Composite Effect of BenDaniel Duke Boundary Condition and Material Composition on Eigenenergy of Multiple Quantum Well Structure

Arpan Deyasi, Swapan Bhattacharyya

Abstract*— Numerical simulation is carried out to determine of first three eigenstates of a multiple quantum well structure for both constant and variable effective mass cases where BenDaniel-Duke boundary condition is introduced for computation of effective mass mismatch along with the consideration of potential barrier dependence on material composition of higher band-gap material. Dimensional asymmetry is introduced to observe the change in eigenvalue, and no. of layers is also varied to observe the same in absence of electric field. GaAs/$Al_xGa_{1-x}As$ material composition is considered for simulation purpose to estimate tunneling probability. Variation of mole fraction provides a shift in eigenenergies for resonance transmission.

Index Terms*— Multiple Quantum Well Structure, Eigenenergy, BenDaniel Duke Condition, Material composition

I. INTRODUCTION

Recent theoretical works on the resonant tunneling in multibarrier heterostructures generates a lot of interest amongst researchers, as it helps to characterize the electrical and optical properties of ultrathin semiconductor devices, which can be developed by advanced material growth techniques, particularly molecular beam epitaxy and metallo-organic chemical vapor deposition [1]-[3]. Design of these nanoscale devices is based on the calculation of transition probabilities which requires exact evaluation of confined energy levels, and these may be varied by tailoring the material composition and thicknesses of intermediate layers. Thicknesses of the layers are comparable to the de-Broglie wavelength, and due to the relatively larger mean free path of electrons compared to the thickness, electrons travel throughout the structure maintaining phase coherence [4]. This leads to the formation of energy minibands, which ultimately determine transmission probability of the device. Computation of eigenenergy thus becomes the key factor for analysis of multiple quantum well structures, where material parameters along with near accurate picture of band diagram become important from simulation perspective, and the method adopted for the simulation also plays a vital role when level of accuracy is concerned.

Pioneering theoretical works on multibarrier ultrathin structures was carried out by Easki and Tsu [5]-[6] where electronic transport proceeds via resonant tunneling mechanism, producing a series of energy levels and associated subbnads due to quantization of carriers in the direction of confinement. This was later followed by several workers for development of a complete mathematical model on barrier transmission [7]-[8] for 1-D potential configuration. Later Mcllroy [9] analyzed the effect of carrier wavefunctions with special attention on wavefunction overlapping. Anemogiannis [10] also calculated the eigenstates and lifetime considering the scattering phenomenon.

MQW structure in presence and absence of electric field can generally be analyzed by Transfer Matrix Technique [7]-[8], [11]-[13] where time-independent Schrödinger's equation with proper boundary conditions is solved; which is also suitable for computation of eigenstates of dimensionally asymmetric structures. MQW structure subjected to unbiased conditions can be analyzed by different numerical procedures as suggested by previous workers like Variational Method [13], Airy's function approach [7], [15], Finite Element Method [16], Transfer Matrix Technique [11]-[13], [17]-[18], Weighted Potential Method [19]. Gildenblat [7] investigated the energy dependence and symmetry properties of the transfer matrix describing the tunneling and reflection processes in multiple asymmetric localized potential barriers. The idea of high-Q electron energy filter proposed by Shen [4] by increasing no. of well and barrier layers. Y.J.Hong et. al. [20] analyzed the structure in a different generalized approach to study resonant tunneling phenomenon, which can be used for computation of eigenstates of double barrier, double quantum well problems with proper boundary conditions.

The present paper deals with determination of eigenenergy of a superlattice structure in absence of applied electric field for $GaAs/Al_xGa_{1-x}As$ material composition, which is a reasonable experimental realization of the 1D confinement. BenDaniel Duke boundary condition [21] have been applied to solve the Schrödinger equation for the electronic envelope function and predict the electronic properties of multiple quantum well device, and a comparative study shows the importance of the

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condition when resonant tunneling is concerned. Several theoretical workers incorporated this method [22]-[24] along with the material parameters for computation of electron energy states, where dimensional asymmetry and layer number variation are introduced to observe the change in eigenvalue. Contact barriers are also taken into account to predict accurate transmission probability.

II. THEORETICAL CONSIDERATION

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

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

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

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

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

For the multiple quantum well structure under consideration,

$$\kappa_1=\frac{\sqrt{2m_b^*(V-E)}}{\hbar} \quad (3.1)$$

&

$$\kappa_2=\frac{\sqrt{2m_w^*E}}{\hbar} \quad (3.2)$$

where κ1 and κ2 are the wavefunctions, solution of equation (2) for different regions of the structure gives the eigenenergy of the device in absence of electric field.

