A THEORETICAL DESIGN OF QUANTUM WELL WITH EQUISPACED ENERGY LEVELS IN THE CONDUCTION BAND OF $Al_XGa_{1-X}Sb$ AND $Al_X\ In_{1-X}Sb$†

Arthur Imooah Ejere[1] and Godfrey E.Akpojotor[2]

[1]Department of Physics, University of Benin, Benin city, Nigeria
[2]Department of Physics, Delta State University, Abraka, Nigeria

Abstract

Equispaced energy levels Quantum well (QW) is realized in the conduction band of semiconductor nanostructures. The procedure starts with the effective-mass Schrodinger equation, with the local conduction-band edge as the potential experienced by an electron in the QW made to coincide with another effective-mass Schrodinger equation with a linear harmonic oscillator potential. In this paper, an attempt has been made to model some semiconductor ternary alloys ($A_x B_{1-x}C$) using this procedure, with the Dingle partition of 85:15 ratio for conduction band and valence band respectively. Two models are derived, one with a confining potential that may be realized by appropriate grading of the $Al_xGa_{1-x}Sb$ and $Al_x\ In_{1-x}Sb$ and the other with a non-confining potential where the electron effective-mass tends to zero as z tends to infinity [m $(z \rightarrow \pm\infty) \rightarrow 0$]. This latter type of model is not realizable.

KeyWords: Semiconductor nanostructures, ternary alloys, Effective Mass Schrodinger equation.

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1. INTRODUCTION

Controlled confinement of electrons in one dimension by semiconductor heterojunctions such that, a well with width of the order of the de Broglie wave length of electron is formed can be realized. This constitutes a quantum well (QW). An electron in this well displays quantum phenomena (Dingle et al, 1974; Basu, 1997; Marquezimi et al, 1996). The nano-structuring of semiconductor materials was first introduced by Shockley (1951) and later by Kroemer (1957). QW and nanostructures generally are broadly tailorable, that is, there is the possibility of implementing a design such that the quantized states and the corresponding wave functions respond to the design (Nenad, 2007; Nurmikkor and Gunshor, 1994). The application of the QW has continue to advance in optoelectronics such as infrared photodetectors, infrared imaging, laser photodetectors and diode lasers (Choi, 1997). All these devices operate optimally with coherent emission. One approach to achieve coherent emission is to design these devices with equispaced QW. The purpose of this paper is to theoretically design and give the signatures for equispaced QW. This will involve presenting the calculated effective mass function m(z), potential function V(z) and the electron wave function $U_i(z)$ for two ternary alloys QWs (Milanovic and Ikonic, 1996; Milanovic et al, 1996; Ejere and Idiodi, 2011).

This rest of the paper is organized as follows. In section 2, we present the theoretical formulation of the design. The calculated results which depict the signatures for the equispaced QW will be presented in Section 3 and this will be followed by a brief conclusion in section 4.

2. THEORETICAL FORMULATION

Consider the 1-D time-independent Schrodinger equation

$$\frac{-\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m}\frac{d\psi}{dz}\right)+\theta\left(m-m_{BC}\right)\psi=E\psi \qquad (1)$$

We seek the function $m(z)$ and therefore $V(z)$ such that the energy spectrum of Eq. (1) has equidistant states same as 1-D Harmonic Oscillator (1-DHO) (Powell

and Crasemann, 1962; Milanovic and Ikonic, 1996; Yariv, 1988; Einevoll et al, 1990; Renan et al, 2000; Paul, 2005).

For convenience let us express, the following units are used:

Energy in eV units,

Length in $\overset{o}{A}$ units, and

Effective mass in free electron mass units,

Taking into account these units, Eq.(1) becomes

$$\frac{d}{dz}\left(\frac{1}{m}\frac{d\psi}{dz}\right)+q\left[E-\theta\left(m-m_{BC}\right)\right]\psi=0 \qquad (2)$$

By putting $z=g(y)$ (introducing a new coordinate) into Eq.(1) and consequently introducing a new function u(y) (Eugene, 1970 and Abramowitz and Stegun, 1972):

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

Eq.(2) becomes,

$$\frac{d^2u}{dy^2}+\left[A(y)+qmg'^2\left\{E-\theta\left(m-m_{BC}\right)\right\}\right]u=0 \qquad (3)$$

where,

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

Potential V for 1-DHO denoting equispaced level is given by

$$V=\frac{1}{2}m_{LHO}\left(\frac{\Delta E}{\hbar}\right)^2 y^2+V_o \qquad (5)$$

Substituting for V in the schrodinger equation

$$\frac{d^2u}{dy^2}-q\left[E-V_o-\frac{q}{4}\ m_{LHO}(\Delta E)^2y^2\right]m_{LHO}\,u=0 \qquad (6)$$

Equations (2) and (6) must coincide and equations (3) and (6) must also coincide. Their solutions can be obtained as

$$\therefore m(z)=m_{BC}\ Cosh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\,z\right) \qquad (7)$$

$$V(z) = \theta\, m_{BC}\ Sinh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ \ z\right) \tag{8}$$

The equations, (7) and (8) gives the ideal of a physically realizable QW structure. The deviation of the real structure from the idealized one is due to the accumulation of electrons in the lower gap material side at the two heterointerfaces, which lead to band bending at the interfaces (Das Sarma et al, 1990; Alicia and David, 1990). This deviation will perturb energies of state below the barrier top, which remain bounded, while those above would dissolve into continuum. Yet only those which are close to the barrier top will be seriously affected by truncation (Lee et al, 1996). Therefore the influence of truncation is negligible for all practical purposes (Milanovic and Ikonic, 1996; Paul, 2005; Reeno et al., 2007; James et al, 2010).

