Calculating Transmission Coefficient of Double Quantum Well Triple Barrier Structure Having Parabolic Geometry using Propagation Matrix Method

R. Karmakar, A.Biswas, S.Mukherjee, A.Deyasi

Abstract*— Transmission probability of a parabolic double quantum well triple barrier structure in presence of finite thick contact barriers is computed using propagation matrix method for GaAs/Al$_x$Ga$_{1-x}$As material composition. This provides the idea of tunneling at energies less than barrier potential. Effect of different barrier thicknesses and well widths are independently studied on transmission coefficient, and also for a specified structure, material composition of barriers is varied to observe the tunneling effect. Propagation matrix method is used for simulation purpose, and computation is performed considering effective mass mismatch at junctions following BenDaniel Duke boundary conditions. Conduction band discontinuity is also incorporated in the analysis by virtue of that consideration. Contact and middle barrier widths are varied for the same composition for different applications.

***Index Terms*— Effective Mass Mismatch, Parabolic Quantum Well, Propagation Matrix, Transmission Coefficient**

I. INTRODUCTION

Introduction of semiconductor nanostructure in existing VLSI technology may revolutionize the miniaturization techniques which lead to the design and possible implementation of novel electronic and photonic devices. Carrier confinement along reduced dimensions can be easily realized by quantum wells, wires, rings and dots which already provide several microelectronic and optical applications [1]-[4]. Researchers already made a lot of theoretical and experimental works in this context, precisely for one-dimensional confined structures [5]-[7]. Physical properties of heterostructure devices can be estimated from the knowledge of quantum transport processes, and precise estimation of transmission coefficient is essential for the device with incorporation of physical parameters [8]-[10]. Relative interdependency of these data should be taken into account when mathematical modeling is performed for increasing the level of sophistication.

Intense theoretical researches were already carried out to estimate electronic and optical properties of parabolic quantum wells. Occurrence of tunneling resonance was explained by Cruz [11], and QCSE was explained by Yamaguchi [12] in recent years. Effect of electric field on Stark resonance condition is also calculated by Yuen [13]. Absorption coefficient for interband optical transitions was important in designing optical transmitter using parabolic quantum well structures [14]-[16], and it is also compared with different quantum well shapes [17]. Intraband transitions in parabolic multiquantum well structures is calculated for designing novel infrared detector [18], and interband optical transitions in presence of midinfrared field [14] was computed for that sole purpose.

Several techniques have already been used by researchers to analyze double quantum well triple barrier structure such as Variational method [12], Fourier Series method [17], [19], Transfer Matrix approach [11], Propagation Matrix method [20], Finite Difference method [21] etc. Comparing all these methods, PMM is considered is as one of the accurate techniques as it can effectively be used to solve second-order differential equations. With this technique, transmission probability is computed for double quantum well triple barrier structure along with the incorporation of dimensional asymmetry.

The paper deals with theoretical computation of transmission coefficient of double quantum well triple barrier structure for GaAs/AlxGa1-xAs material composition for parabolic geometry. Contact barriers are assumed having finite thicknesses and well width is considered dimensionally greater than barrier width. Introduction of the concept of variable effective mass in the barrier and well layers makes the analysis more realistic from application point of view. Since effective mass of barrier material, and conduction band discontinuity of the heterostructure, both are assumed function of material composition, so mole fraction variation provides a good theoretical idea about resonant tunneling. Comparative analysis is also carried out for different barrier thickness for some particular well width and vice-versa considering effective mass mismatch at junctions.

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Contact barrier width is made different than middle barrier width to observe the change in transmission probability. Logarithmic scale of transmission coefficient is chosen to study the generated profiles.

II. MATHEMATICAL MODELING

Motion of a single electron in one dimension can be computed by using Schrödinger's time-independent equation:

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z)+V(z)\psi(z)=E(z)\psi(z) \qquad (1)$$

Incorporating the concept of effective mass mismatch, i.e. spatial variation of effective mass in Schrödinger's equation, we obtain

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m^*(z)}\frac{\partial}{\partial z}\psi(z)\right]+V(z)\psi(z)=E(z)\psi(z) \qquad (2)$$

In order to avoid differentiating discontinuous functions and producing infinities, solution of Schrödinger's equation (2) requires envelope function approximation that is both $\psi(z)$ and $(1/m^*)(\partial\psi(z)/\partial z)$ are continuous by considering electron transport across the heterojunction.

