterojunction structures can considerably increase device efficiency[3].

One important application of heterojunction is to use ΔE_c and ΔE_v to form barriers for carriers. A quantum well is formed by two heterojunction or three layers

of materials such that the middle layer has the lowest E_c for an electron well or the highest E_v for a hole well. A quantum well thus confines electrons or hole in a two-dimensional (2-D) system. When electron are free to move in a bulk semiconductor in all directions (3-D), their energy above the conduction-band edge is continuous.

In a quantum well, carriers are confined in one direction and the energy within this well is no longer continuous with respect to x-direction, but becomes quantized in subbands.

The most-important parameters for a quantum well are the well width and well height, It should be noted that the carriers can "leak" out of the well tunneling with finite probability.

When quantum wells are separated from one another by thick barrier layers, there is no communication between them and this system can only be described as multiple quantum wells. However, when the barrier layers between them become thinner, the wavefunctions start to overlap, a heterojunction superlattice is formed. The superlattice has two major differences from a multiple quantum-well system (1) the energy levels are continuous in space across the barrier, and (2) the discrete levels widen into minibands.

Crystalline semiconductor superlattices are usually constructed by growing two compounds, such as $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ where the lattice constants are almost identical. It has been reported by Esaki[4] that the model on superlattices is analogous to the Kroger-Penny model with the following conditions: (i) the barrier height is the energy mismatch in the conduction band edges of two materials with different compositions, (ii) the well and barrier regions are different and they correspond to the effective mass at the conduction band edges respectively.

Intensive research work has been carried out for the development of efficient optoelectronic devices based on quantum nanostructures. Recently, wide band gap III-V nitride semiconductor material[5] have received much attention due to their high potential for applications in optoelectronic devices, which covers wide range of spectrum from green-ultraviolet spectral region(307nm-550nm). These nitrides provide potential for the expansion of semiconductor technology for various applications ranging from televisions, traffic signals, scanners, flashlights, high-density optical storage memories and automotive backlighting [6]. The recent development in the field of GaN-based light emitting devices have stimulated several experimental and theoretical studies on GaN/AlGaIn heterostructures [7].

The resonant tunneling of an electron wave through multiple potential barriers is one of the basic phenomena in quantum mechanics. The theory of resonant tunneling was originally developed by Tsu and Esaki in the early 1970s[8]. Aishima and Fukushima [9] later extended the method to resonant tunneling structures with barriers and wells of different heights .

The wave function intensity has been calculated by squaring the wave function amplitude for the varying number of wells from 1 to 6. Transfer matrix method [10] has been used to obtain solutions of Schrodinger equation in well and barrier regions. The simulation is carried out using MATLAB software. Transmission coefficients have been determined for superlattice structures of different barrier heights.

The present work includes the followings. In the section 2, we explained the theoretical analysis of solving Schrodinger equation using TMM was presented. In the section 3, the theoretical model is simulated to understand the effects of some parameters, like barrier height, barrier effective mass, and number of wells on the eigen states values. Also, the transmission coefficients have been discussed for superlattice structures of GaN/Al_xGa_{1-x}N. Finally, the conclusions are summarized in the section 4.

2. Transfer Matrix Method

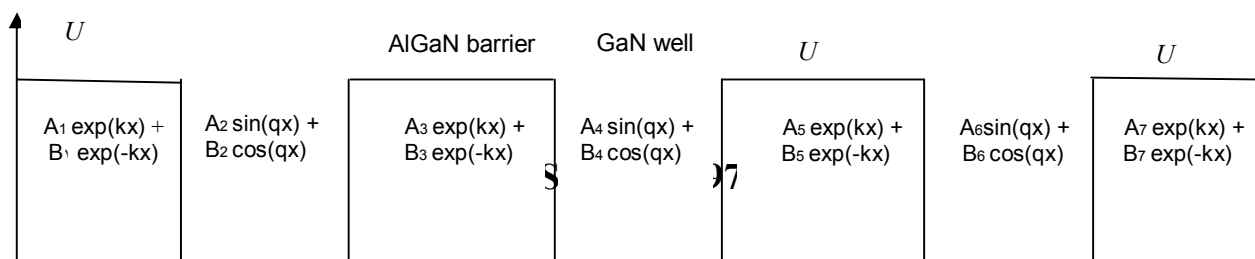
To understand the physical properties of device structures, it is important to simulate the expected performance on a computer. Here, we use TMM for its simplicity and to provide a reasonable accuracy. The variation of the effective mass and the barrier height due to the aluminum concentration have been included in our calculations. The fundamental equations that describe the electron spatial behavior is [1]

