



ANALYTICAL MODELING FOR NANOSTRUCTURE QUANTUM WELLS WITH EQUISPACED ENERGY LEVELS IN SEMICONDUCTOR TERNARY ALLOYS ($A_x B_{1-x} C$)

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ABSTRACT

The purpose of this study is to formulate an Analytical model of equispaced energy levels quantum wells (QWs) in semiconductor ternary alloys ($A_x B_{1-x} C$). The procedure is by mapping the envelop function Schrodinger equation for realistic QW, with the local conduction band edge as the potential experienced by an electron in the QW into an effective mass Schrodinger equation with a linear harmonic oscillator potential by the method of coordinate transformation. The electron effective mass and potential are then obtained as the signature for the equispaced energy level for QWs in semiconductor ternary alloys.

Keywords: Semiconductor nanostructures, Ternary alloys, Quantum wells, Equispaced energy levels, Effective mass.

1. INTRODUCTION

Confinement of electrons in nanostructures gives rise to quantum effects [1-3]. One of these effects is that experimental measurement involving these confined electrons are influenced by their environment and consequently prone to errors [4, 5] such as decoherence [6-8]. Consequently, many of the application of these nanostructures especially those that require emission and absorption are often affected by decoherence which usually affect quantum system. The nano-structuring of semiconductor materials was first introduced by Shockley [9] and later by Kroemer [10], however the progress of nanofabrication technology was affected by decoherence [9-12]. This has instigated the search for designs which may reduced the decoherence which cannot in principle be eliminated for the obvious reasons of the size of the nanostructure and that there is no physically isolated quantum system in nature [6, 13]. One possible way to reduced the effect of decoherence may be to design semiconductors nanostructure with equispaced energy levels which will lead to coherent emission and absorption.

The mapping of the Schrodinger equation set up for the semiconductor nanostructure into appropriate dimensional simple harmonic oscillator (SHO) by coordinate transformation approach yield equispaced energy levels in a QW and the eigenfunction are given by the well-known hermite polynomials. Since the goal of physics is to account for all physical phenomena, irrespective of their complexities, with the few known ones, mapping of semiconductors nanostructure into the SHO will enable us to obtain its appropriate solution for the effective mass function $m(z)$, potential function $v(z)$, grading function $x(z)$ and the electron wave function $u(z)$ are signature for the equispaced energy levels for the semiconductor ternary alloys QWs [14-17] the reasons for calculating the effective masses is because they can be used as inputs for further single band calculations so as to obtain the electronic structure when the absolute size of the structures is known [23] further, the carrier effective masses of a QW is strongly connected to the carrier mobility, is one of the most important devices parameters. The reason being that low carrier effective mass means the parent materials is highly

suitable for high speed carrier mobility applications. Our choice of ternary alloys QWs for this preliminary study is motivated not only by the need to generalized previous studies [16, 17] of 1D for the semiconductor ternary alloys ($A_x B_{1-x} C$) but also because many of the physical effect in quantum well structures can be seen at room temperature and can be exploited in real device.

2. ANALYTICAL MODELLING

For an electron confined in a QW, the Schrodinger equation is given as,

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

$$E_n = \frac{-\eta^2}{2m} \left[\frac{n\pi}{L_z} \right]^{-2} \text{ and } \psi_n = A \sin \left[\frac{n\pi z}{L_z} \right] \quad (2)$$

where $n=1, 2, 3, \dots$

In Eq. (1), $V(z)$ is the structural potential (i.e. the "quantum well" potential) seen by the electron in the well with confinement in the z direction, m is the electron effective mass, and E and ψ are the eigenenergy and eigenfunction respectively.

Eq. (2) is an ideal case solution of treating the QW (with L_z as well width) as a well with infinite barrier potential well. This solution is not realistic because of the increase effect of decoherence.

In the semiconductor ternary alloy $A_x B_{1-x} C$, the x is the mole fraction of the semiconductor alloy composition. It is the grading function which linearly depends on the conduction band edge hence the potential $V(z)$ experienced by the electron in the QW;

$$x(z) = \frac{V(z)}{\Delta V} \quad (3)$$

Where ΔV , is the potential difference between the materials AB and BC.

The $x(z)$ is also related to the electron effective mass $m(z)$ as

$$V(z) = \phi [m(z) - m_{BC}] / \Delta m \quad (4)$$

where $\Delta m = m_{BC}$ is the difference of effective mass between the materials AB and BC.