Let the envelope-functions in well and barrier regions be $\psi_w(z)$ and $\psi_b(z)$ respectively, then the BenDaniel duke conditions can be written as-

$$\psi_w(z)\big|_{interface}=\psi_b(z)\big|_{interface} \quad (4.1)$$

and

$$\frac{1}{m_w^*}\frac{d\psi_w(z)}{dz}=\frac{1}{m_b^*}\frac{d\psi_b(z)}{dz} \quad (4.2)$$

Imposing equations (4.1) and (4.2) on (2), we can obtain eigenstates of the structure under consideration.

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

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m_b^*(z)}\frac{\partial}{\partial z}\psi(z)\right]+V_b(z)\psi(z)=E(z)\psi(z) \quad (5)$$

and

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m_w^*(z)}\frac{\partial}{\partial z}\psi(z)\right]+V_w(z)\psi(z)=E(z)\psi(z) \quad (6)$$

where m_b^* & m_w^* are the effective masses of barrier and well regions, and V_b & V_w are potentials respectively.

Effective mass of higher bandgap material is considered as a function of mole composition of Al & Ga, which also determines the conduction band discontinuity, taken into account for computation purpose, as it determines the potential barrier height; i.e., composite band diagram of the superlattice.

III. NUMERICAL ANALYSIS

Numerical computation of first three eigenenergy states of multiple quantum well structure having 8 wells and 7 barriers starts with a realistic consideration of finite thickness of contact barriers and they are made of $Al_xGa_{1-x}As$ material, which is generally not considered in various literatures for simplification purpose, but extremely important from experimental point-of-view. Variation of barrier width for constant well width and barrier height for both constant and variable effective mass cases provide same nature where eigenvalue has a greater magnitude when effective mass mismatch at junctions are taken into account.

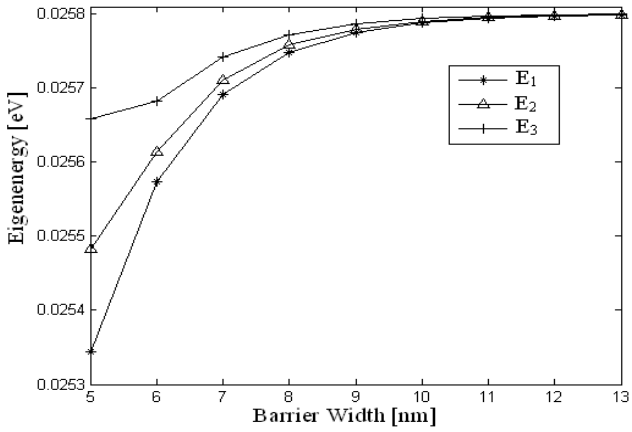

Fig 1: Eigenenergy profile for first three eigenstates with barrier width for constant effective mass

When barrier and well have comparable dimensions, eigenstates form a miniband, but as the dimensional mismatch increases by decreasing barrier width, the miniband collapses and distinguishable energystates may be observed for both the conditions. These are described in fig 1 & fig 2.

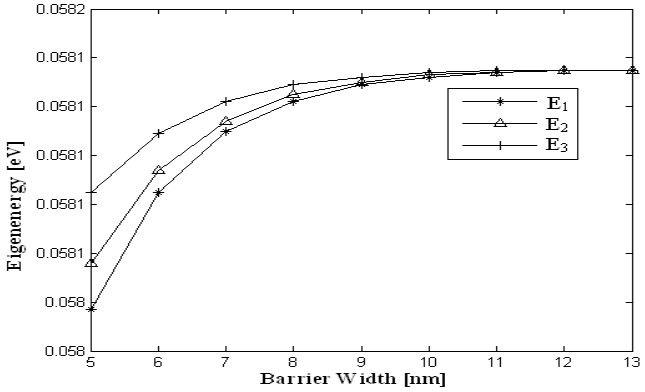

Fig 2: Eigenenergy profile for first three eigenstates with barrier width for variable effective mass

Variation of well width shows a much reduced effect on eigenenergy when separation between the states are concerned, i.e. miniband exists irrespective of well width when barrier has a considerable dimension. With increment of well width for both the effective mass condition, eigenvalues decrease exponentially. Fig 3 shows the constant effective mass case.

