

ON THE QUANTUM CONFINEMENT EFFECT OF MISSEN ELECTRON AND ELECTRON
CHARGE CARRIERS IN A TYPICAL SYNTHETIC SEMICONDUCTING SYSTEM

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ABSTRACT

An investigation on the quantum confinement effect of electron and missen electron, when decoupling has not taken place in a synthetic semiconductor structure of GaAs/AlGaAs has been carried out. We have derived analytical expressions of bound state energies from a careful study of the transcendental equation which reproduce impressively well, the numerical solutions of the corresponding transcendental equation for all confinement sizes and potential barrier without any adjustable parameter. These expressions depend on a unique parameter which contains the barrier height and well width. The investigation reveals that the optical absorption data in conjunction with computed energy level based on non-parabolic effective mass theory yielded the needed information (tunneling, exerted force on the wall just before tunneling, critical layer thickness, misfit dislocations etc) about the quantum confinement effect in the structure. Steeper graphs were obtained due to the large band offset (energy gap difference between the composite materials). Also, confinement energy is inversely proportional to the effective mass whereas, confinement potential depends on the direction of the structure.

Keywords: Missen–Electron, Supper Lattices (SL), Multiple Quantum Well (MQW), Quantum Size Effect (QSE), Parabolic.

INTRODUCTION

Nanotechnology has made an intensive impact over the properties of wide band gap semiconductor materials which play an important role in opto–electronic devices. Exploring the band gap engineering, creating artificial constraints on the carrier movement, tailor made combinations of hetero–structure materials are the significant tools to enhance the structural and optical properties of semiconducting materials according to the applications. There have been the establishment and development of nanostructures, which are called

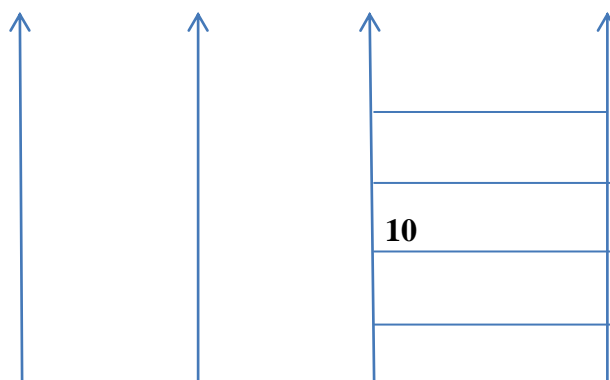
super lattices (SL) or Multiple Quantum Wells (MQW) depending on the width of the barrier layers or simply called Hetero-structure. In the study of the properties of electrons, phonons and excitations in either an infinite crystal or one with a periodic boundary condition, in the absence of defects, these particles or excitations are described in terms of Bloch waves, which can propagate freely throughout the crystal. Suppose the crystal is finite and there are now two infinite barriers, separated by a distance L , which can reflect the Bloch waves along the Z -direction. These waves are then said to be spatially confined. Three types of models are said (Adelabu, 1993) to be used to calculate the confinement energies of electron and hole (Missen-electron) in a super lattices or Multiple Quantum Well in addition to the infinite potential well and particles in box models. These are:

- i. Kronig- Penney Model (Kronig and Penney, 1930)
- ii. Kane Model in the Envelope Function Approximation
- iii. Tight Binding Model (Schuurmans and Hooft, 1985; Schulman and Chang 1985).

This paper presents the report of investigations on the quantum confinement effect of charge carriers in GaAs/AlGaAs quantum well (QW) systems using the effective mass band structure calculation including non-parabolic in both the well and barrier layers.