$$\frac{d^2 \varphi(x)}{dx^2} + \left(\frac{8m^* \pi^2}{h^2} \right) (E - U) \varphi(x) = 0 \quad \text{in the AlGaIn barrier} \quad (1)$$

$$\frac{d^2 \varphi(x)}{dx^2} + \left(\frac{8m^* \pi^2}{h^2} \right) E \varphi(x) = 0 \quad \text{in the GaN well} \quad (2)$$

Where $\Psi(x)$ is the wave function.

At this junction, E is the energy of electron, conduction band potential is zero and effective mass of electron m^* equal to m_w in the well region and in the barrier region conduction band potential is U and m^* is m_b . $\Psi(x)$ as in the sets of equations (1) and (2)



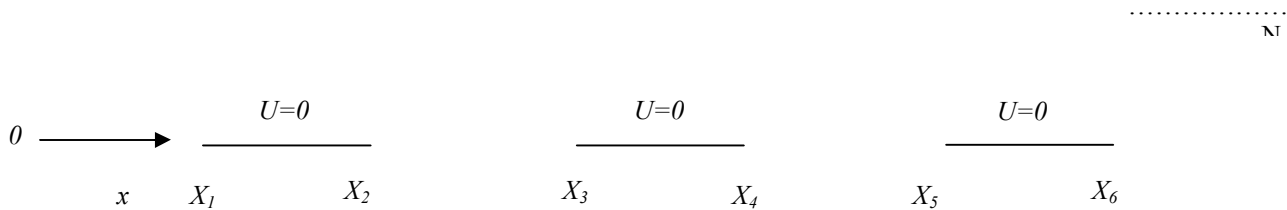


Figure1. Superlattice nanostructure consisting of three Quantum wells with solutions.

For the proper confinement of the electrons in the well, the energy E must be less than barrier height U . The superlattice nanostructures considered for the theoretical analysis for 3 wells is shown in Fig.1. The general solutions of the Schrodinger equation for this quantum nanostructure are as follows:

$$\left. \begin{aligned} \varphi_1(x) &= A_1 \exp(kx) + B_1 \exp(-kx), & x < 0 \\ \varphi_2(x) &= A_2 \sin(qx) + B_2 \cos(qx), & 0 < x < x_1 \\ \varphi_3(x) &= A_3 \exp(kx) + B_3 \exp(-kx), & x_1 < x < x_2 \\ \varphi_4(x) &= A_4 \sin(qx) + B_4 \cos(qx), & x_2 < x < x_3 \\ \varphi_5(x) &= A_5 \exp(kx) + B_5 \exp(-kx), & x_3 < x < x_4 \\ \varphi_6(x) &= A_6 \sin(qx) + B_6 \cos(qx), & x_4 < x < x_5 \\ \varphi_7(x) &= A_7 \exp(kx) + B_7 \exp(-kx), & x > x_5 \end{aligned} \right\} \quad (3)$$

Where, $q^2 = (8m^*\pi^2/\hbar^2)E$ and $k^2 = (8m^*\pi^2/\hbar^2)(U - E)$ are wave vectors in quantum well and barrier region, respectively. The following continuity conditions must be hold for each interface located at position x_i

$$\begin{aligned} \varphi_i(x_i) &= \varphi_{i+1}(x_i) \\ \frac{1}{m_i^*} \frac{d\varphi_i(x)}{dx} \Big|_{x_i} &= \frac{1}{m_{i+1}^*} \frac{d\varphi_{i+1}(x)}{dx} \Big|_{x_i} \end{aligned}$$

Where i represent the i th interface that takes value of $i=1,2,3,\dots,2nw$ where nw is number of wells. Applying the above continuity conditions wave function and its derivation at each interface between well and barrier regions, one can obtain the following recursive relation between the arbitrary coefficients (A_i s and B_i s) in a matrix form as follows:



$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \prod_{i=1}^{2n_w} M_{2i-1}^{-1} M_{2i} \begin{bmatrix} A_{2n_w+1} \\ B_{2n_w+1} \end{bmatrix} \quad (4)$$