In the barrier and well regions, modified Schrödinger's equation's are-

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m_b^*(z)}\frac{\partial}{\partial z}\psi(z)\right]+V_b(z)\psi(z)=E(z)\psi(z) \qquad (3)$$

and

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m_w^*(z)}\frac{\partial}{\partial z}\psi(z)\right]+V_w(z)\psi(z)=E(z)\psi(z) \qquad (4)$$

where m_b^* & m_w^* are the effective masses of barrier and well regions, and V_b & V_w are potentials respectively. For the double quantum well triple barrier structure under consideration as shown in fig, wavevector for the problem may be defined as:

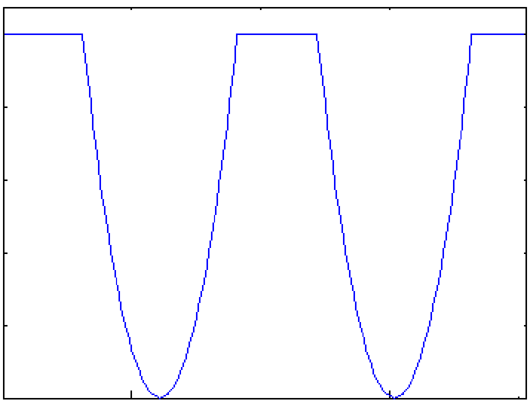

Fig 1: Schematic picture of double quantum well triple barrier structure having parabolic geometry with GaAs/$Al_xGa_{1-x}As$ composition

$$k_j=\left[\frac{2m^*\left(E-qV_j\right)}{\hbar^2}\right]^{0.5} \qquad (5)$$

The wave functions in regions *j* and *j* + 1 are

$$\psi_j=A_j\exp[ik_jx]+B_j\exp[-ik_jx] \qquad (6.1)$$

$$\psi_{j+1}=C_{j+1}\exp[ik_{j+1}x]+d_j\exp[-ik_{j+1}x] \qquad (6.2)$$

where A and C are coefficients for the wave function traveling left to right in regions j and j+1 respectively; B and D are the corresponding right-to-left traveling-wave coefficients. We assume that BenDaniel Duke boundary conditions are satisfied in all the junctions.

Propagation between potential steps separated by distance L_j carries phase information only so that

$$\psi A_j\exp[ik_jL_j]=\psi C_j \qquad (7.1)$$

and

$$\psi B_j\exp[-ik_jL_j]=\psi D_j \qquad (7.2)$$

This can be formulated as-

$$\begin{bmatrix}A_j\\B_j\end{bmatrix}=M\begin{bmatrix}C_{j+1}\\D_{j+1}\end{bmatrix} \qquad (8)$$

where

$$M=\begin{bmatrix}\exp[-ik_jL_j] & 0\\ 0 & \exp[ik_jL_j]\end{bmatrix} \qquad (9)$$

Thus, propagation matrix for j^{th} region can be written as:

$$Pj=\frac{1}{2}\begin{bmatrix}\left(1+\frac{m_j}{m_{j+1}}\frac{k_{j+1}}{k_j}\right)\exp[-ik_jL_j] & \left(1-\frac{m_j}{m_{j+1}}\frac{k_{j+1}}{k_j}\right)\exp[-ik_jL_j]\\ \left(1-\frac{m_j}{m_{j+1}}\frac{k_{j+1}}{k_j}\right)\exp[ik_jL_j] & \left(1+\frac{m_j}{m_{j+1}}\frac{k_{j+1}}{k_j}\right)\exp[ik_jL_j]\end{bmatrix} \qquad (10)$$

A flow of propagation matrix in different region of the concerned structure provides the transmission matrix which can be defined as-

$$T(E)=\frac{1}{(P_{11})^2} \qquad (11)$$

III. RESULTS AND DISCUSSIONS

The quantum structure considered for numerical computation of transmission coefficient is double well triple barrier one, where well is made by lower bandgap GaAs material, and barrier is fabricated by higher bandgap $Al_xGa_{1-x}As$ material. In this context, for better result, conduction band discontinuity is considered at the junctions, and effective mass mismatch is also taken into account following BenDaniel Duke boundary condition.

The quantum structure is first considered with dimensional symmetry, i.e., equal well and barrier widths at the top of conduction band structure, and transmission coefficient is calculated for equal effective mass and disparity in effective mass considerations. Fig 2 reveals the comparative study, which indicates that probability of transmission reduces when realistic concept is considered.