The $x(z)$ is also related to the electron effective mass $m(z)$ as:

$$V(z) = \phi [m(z) - m_{BC}] \quad (5)$$

Further, to conserve the electron flux, we have to choose barrier continuous case $\frac{1}{m} \frac{d\psi}{dz}$ which will lead

to envelop function Schrodinger equation for realistic QW with a position dependent effective mass related to the position dependent potential [14,18].

$$-\frac{\eta^2}{2m} \frac{d}{dz} \left(\frac{1}{m_z} \frac{d\psi}{dz} \right) + \phi [m(z) - m_{BC}] \psi = E\psi \quad (6)$$

We seek the function $m(z)$, $x(z)$ and $V(z)$ such that the energy spectrum of (6) has equidistant states as one dimensional SHO [14,19]. For inconvenience the following unit are used energy in eV length in A and effective mass in free electron mass. Taking into accounts these units Eq.(6) becomes

$$\frac{d}{dz} \left(\frac{1}{m_z} \frac{d\psi}{dz} \right) + q \{E - \phi\} [m(z) - m_{BC}] \psi = 0. \quad (7)$$

Now if we introduce the coordinate transformation $z = g(y)$ and consequently introduce a new function $u(y)$ [20, 21]:

$$u(y) = \psi(y) \exp \left[-\frac{1}{2} \int_{y_0}^y \frac{1}{mg'} \frac{dmg'}{dy} dy \right] \quad (8)$$

Eq. (7) becomes

$$\frac{d^2u}{dy^2} + [A(y) + qmg'^2 \{E - \phi [m(z) - m_{BC}]\}] u = 0 \quad (9)$$

where

$$A(y) = \frac{1}{2} \frac{d}{dy} \left[\frac{1}{mg'} \frac{dmg'}{dy} \right] - \frac{1}{4} \left[\frac{1}{mg'} \frac{dmg'}{dy} \right]^2 \quad (10)$$

The potential for the one Dimension (1D) SHO denoting equispaced energy level is given by [14,15].

$$V = \frac{1}{2} m_{IDSHO} \left(\frac{\Delta E}{\eta} \right)^2 y^2 + V_o \quad (11)$$

Taking Eq. (11) into account Eq. (9)), it will become

$$\frac{d^2u}{dy^2} + q \left[E - V_o - \frac{q}{4} m_{IDSHO} \left(\frac{\Delta E}{\eta} \right)^2 y^2 \right] m_{IDSHO} u = 0 \quad (12)$$

Eqs. (7) and (12) must coincide and Eqs. (9) and (12) must also coincide. Then their solutions can be obtained respectively as

$$m(z) = m_{BC} \text{Cosh}^2 \left(\frac{\Delta E}{\eta} \sqrt{\frac{q}{\phi}} z \right) \quad (13)$$

and

$$V(z) = \phi_{BC} \text{Sinh}^2 \left(\frac{\Delta E}{\eta} \sqrt{\frac{q}{\phi}} z \right) \quad (14)$$

Now taking into account Eqs. (4) and (3), the grading function becomes:

$$x(z) = \frac{m_{BC}}{\Delta m} \text{ Sinh}^2 \left(\frac{\Delta E}{\eta} \sqrt{\frac{q}{\phi}} z \right) \quad (15)$$

Eqs. (13) - (15) are the desired electron effective mass potential experienced by the electron and the grading function respectively to achieve a physically realizable equispaced energy level QW ternary semiconductor. The wave function corresponding to the eigenstates is given by:

$$\psi_1(z) = \left(\frac{1}{i!2} \right)^{\frac{1}{2}} [q\Delta Em]^{1/4} U_1(z) \quad (16)$$

where the eigenfunctions $U(z)$ are the well-known Hermite functions.

$$U_1(z) = \left(\frac{1}{i!2} \right)^{\frac{1}{2}} [q\Delta Em(z)]^{1/4} H_1(z) e^{-\frac{1}{2}(z)} \quad (17)$$