Where $M_i^{-1} = \begin{bmatrix} \sin(qx_i) & \cos(qx_i) \\ \frac{q}{m_w} [\cos(qx_i)] & \frac{-q}{m_w} [\sin(qx_i)] \end{bmatrix}$

and $M_i = \begin{bmatrix} e^{kx_i} & e^{-kx_i} \\ \frac{k}{m_b} [e^{kx_i}] & \frac{-k}{m_b} [e^{-kx_i}] \end{bmatrix}$

Equation (4) can be written as

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = M \begin{bmatrix} A_{2n_w+1} \\ B_{2n_w+1} \end{bmatrix} \quad (5)$$

Here,

$$\begin{aligned} A_1 &= M_{11} A_{2n_w+1} + M_{12} B_{2n_w+1} \\ B_1 &= M_{21} A_{2n_w+1} + M_{22} B_{2n_w+1} \end{aligned} \quad (6)$$

To obtain the bound states, we must apply the boundary conditions on the wave function that the wave function must tend towards zero at the outer barriers that means the coefficients of the growing exponentials must be zero. In this case, with the origin at the 1st interface implies that $B_1 = 0$ and for last barrier $A_{2n_w+1} = 0$. Hence, the above equation would imply that $M_{22} = 0$. As all of the elements of M are function of k and q , which are both in turn are functions of the energy E , therefore energy satisfies the following non-linear equation, [1]

$$M_{22}(E) = 0 \quad (7)$$

Are called eigen states. which is determine through the Bisection numerical iterative method. The arbitrary coefficients will be follow simply by using eq.(4) and the envelope wave function has been deduced. Multiplying matrices together for the whole potential profile, the wave functions, corresponding to the eigenvalues are found for the whole system. For systems where the states are not bound and properly confined.

The transmission coefficient T is the ratio of the probability current density for the transmitted beam of particles to the probability current density for the incident beam thus:

$$T(E) = \frac{q}{k} \frac{|A_7|^2}{|A_1|^2} \quad (8)$$

TMM can be used to calculate the transmission coefficients as, or for our superlattice structure is,

$$T(E) = \frac{1}{M_{11}^* M_{11}} \quad (9)$$

where, M_{11} the first matrix element and M_{11}^* is its complex conjugate.

The motive behind using the TMM is to obtain the electron energy accurately and to analyze the transmission coefficients concurrently. The transmission



coefficients is necessary to study the tunneling of the electron through the superlattice. The transmission coefficient has been an important quantity since it provides most of the relevant information of the transport process in superlattice and it is characterized by a series of resonance peaks at specific incidence energies.

3. Results and Discussion

We have carried out detailed analysis of superlattice nanostructures in which thickness of well region and barrier is of the order of nanometers. The variation of electron energy with effective mass of electron in the barrier region has been studied for superlattice structure in Figure 2. The values of well and barrier width are optimized to be 2nm and 6nm respectively. The value of energy E was found to be decreasing with the increase in barrier mass. As the molar concentration of aluminum increases the barrier mass is increased. We have considered barrier height of 0.3112 eV for the superlattice consisting of 1,2,...,6 periods. The effective mass of the electron in GaN well region is taken to be $0.2m_0$. The decrease in the energy value is due to the inverse relation between energy and effective mass.

Figure 3. depicts the dependence of energy on the barrier height. Effective mass of electron in the barrier region and well region are $0.256m_0$ and $0.2m_0$ respectively for the superlattice consisting of 1,2,...,6 periods. It reveals that value of energy E is increasing with corresponding increase in barrier height.

The variation in energy with number of wells is shown in Figure 4 as number of wells is increased from 1 to 8. When the number of wells is increased, the energy is decreased due to the increasing in the whole structure length and a new energy state is generated when a new QW, is added to the structure. And for a superlattice when the number of periods became very large (approaches to infinity) a mini band will be generated. We notice that the width of the miniband is reduced with increasing the number of wells.

When the barrier thickness separating between two wells is large, the eigenfunctions have the same eigenvalue (they are degenerate) and the tunneling in such structure is very poor. To improve the tunneling properties, the separating distance must be reduced. This will allow the wavefunctions to overlap and the degeneracy will be removed, and in consequence, we will see two separate eigenstates.

Figure 5. demonstrates the ground state wave function intensity in MQW superlattice structure, for 1,2,...,6 wells, all have even symmetry.