THEORETICAL BACKGROUND AND CALCULATION

Quantum size effects in semiconductors occur when the size of the particle is small in comparison with Bohr excitonic radius which is the natural length scale of the Electron – Missen electron pair (Dingle *et al* 1975). This effect is a direct consequence of the confined electron and hole motions in three-dimensional space. Quantum confinement effect is characterized by electronic transitions which have been shifted to higher energies upon decrease of the size of the particle. Qualitatively this Confinement effect is similar to the problem of particle in a box (Beck *et al* 1992). Energy band calculations in Low dimensional structures (LDS) have been the subject of some earlier publications among which are those of Adelabu *et al* (1989, 1996 and 2002). Fig a represent a model for infinite potential well while fig b represent a model for finite potential well, capped at $n = 4$. Calculations of the energy band structure establish the key features of the electronic structures of solids. Thus, this provides the quantitative interpretations of numerous experimental results, which also guides further investigations.



n=4	E4
n=3	E3
n=2	E2
n=1	E1

Fig a. Infinite Potential Well

Fig b. Finite Potential Well

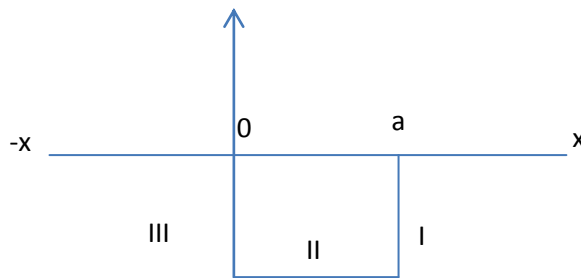


Fig c. Coordinate System of a Potential Well

The Schrodinger equation of the coordinate system in the potential well as shown in figure c is;

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi}{dz^2} + V\psi = E\psi$$

Where

$$\begin{aligned} V = 0 & \quad \text{for } x > a \text{ (region I)} \\ V = -V_0 & \quad \text{for } 0 < z < a \text{ (region II)} \\ V = 0 & \quad \text{for } z < 0 \text{ (region III)} \end{aligned}$$

For bound states, we need $-V_0 < E < 0$. Let

$$k^2 = \frac{2m^*(E + V_0)}{\hbar^2}$$

and

$$k^2 = \frac{2m^*E}{\hbar^2}$$

The Schrodinger equation thus becomes;

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{for (region II)}$$

and

$$\frac{d^2\psi}{dx^2} - k^2\psi = 0 \quad \text{for (region III)}$$

that have solution

$$\psi = A \sin kz + B \cos kz \quad \text{for } 0 < z < a .$$

$$\psi = Ce^{-kz} + De^{kz} \quad \text{for } z < 0 \text{ and } z > a .$$

The requirement that $\psi \rightarrow 0$ as $z \rightarrow \pm\infty$ demands that

$$\psi = Ce^{-kz} \quad \text{for } z > a \text{ (region I),}$$

$$\psi = De^{kz} \quad \text{for } z < a \text{ (region III)}$$

The boundary conditions that ψ and ψ' be continuous at $z = 0$ and $z = a$, then give,

$$A \sin ka + B \cos ka = Ce^{-ka} ,$$

$$-A \sin ka + B \cos ka = De^{-ka} ,$$

$$Ak \cos ka - Bk \sin ka = -Ck e^{-ka} ,$$

$$Ak \cos ka + Bk \sin ka = Dk e^{-ka};$$

For solutions for which not all A, B, C, D vanish, it is imperative to have either $A = 0, C = D$ or $B = 0, C = -D$.

Solving the Schrodinger wave equation with all the necessary boundary conditions give the eigenvalue as:

$$E_n = \frac{\pi^2 \hbar^2}{2m^*} \left(\frac{n}{L_z}\right)^2$$

\hbar = reduced planck constant.

n = Quantum number

m^* = Free electron mass

m_0 = the effective mass

L_z = well width

In this article, the confinement energies with the well width for electron and hole are computed, using the infinite potential well expression for the artificial semiconductor GaAs/AlGaAs using difference of 1°A for well width between 0-500°A; with GaAs as the well and AlGaAs as the barrier. A Matlab programming for the above equation was written to generate the confinement eigenvalues with the varying well width at different energy levels n=1,2,3,4,5.