For $i = 0, 1, 2$;

$$H_0(z) = 1, H_1(z) = 2z \text{ and } H_2(z) = 4z^2 - 2 \quad (18)$$

Thus the corresponding eigenfunctions are

$$\psi_0(z) = [q\Delta Em_{BC}]^{1/4} \text{ Cosh}^{\frac{1}{2}} \left(\frac{\Delta E}{2} \sqrt{\frac{q}{\phi}} z \right) e^{-\frac{1}{2}(z)} \quad (19)$$

$$\psi_1(z) = 2 \left[\frac{1}{4} q\Delta Em_{BC} \right]^{1/4} \text{ Cosh}^{\frac{1}{2}} \left(\frac{\Delta E}{2} \sqrt{\frac{q}{\phi}} z \right) e^{-\frac{1}{2}(z)^2} \quad (20)$$

$$\psi_2(z) = \frac{2}{2} \left[\frac{1}{4} q\Delta Em_{BC} \right]^{1/4} \text{ Cosh}^{\frac{1}{2}} \left(\frac{\Delta E}{2} \sqrt{\frac{q}{\phi}} z \right) (2z^2 - i) e^{-\frac{1}{2}(z)^2} \quad (21)$$

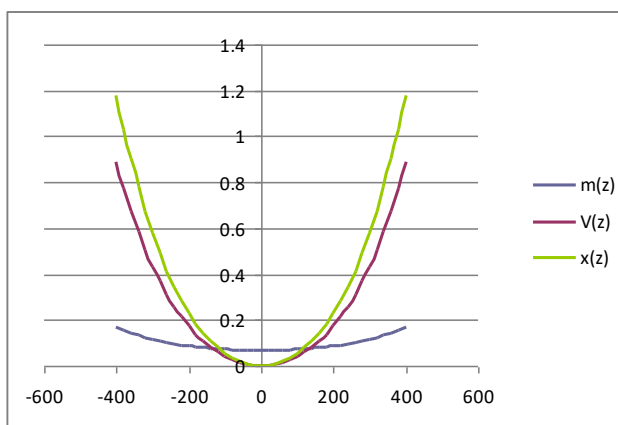


Fig 1a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Al_xGa_{1-x}As$

3. RESULTS AND DISCUSSION

The calculation of the electron effective mass grading function potential and wave functions are performed by a method that has been previously described [15] the electron effective mass the potential and the wave functions (at $i=0, 1$ and 2) are obtained from Eq.s (213) (219) (220) and (221) respectively using a common value in the literature for $\Delta E = 30$ meV [22] the values of the material effective masses and minimum band gaps are obtain from David (1991) [27] and band off-set (the last column of Table 1) from [14,15]. Graphs of the electron effective mass and potential dependence on the chosen direction of confinement for nine ternary semiconductors QWs. All the graphs of Fig 1a to Fig 9a are parabolic and have equispaced states both for the effective mass and potential with that of the former having a wider spread.

The trend here is that the grading function which linearly depends on the conductor band edge hence the potential has a linear relation with the electron effective mass [18]. Since band edge dependence on material composition is indispensable in band gap engineering [23], the equispaced states electron effective mass will be very useful in obtaining equispaced energy levels in QWs.

The calculated dependence of the normalized wave functions $U(z)$ of the first three bound states (Figs. 1(b) to 9(b)) on the direction of confinement provides as a check on our formulation. For it is a common knowledge that irrespective of the variation of the energy levels, the sinusoidal path of the wavefunction for each of the level should not be affected. Therefore the achievement of the expected path for the wave function from our formulation implies that our coordinate transformation was successful.

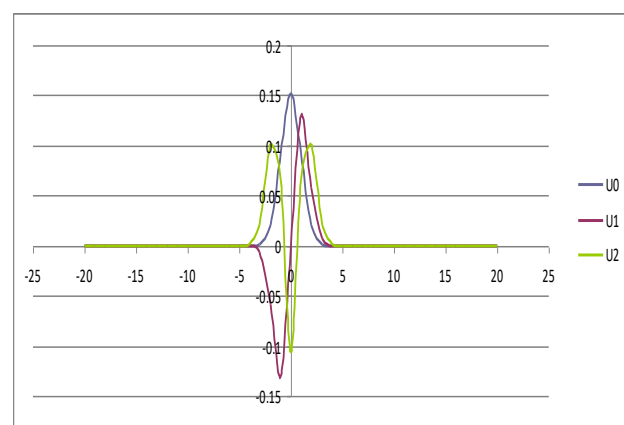


Fig. 1b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ for $Al_xGa_{1-x}As$