The wave function intensity was computed by squaring the amplitude of wave function. The electrons are confining in well region because energy is less than the conduction band potential. The solution of Schrodinger equation consist of growing and decaying terms due to which wave function intensity increase in well region and decreases in barrier region. Due to interaction of wave functions between adjacent well regions in superlattice, wave functions will



overlap with each other. Therefore wave functions intensity in each well never reaches to zero.

In such superlattice structures, the wave function intensity is dominant in the central well for better confinement in the middle of the whole structure than other well regions.

Figures 6. and 7. The eigenfunction correspond to 1st excited state has odd symmetry, while the second excited state wave functions intensities, respectively for superlattice structure consisting of 3,4,...6 wells.

Figure 8. shows the dependence of transmission coefficient on the energy of an incident electron for different value of barrier heights. One way of quantifying the proportion of electrons that tunnel through is in terms of transmission coefficient, which is defined as the probability that any single electron impinging on a barrier structure will tunnel and contribute to the current flow through the barrier. Transmission coefficient has been deduced for the 3well superlattice structure. The barrier heights of 0.1503eV, 0.3112eV, 0.4827eV have been estimated corresponding to Aluminum mole fractions of 0.1, 0.2 and 0.3 in the AlGaN barrier respectively. For higher values of energy, transmission coefficient becomes oscillatory and peaks will be appeared corresponds to resonant tunneling. For asuperlattice will two wells, each resonant peak will be splitted into peaks, as shown in the figure. Transmission coefficient was found to be changing from 0.5599 to 0.9594 for $V=0.1503\text{eV}$, from 0.1231 to 0.9981 for $V=0.3112\text{eV}$, and from 0.0048 to 0.9659 for $V=0.4827\text{eV}$.

Fig 9 shows the wave function intensity of four quantum well superlattice and compared with [1]. Since the wave functions must have even or odd symmetry due to the symmetry of the superlattice, therefore, we can conclude that our calculations are more accurate than that presented in [1].

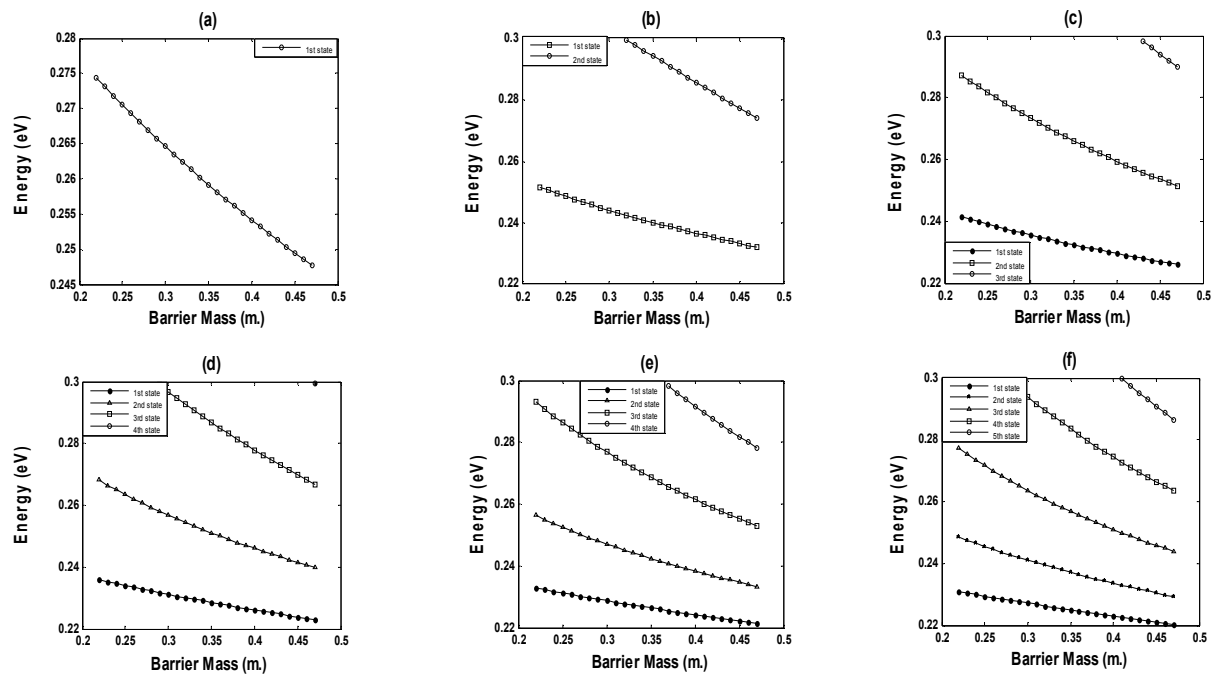


Figure 2. Variation of energy with barrier effective mass in superlattice MQW's, of(a)one (b)two (c)three (d)four (e)five (f)six QWs.