Parameters

Electron mass = $0.067m_0 = 6.097e-32$

Missen electron mass = $0.532m_0 = 4.8412e-31$

Where $m_0 = 9.1e-31\text{kg}$

NUMERICAL RESULTS AND DISCUSSIONS

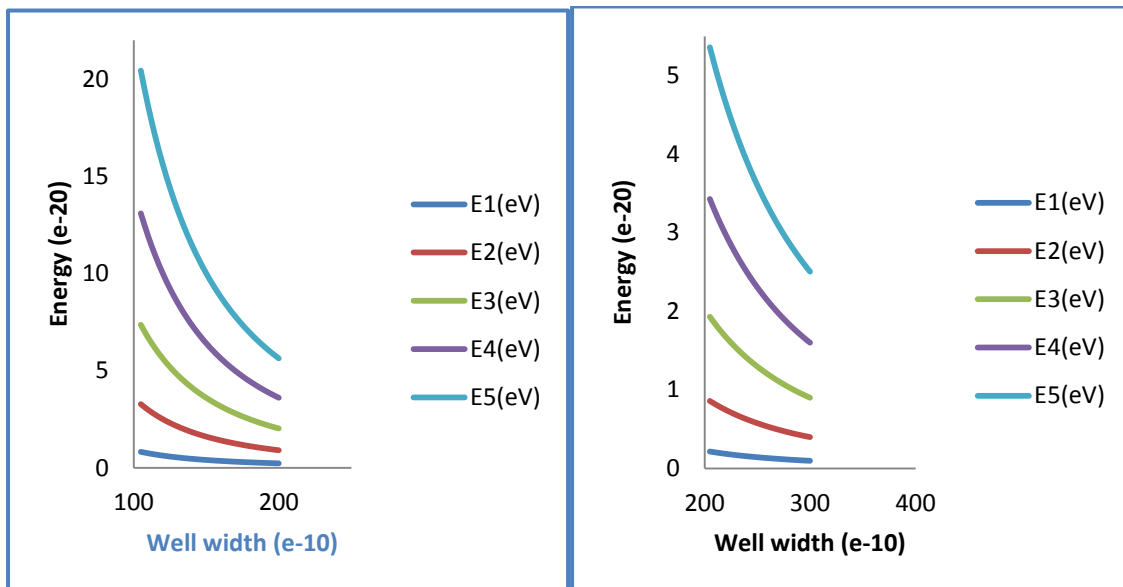


Fig 1. Electron energy against Well width