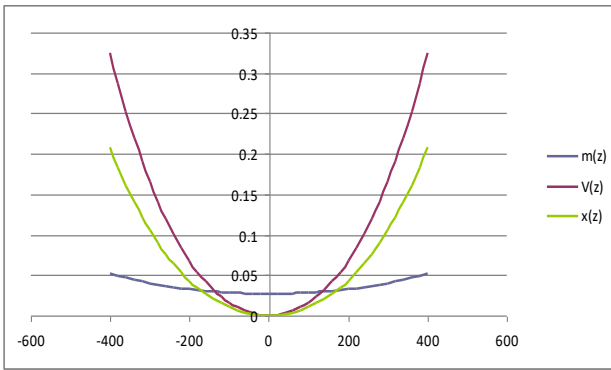


Fig 2a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Al_xIn_{1-x}As$

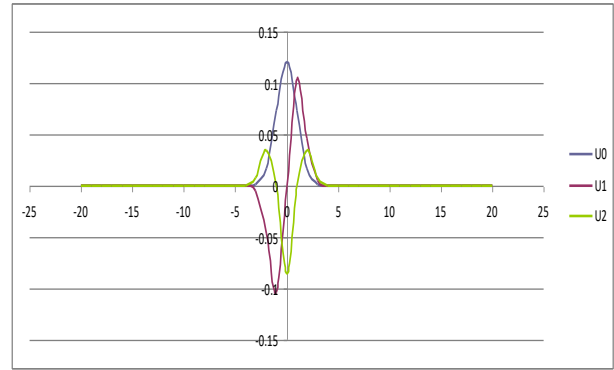


Fig. 2b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ for $Al_xIn_{1-x}As$

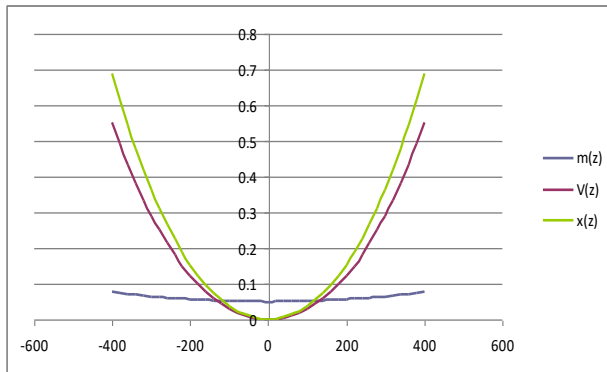


Fig 3a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Al_xGa_{1-x}Sb$

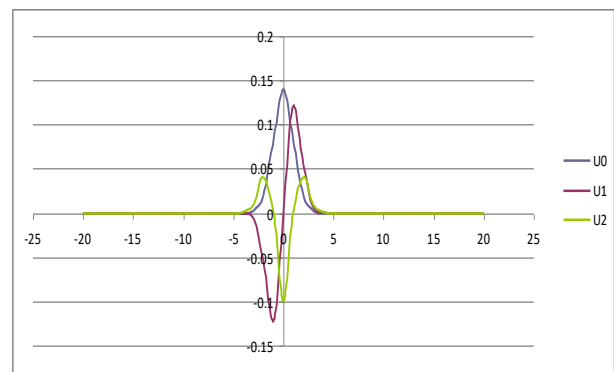


Fig. 3b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ for $Al_xGa_{1-x}Sb$