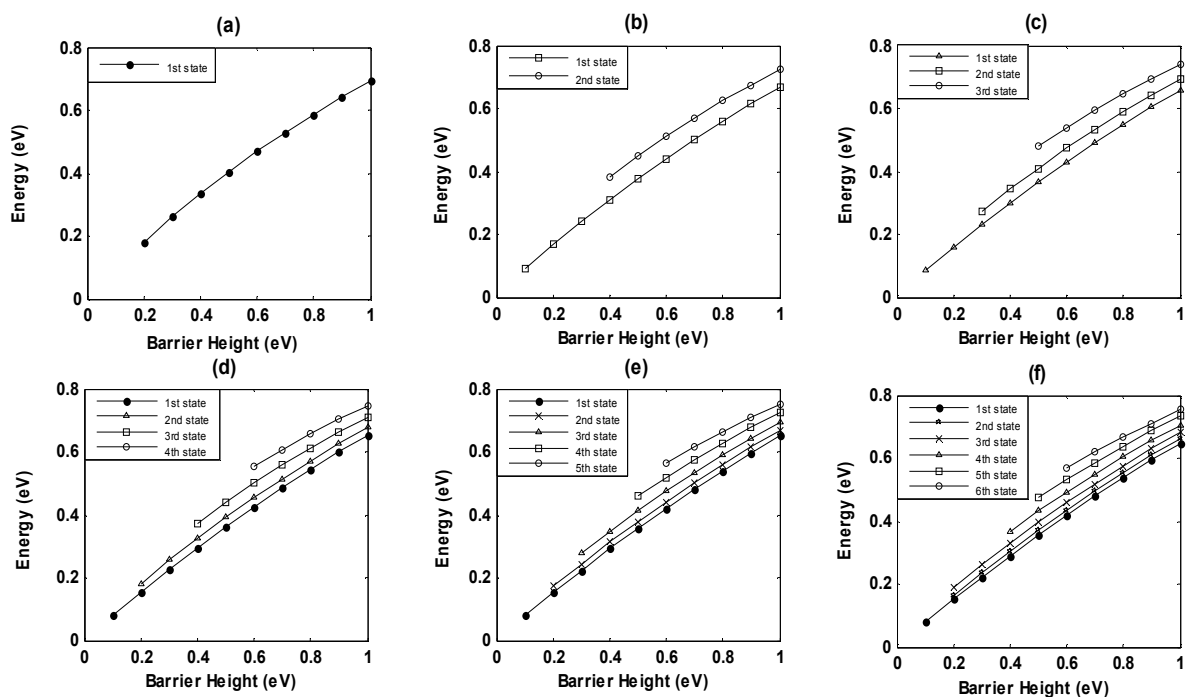
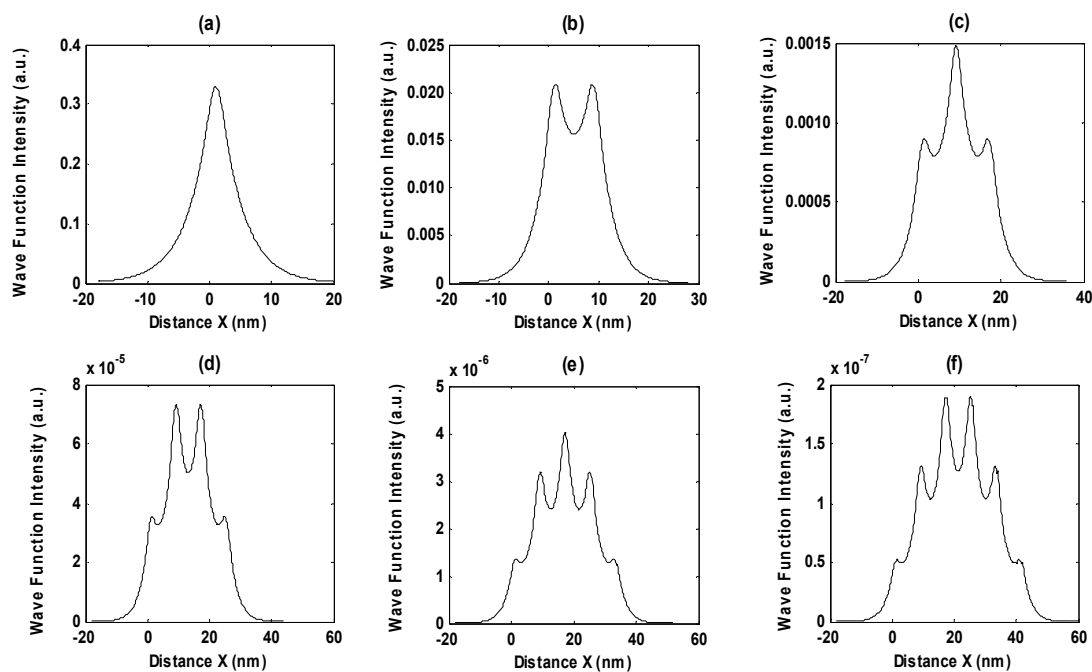