Fig 2. Electron energy against Well width

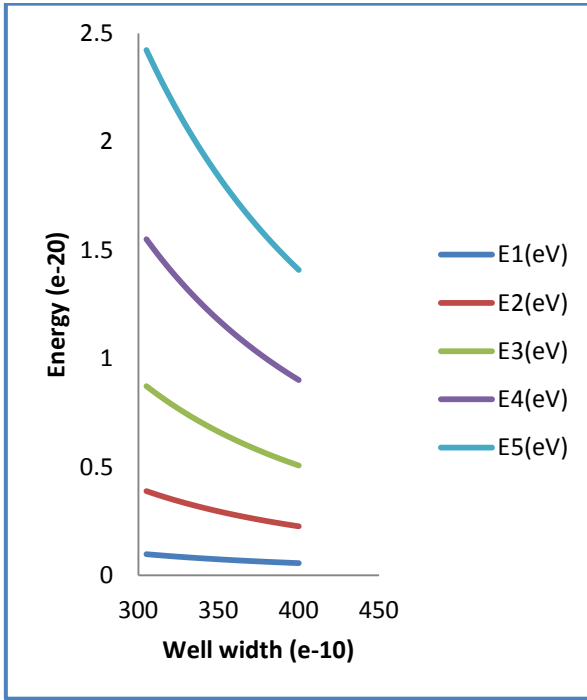


Fig 3. Electron energy against Well width

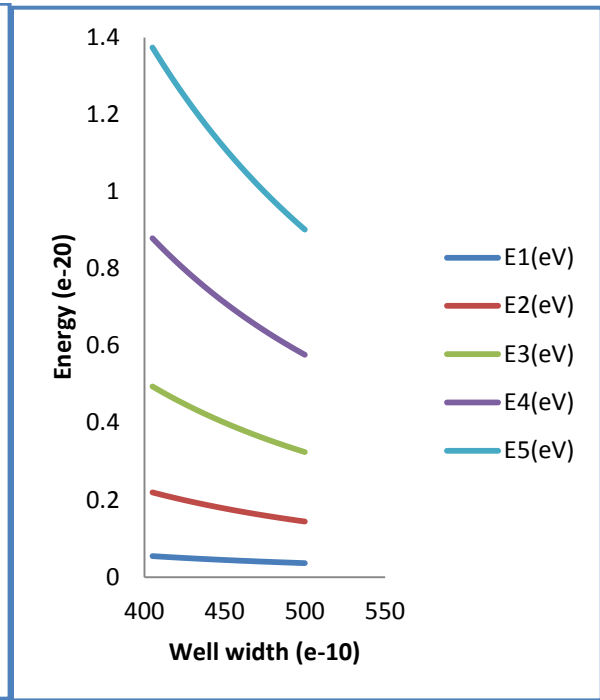
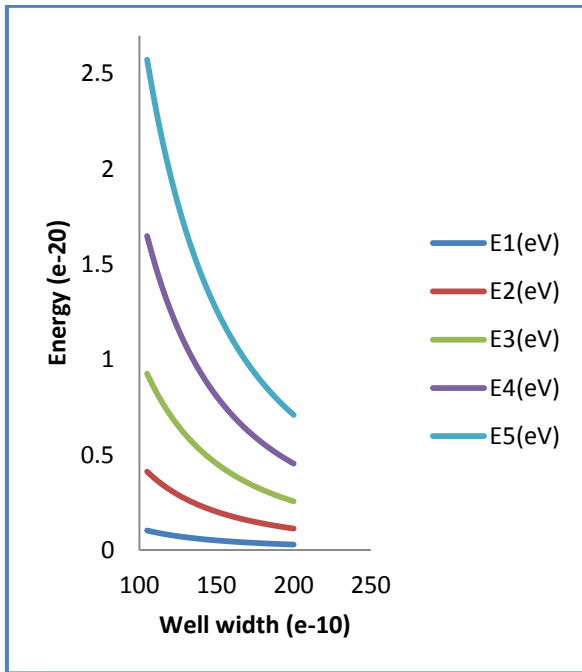