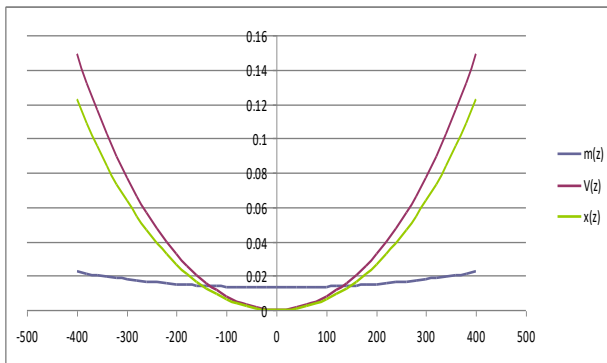


Fig4a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Al_xIn_{1-x}Sb$

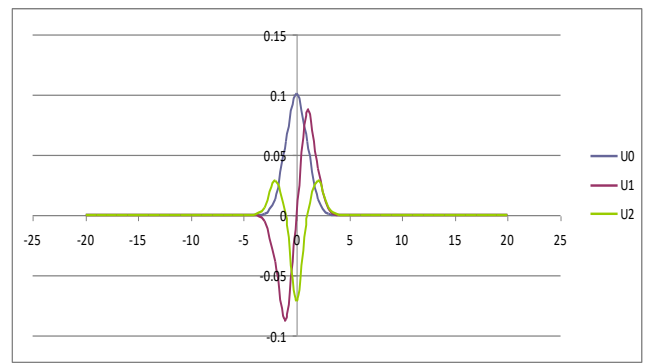


Fig.4b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ for $Al_xIn_{1-x}Sb$

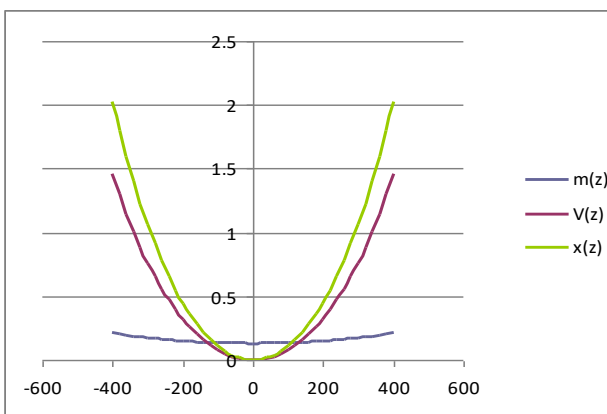


Fig 5a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Cd_xZn_{1-x}Se$

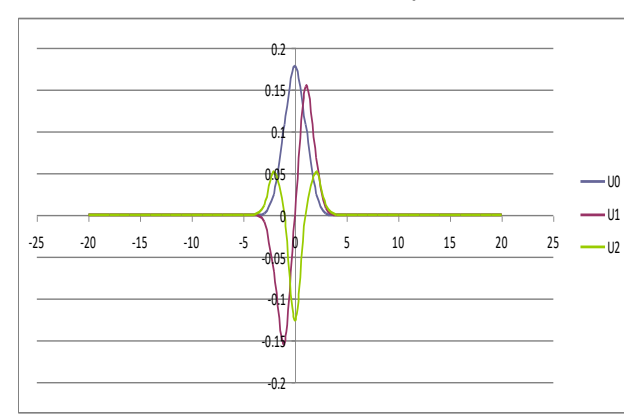


Fig. 5b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ for $Cd_xZn_{1-x}Se$

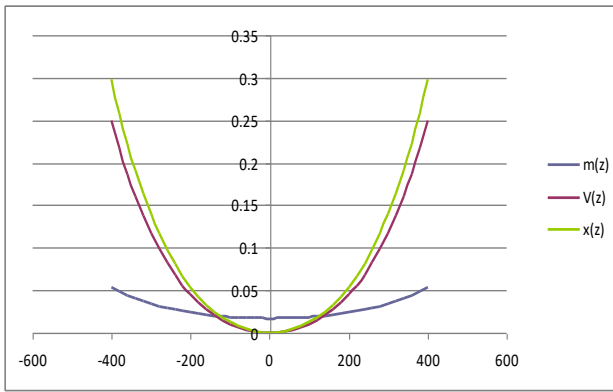


Fig 6a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Cd_xHg_{1-x}Te$

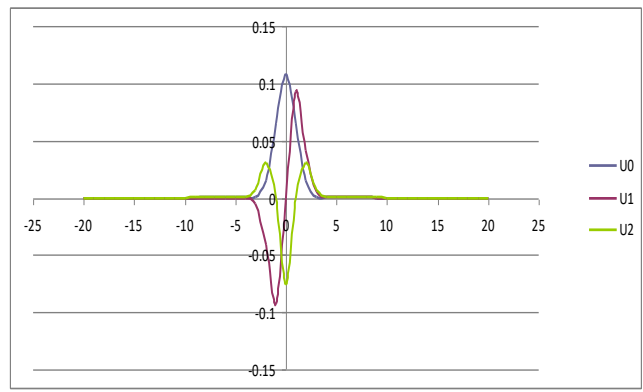


Fig. 6b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ for $Cd_xHg_{1-x}Te$