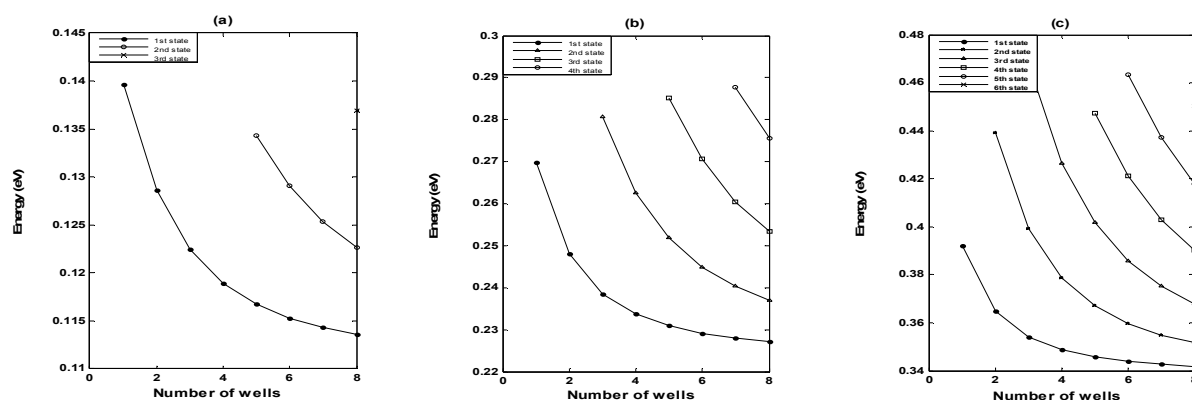