Fig 4. Electron energy against Well width



5. Missen-electron energy against Well width

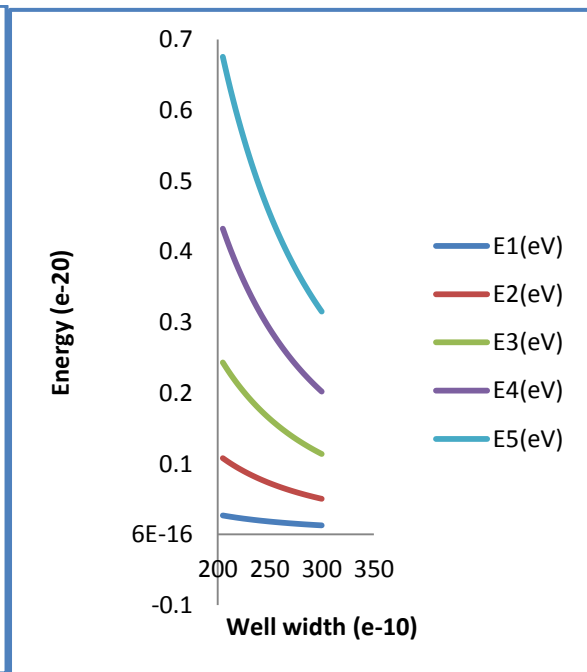


Fig 6. Missen-electron energy against Well width

Fig

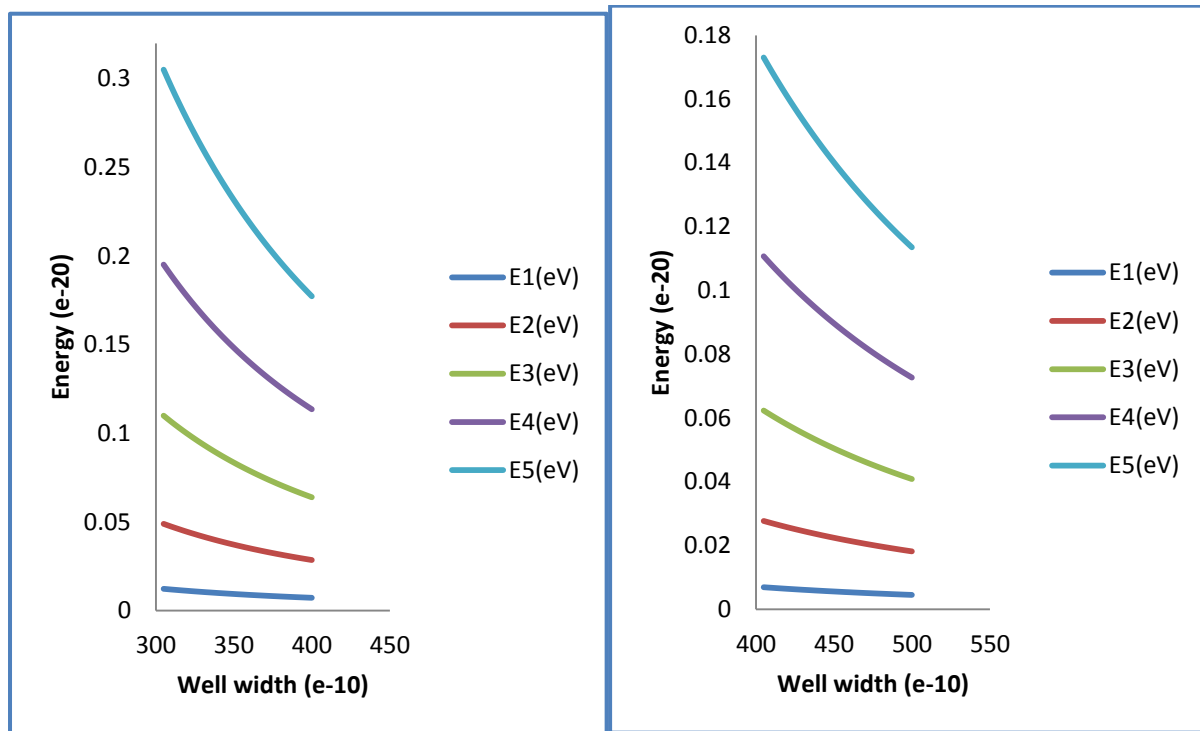


Fig 7 Missen-electron energy against Well width

Fig 8. Missen-electron energy against Well width

An electron or missen electron confined in a one-dimensional synthetic semiconducting system have its eigenstate computed and the results are presented in the figures 1,2,3,4,5,6,7,8. The eigenvalues for electrons as generated from the written program is as presented in figures 1,2,3, 4 while the eigenvalues for missen electrons are presented in figures 5,6,7,8. As evident from all the figures, the eigenvalues for the electrons and missen-electron increases as the energy level increases for any particular well width and the eigenvalues decreases as the well width increases for each particle at a particular energy level. The graph is steeper and infinitesimal due to the large energy gap difference between the composite materials. This difference is known as band offset. This shows that energy cannot be zero for any of the particles as the well width approaches zero under any consideration.

CONCLUSION

The eigenvalue for the electrons and missen electrons increases as the energy level increases for any particular well width and the eigenvalues decreases as the well width increases for each particle at a particular energy level. The number of bound states lying within the well decreases as the well width becomes smaller. Confinement energy is inversely proportional to the effective mass while confinement potential depends only on the direction.

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