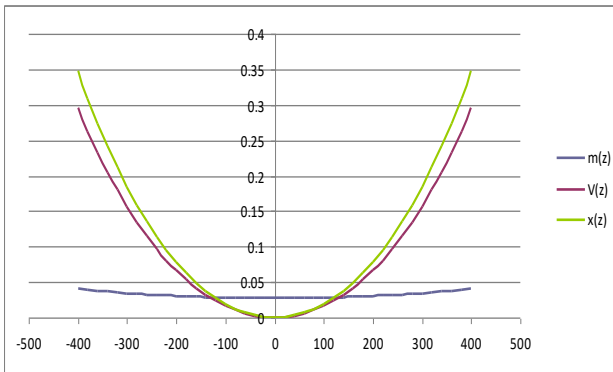


Fig7a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Ga_xIn_{1-x}As$

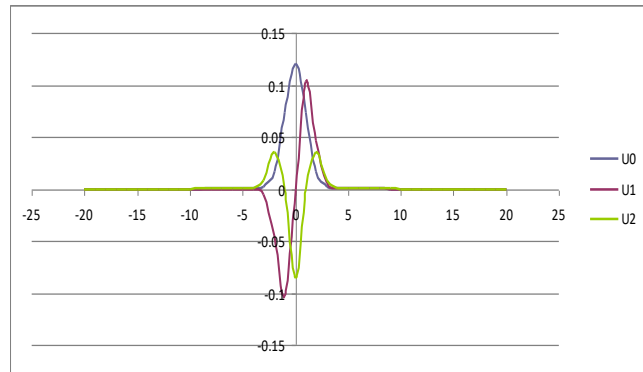


Fig.7b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ $Ga_xIn_{1-x}As$

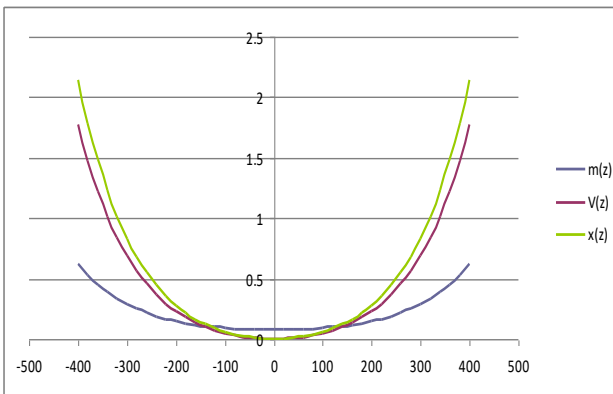


Fig 8a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Ga_xIn_{1-x}P$

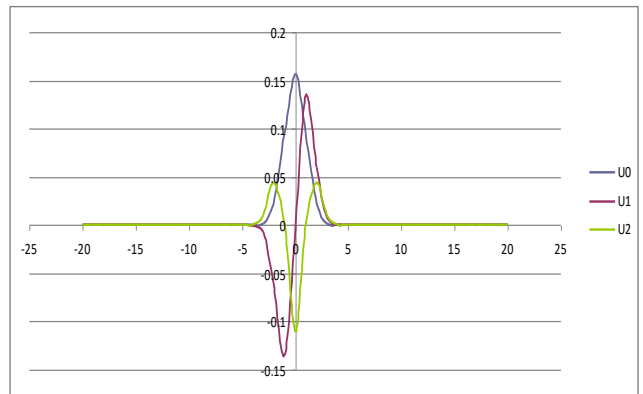


Fig.8b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ $Ga_xIn_{1-x}P$

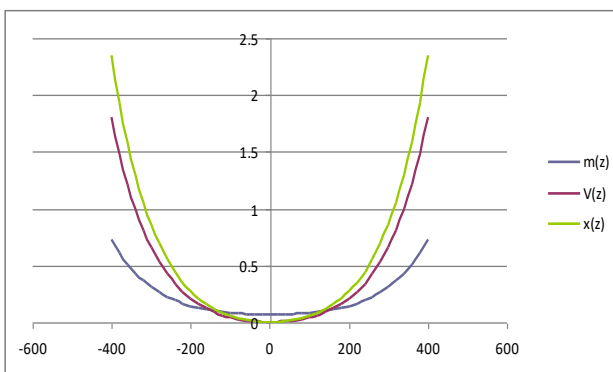


Fig. 9a: The Effective mass $m(z)$, the potential $v(z)$ and the mole fraction $x(z)$ for $Ga_xP_{1-x}As$