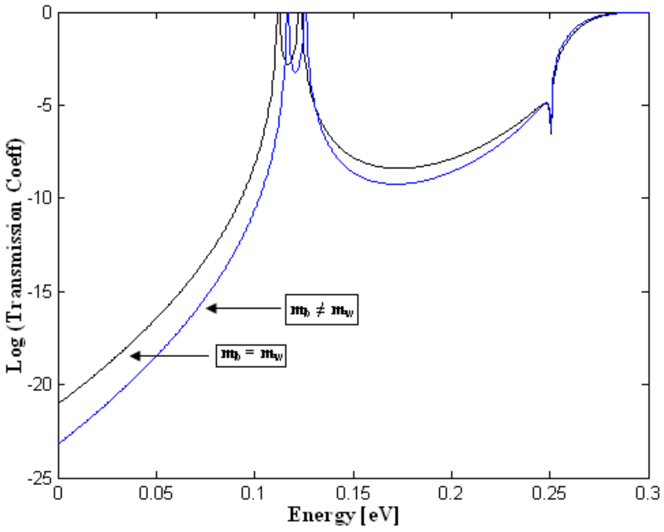

Fig 2: Comparative analysis of transmission coefficient with energy with and without considering effective mass difference at junctions

Introduction of dimensional asymmetry considering BenDaniel Duke condition leads to the variation of transmission coefficient profile within the specified energy range. Fig 3 shows that with higher barrier width, transmission probability reduces when well width is kept constant for potentially symmetric structure.

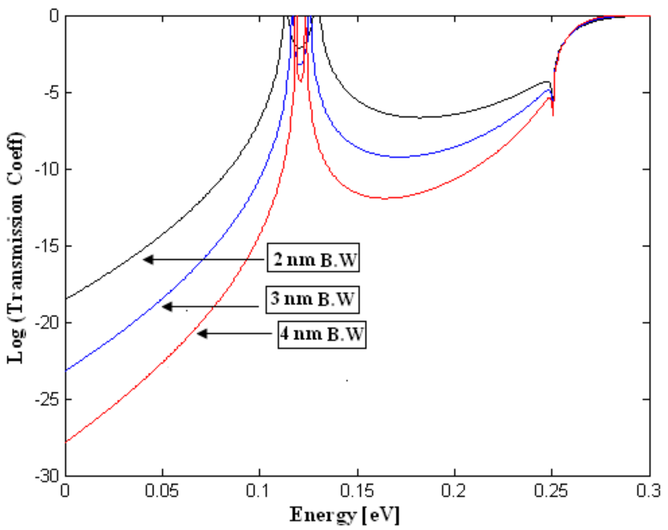

Fig 3: Transmission coefficient profile with energy for different barrier width for GaAs/$Al_{0.3}Ga_{0.7}As$ material composition

Similarly, well widths are varied in the same manner and it is revealed from fig 4 that with increase of well dimension, resonant tunneling phenomenon is evident at lower energy values. This is also plotted for potentially symmetric structure.

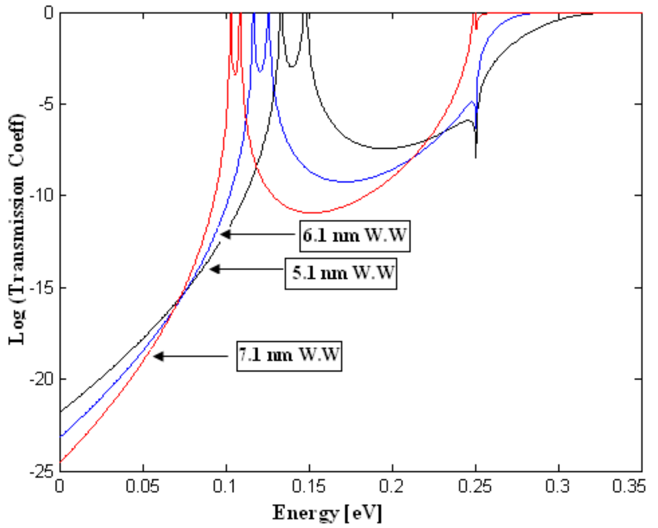

Fig 4: Transmission coefficient profile with energy for different well width for GaAs/$Al_{0.3}Ga_{0.7}As$ material composition

By varying potentials of both contact barriers and also of the middle barrier for otherwise dimensionally asymmetric structure and it is revealed that transmission probability reduces with increase of Al content in the barrier material. This is plotted in fig 5. This is due to the fact that with increase of Al mole fraction, both potential barrier (i.e. conduction band discontinuity) and effective mass mismatch at the junctions increase, and hence tunneling probability reduces.