The wave function corresponding to eigenstates is given by

$$\psi_i(t) = \left(\frac{1}{i!\,2^i}\right)^{1/2}\ (q\Delta Em)^{1/4}\ U_i(t) \tag{9}$$

The eigenfunctions $U(t)$ are the well-known Hermite funtions.

$$U_i(z) = \psi_i(z) = \left(\frac{1}{i!2^i}\right)^{1/2}\ [q\,\Delta Em(z)]^{1/4}\ H_i(z)e^{-\frac{1}{2}(z)^2} \tag{10}$$

For $i = 0,1,2$

$$H_o(z) = 1,\ H_1(z) = 2z \quad and \quad H_2(z) = 4z^2 - 2 \tag{11}$$

Substituting values for $H_i(z)$ (Powell and Crasemann, 1962; Russel, 1998), into Eq.(11) gives

$$U_0(z) = \psi_0(z) = (q\,\Delta Em_{BC})^{1/4}\ Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ z\right).e^{-\frac{1}{2}(z)^2}$$

$$U_1(z) = \psi_1(z) = 2\left(\frac{1}{4}q\,\Delta Em_{BC}\right)^{1/4}\ Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ z\right).\ z\,e^{-\frac{1}{2}(z)^2}$$

$$U_2(z) = \psi_2(z) = \frac{2}{2}\left(\frac{1}{4}q\,\Delta Em_{BC}\right)^{1/4}\ Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ z\right).(2z^2 - 1)e^{-\frac{1}{2}(z)^2}$$

3. RESULTS AND DISCUSSION

The variation of the effective mass and the potential functions, required to obtain equispaced levels with ΔE = 30meV are obtained. It enables for instance, a cascade of electron transitions with absorption or emission of photons (Q_i and Q_i, 1999).

Table 2.1: some semiconducting properties of selected ternary alloys (David, 1991)

	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	GaSb/Al Sb ($Al_xGa_{1-x}Sb$)	Ga Sb 0.050 m_0 0.67 eV	Al Sb 0.09 m_0 1.6 eV	800
2	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

The values of the Electron effective masses and the minimum band gaps are obtained from David, (1991), while the band off-set (the last column of Table1) are calculated. The work of Milanovic and Ikonic with $Al_xGa_{1-x}As$ agrees with these results. See Ejere and Idiodi, 2011 and Milanovic and Ikonic, 1996.

Figures (1a) - (2c), show the results for two semiconductor ternary alloys One can see that, $m(z \to \pm\infty) \to +\infty$, also the potential $V(z \to \pm\infty) \to +\infty$.

The parabolic shape of the V(z) graph for the two alloys are similar and clearly shows that the eigenstates in the QW are equispaced (Ejere and Idiodi, 2011). The shape of m(z) graph follows the parabolic shape of the V(z) .

Classically, confining potential (CP) for all the semiconductor alloys are obtained. The potentials are confining type and the effective mass follows it. In effect, just as the electron tends to avoid regions where its potential exceeds the total energy, it also avoid regions where the kinetic energy will be large there by exceeding the total energy.