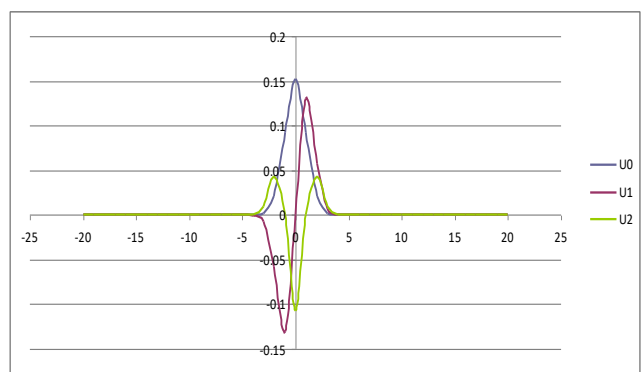


Fig. 9b: The normalized wave functions $U_i(z)$ of the first three bound state with $\epsilon = 0$ $Ga_xP_{1-x}As$

Table 1: Some Semiconducting Properties of Selected Ternary Alloy [27]

| Semiconductor alloy system (Ternary alloy); $A_x B_{1-x} C$ | Electron Effective Mass (M_0) and Minimum band gap (eV) | | Band off set (meV) |
|---|---|---------------------------------|--------------------|
| | M_{BC} | M_{AC} | |
| 1 GaAs/AlAs ($Al_x Ga_{1-x} As$) | Ga As 0.067 m_0 1.35 eV | Al As 0.15 m_0 2.2 eV | 750meV |
| 2 ZnSe/CdSe ($Cd_x Zn_{1-x} Se$) | Cd Se 0.13 m_0 1.74 eV | ZnSe 0.17 m_0 2.58 eV | 720meV |
| 3 HgTe/CdTe ($Cd_x Hg_{1-x} Te$) | Hg Te 0.017 m_0 0.15 eV | Cd Te 0.14 m_0 1.44 eV | 840meV |
| 4 In As/AlAs ($Al_x In_{1-x} As$) | In As 0.027 m_0 0.36 eV | Al As 0.15 m_0 2.2 eV | 1567meV |
| 5 GaSb/Al Sb ($Al_x Ga_{1-x} Sb$) | Ga Sb 0.050 m_0 0.67 eV | Al Sb 0.09 m_0 1.6 eV | 800meV |
| 6 In Sb/Al Sb ($Al_x In_{1-x} Sb$) | In Sb 0.013 m_0 0.165 eV | Al Sb 0.09 m_0 1.6 eV | 1220 |
| 7 In P/Ga P ($Ga_x In_{1-x} P$) | In P 0.077 m_0 1.27 eV | Ga P 0.35 m_0 2.24 eV | 825 |
| 8 In As/Ga As ($Ga_x In_{1-x} Sb$) | In As 0.027 m_0 0.36eV | Ga As 0.067 m_0 1.35 eV | 850 |
| 9 Ga P _x As _{1-x} | Ga As 0.067 m_0 1.35 eV | Ga P 0.35 2.24 eV | 770 |

4. CONCLUSION

QW and nanostructures generally are broadly tailorable to various the design [24]. Which find applications in optoelectronics such as infrared photodetectors, infrared imagine, laser photodetectors and diode lasers [25]. All these devices operates optimally with coherent emission. One approach to achieve coherent emission is to design these devices with equispaced energy level QW. In this study, we have demonstrated a generalized method to obtain equispaced states of the electron effective mass and potential as signatures of equipment energy levels for QWs in semiconductor ternary alloys. As stated above, the calculated electron effective masses can be used as inputs for further single band calculations to obtain the electronic structure when the absolute size of the structures is known ([23,25] . The generalized

formulation here can be extended to other semiconductors nanostructures such as theoretical design of equispaced energy level quantum wires which are two-dimensional confinement [26] and quantum dots which are three-dimensional confinement [13]. It is expected that the equispaced energy level will reduce the effect of decoherence in these semiconductors nanostructures especially in their applications that require coherent emission and absorption. Further, electronic devices such as the resonant tunneling diode are also affected by the position-dependence of carrier effective mass and thus the results are applicable to both optoelectronic and electronic quantum devices with real materials but also with ultracold atoms in optical lattice for the effective mass and potential with that of the former having a wider spread.

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