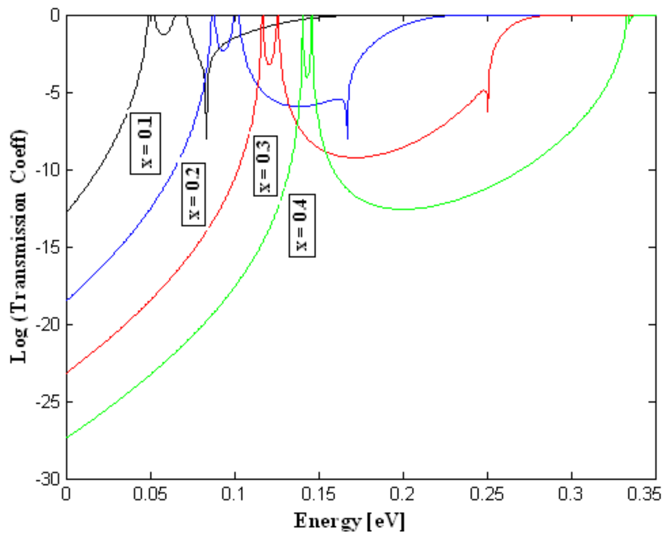

Fig 5: Transmission coefficient profile with energy for specified dimension and GaAs/$Al_xGa_{1-x}As$ material composition

Introduction of dimensional asymmetry between contact and middle barriers makes a variation in the transmission coefficient. Enhancement of middle barrier width restricts transmission, which can be justified from fig 6. The same effect can also be achieved by making higher width of contact barriers, can be observed from fig 7. Shift in resonance condition for these cases are compared with the earlier standard profile.

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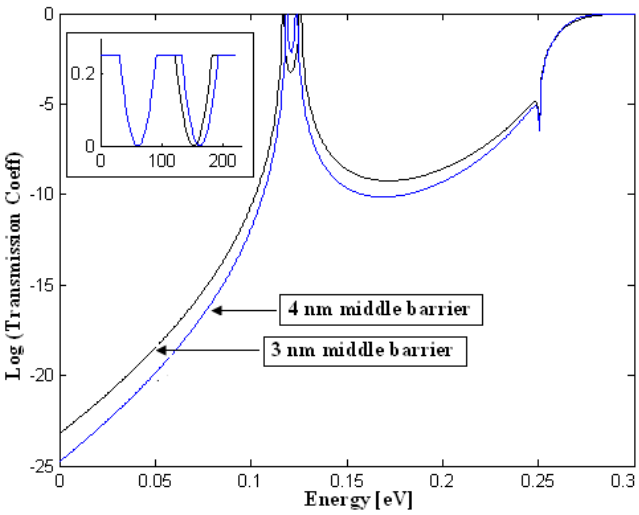

Fig 6: Transmission coefficient profile with energy for different middle barrier width for GaAs/$Al_{0.3}Ga_{0.7}As$ material composition

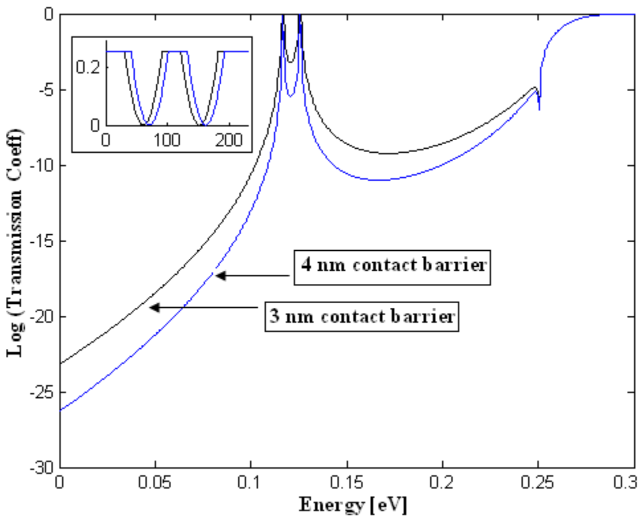

Fig 7: Transmission coefficient profile with energy for different contact barrier width for GaAs/$Al_{0.3}Ga_{0.7}As$ material composition

IV. CONCLUSION

Electronic and photonic properties of DQWTB structure are dependent on material composition and dimensional configuration precisely when parabolic geometry is considered. This analysis is far more important than rectangular structure as step potential configuration is ideal and fabrication limitations in existing microelectronic technology makes the well structure distorted. A close approximation of the fabricated structure is the parabolic geometry, for which the simulation is performed. By considering the mismatch in effective mass, it is observed that transmission probability decreases compared to the case when mismatch is not taken into account. Al composition is varied within type-I heterostructure limitation so that structure can be made potentially different, and resonant tunneling probability is computed for different cases. Existence of quasi-bound states can be verified by studying the origin of resonance peaks, and varying well widths and barrier thicknesses provides pictorial information of these states. This analysis can be further extended to analyze complex one-dimensional confined structures.

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