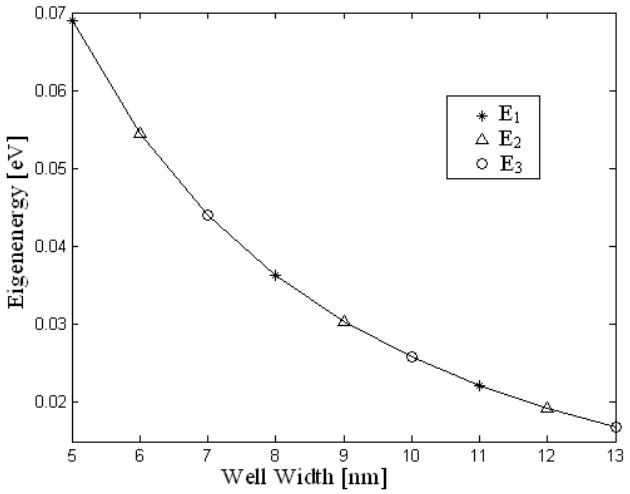

Fig 3: Eigenenergy profile for first three eigenstates with well width for constant effective mass

When Ben-Daniel duke condition is implemented, it is observed that for comparative dimensional considerations, eigenvalues begin to become constant, and for higher well width, they are independent of device dimensions, as concluded from fig 4.

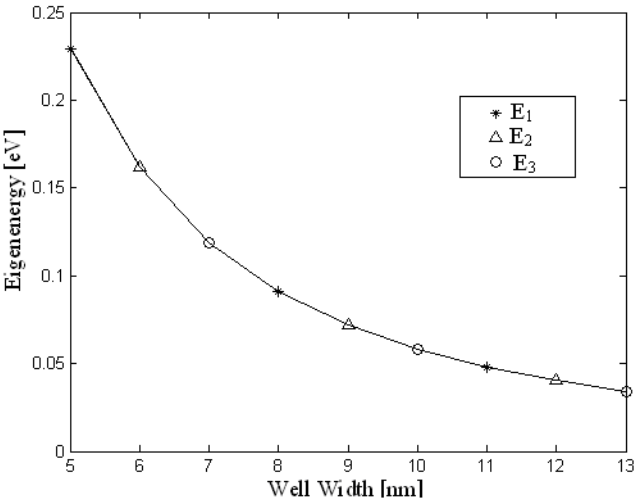

Fig 4: Eigenenergy profile for first three eigenstates with well width for variable effective mass

By increasing number of well layers, it is observed that when effective mass is constant throughout the structure, ground state energy remains almost unchanged, whereas it reduces when higher states are considered. This is shown in fig 5.

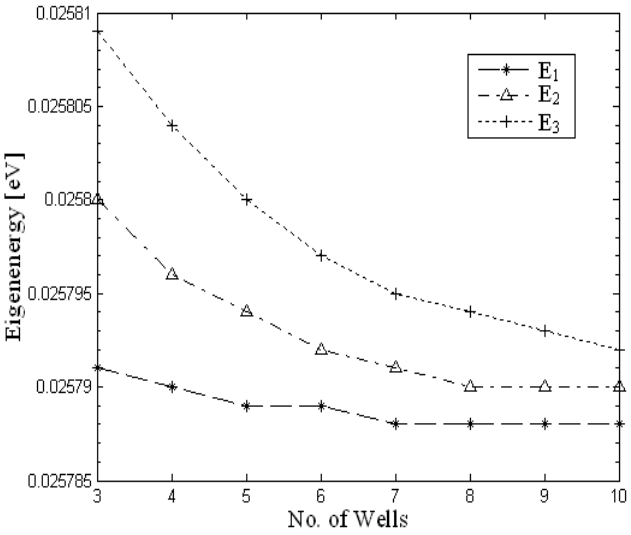

Fig 5: Eigenenergy profile for first three eigenstates with number of well layers for constant effective mass

Considering mismatch at junctions, it is found out that for less number of layers, first two states of eigenenergy decreases, but for higher states, it decreases rapidly, as depicted in fig 6. For sufficient no. of layers, minibands start to form.