Figure 3. Dependence of energy on barrier height in multi wells, for(a)one (b)two (c)three (d)four (e)five (f)six QWs.



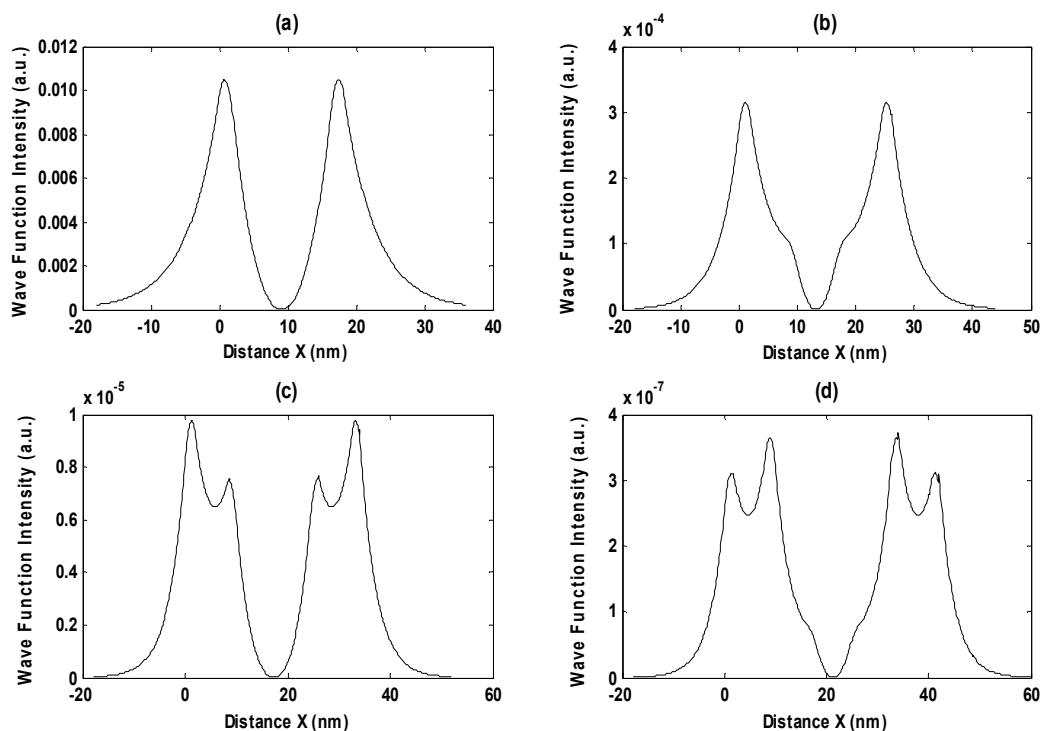


Figure 6. First state excited wave function intensity in multi wells superlattice structure for (a) three (b) four (c) five (d) six QWs.

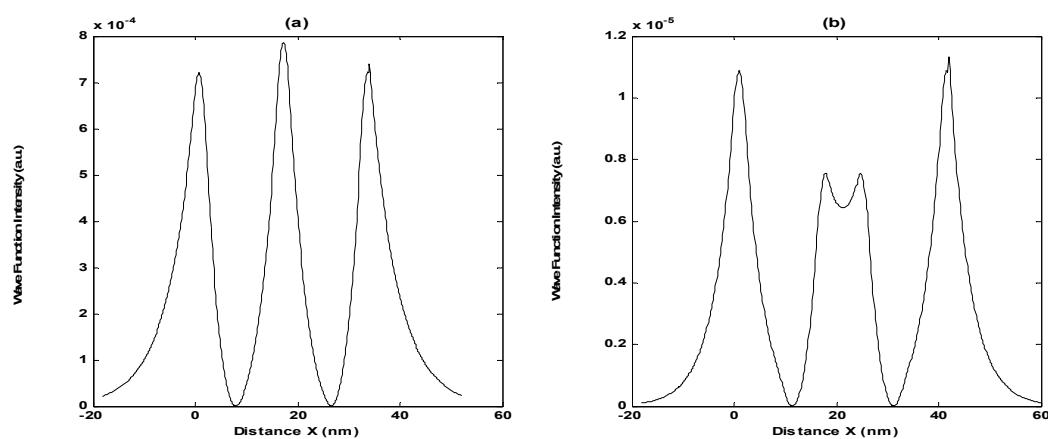


Figure 7. Second state excited wave function intensity in multi wells superlattice structure for (a) five (b) six QWs.

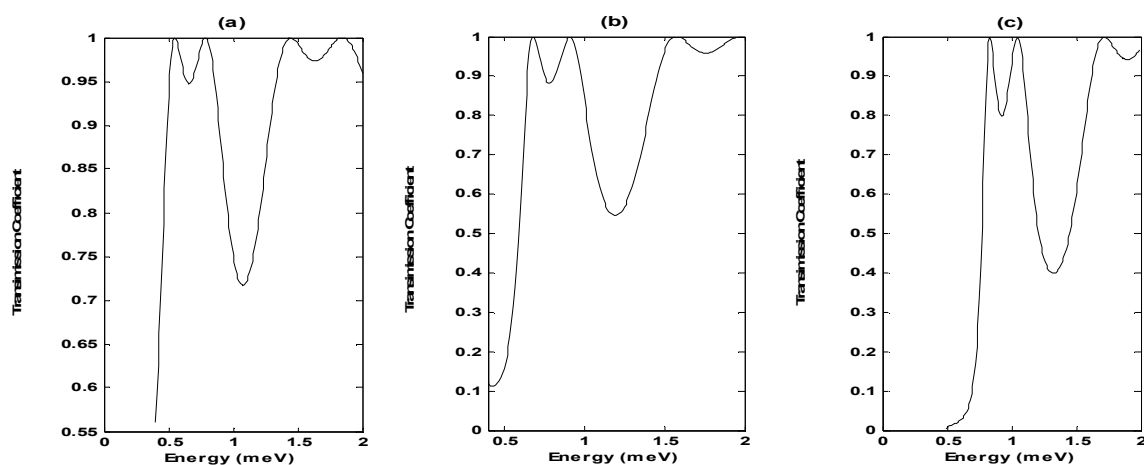


Figure 8. Transmission coefficient as a function of energy for different value of barrier height eV. (a) 0.4827 eV (b) 0.3112 eV (c) 0.1503 eV

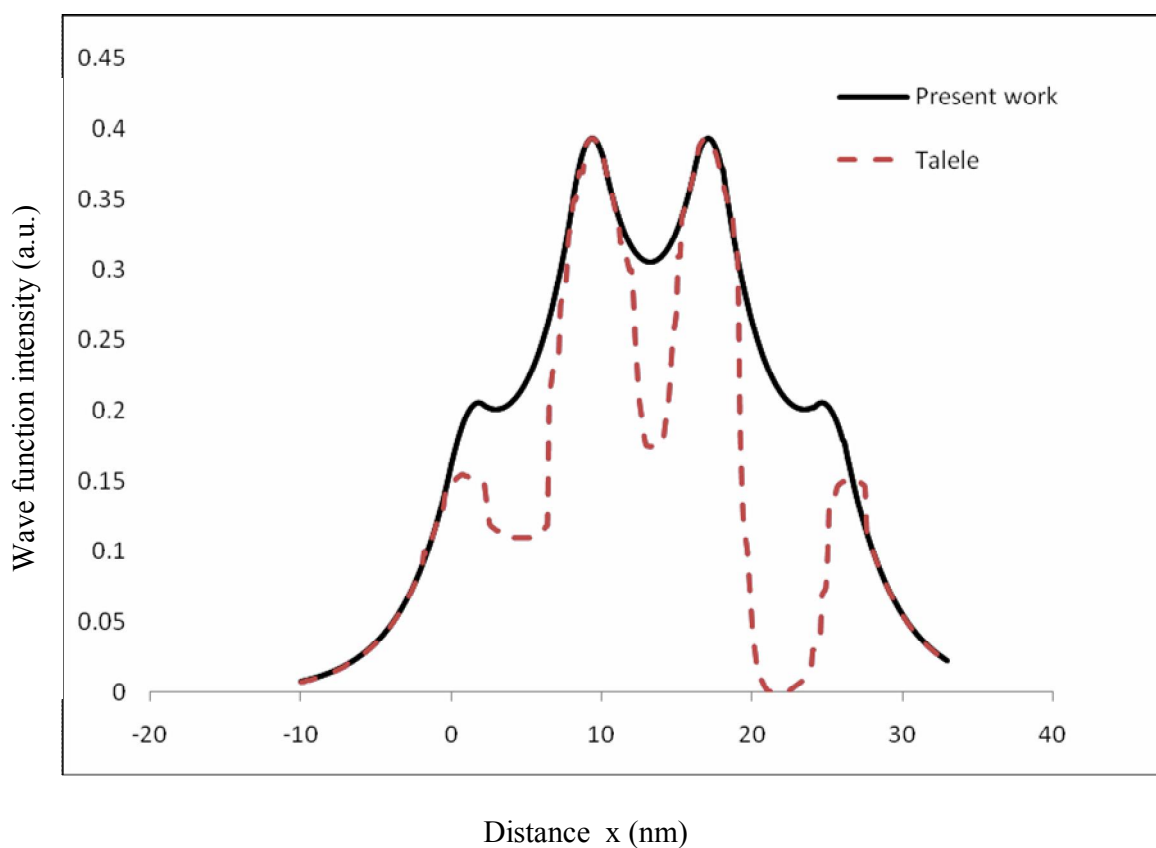


Figure 9. Wave function intensity in 4 QW superlattice.



4. Conclusion

After obtain the results, we concluded :

- 1-TMM uses for theoretical analysis of wave function intensity, energy and transmission coefficients by is effecient and effective.
- 2- When the number of the lattice period $s(N)$ are increase, a new state is appear and collect to the states group, this lead to mini band which as $N \rightarrow \infty$ produce continuous mini band which consist all states.
- 3- The width of each mini band is reduced with increasing number of wells.
- 4- Each resonating tunneling peak for isolated single QW will be splitted into N peaks in superlattice has N QWs and the tunneling properties will be improved.

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