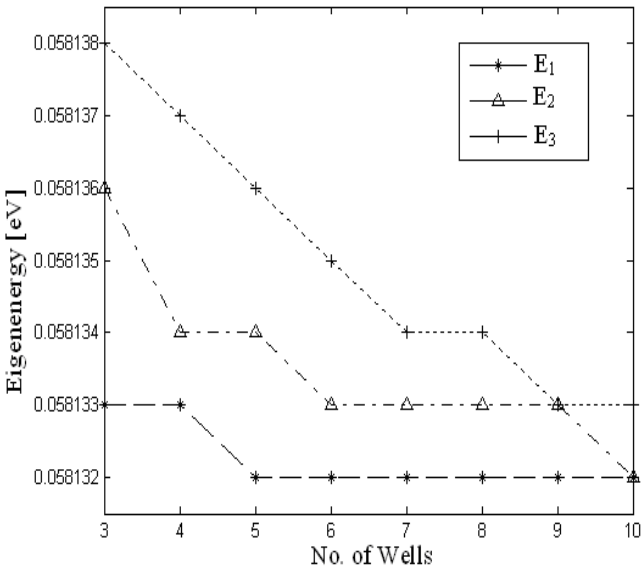

Fig 6: Eigenenergy profile for first three eigenstates with number of well layers for variable effective mass

By varying the potential height of the higher bandgap material, i.e., changing the material composition of AlGaAs, it is observed that eigenenergy starts increasing and for GaAs/$Al_{0.3}Ga_{0.7}As$ composition, eigenstates attain maximum value; then show a decreasing nature. This is pictorially represented in fig 7.

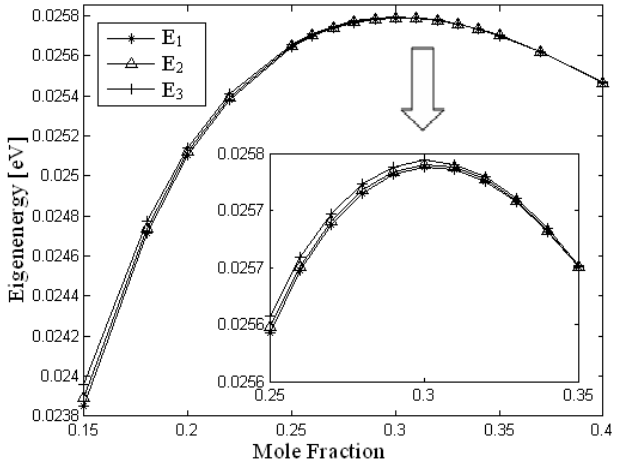

Fig 7: Eigenenergy profile for first three eigenstates with Al mole fraction for constant effective mass

But considering mismatch at heterojunctions, peak of the eigenstates occur at GaAs/$Al_{0.12}Ga_{0.88}$As composition, then a rapid decrement occurs, as shown in fig 8. Simulation is carried out for that range, when AlGaAs remains direct bandgap material. It is also noted that when Al mole fraction exceeds 0.2, miniband formation begins, as difference between consecutive two states becomes extremely small.

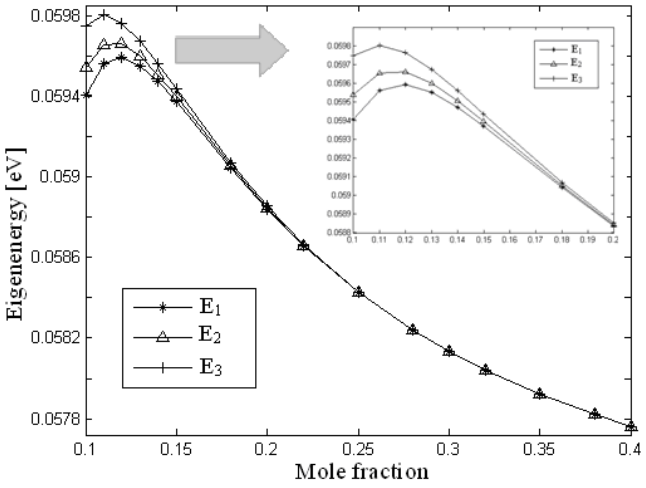

Fig 8: Eigenenergy profile for first three eigenstates with Al mole fraction for variable effective mass

IV. CONCLUSION

From the analysis, it may be concluded that when barrier potential and effective mass are considered as function of material composition for computation of eigenstates, a large variation is observed which is important from fabrication point-of-view. Resonant tunneling can only be possible at eigenstates, and thus proper design and modeling of structure is required for wave-function engineering. Modification of spatial dimension is also included to add flexibility. Finally, it can be stated that incorporation of complex effects such as many-electron interaction, interface scattering etc. have a sensitive effect on eigenenergies and therefore, should be considered in constructing a complete picture about transmission.

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