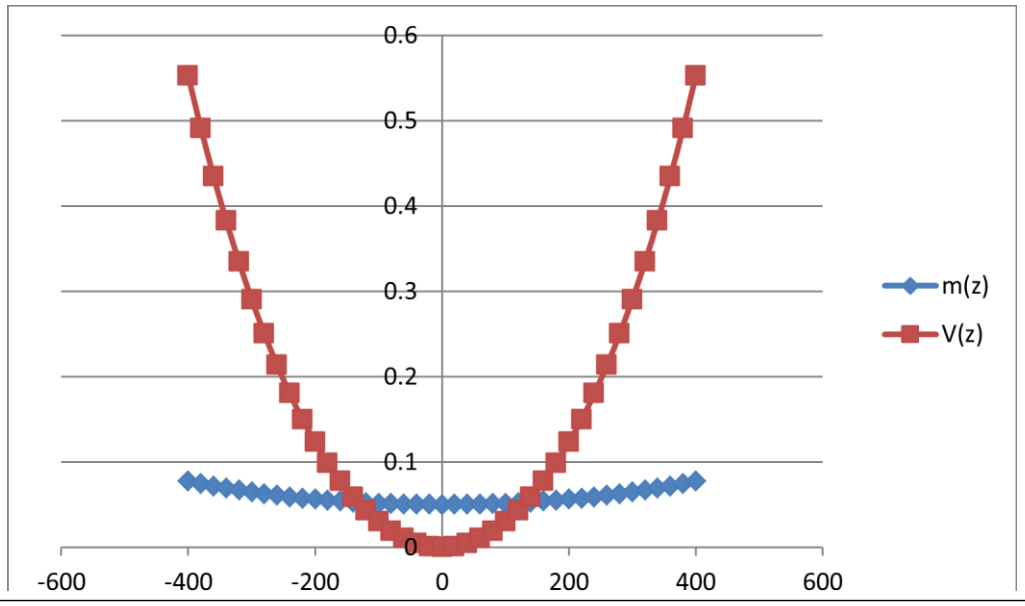

Fig 1a: The Effective mass m (z) and the potential V(z) for $Al_xGa_{1-x}Sb$

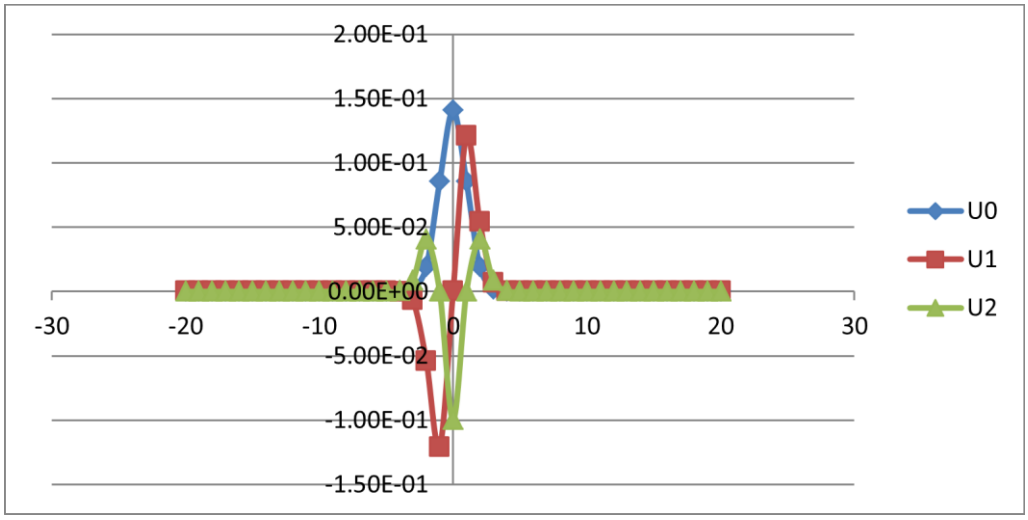

Fig 1b: The normalized wave functions $U_l(z)$ of the first three bound states with $\in = 0$ for $Al_xGa_{1-x}Sb$

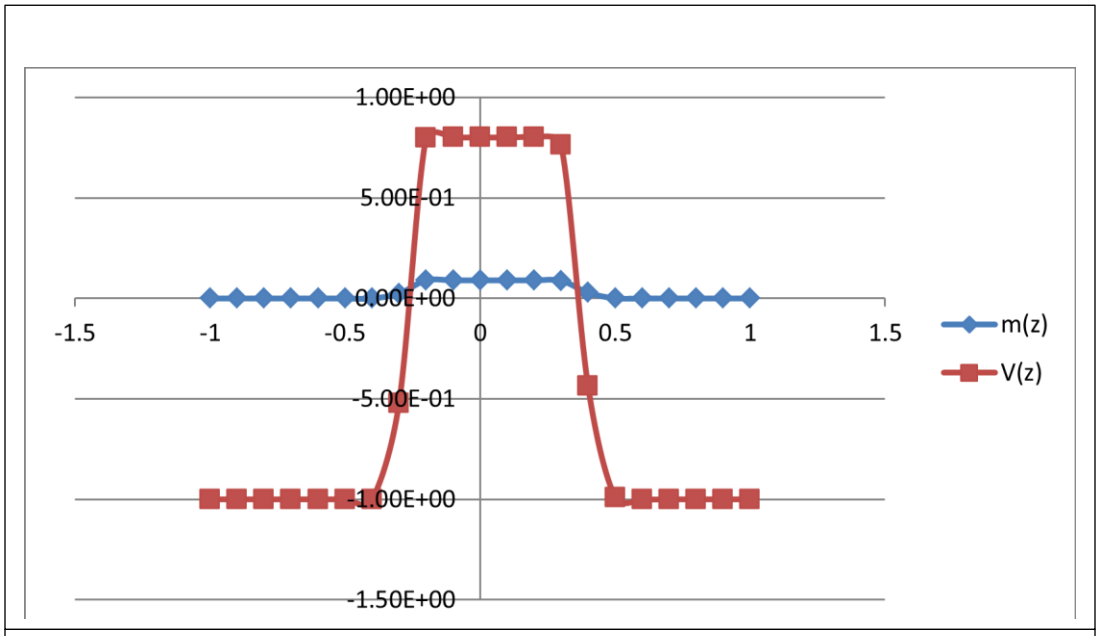

Fig 1c: The Effective mass m (z) and the potential V(z) for $Al_xGa_{1-x}Sb$

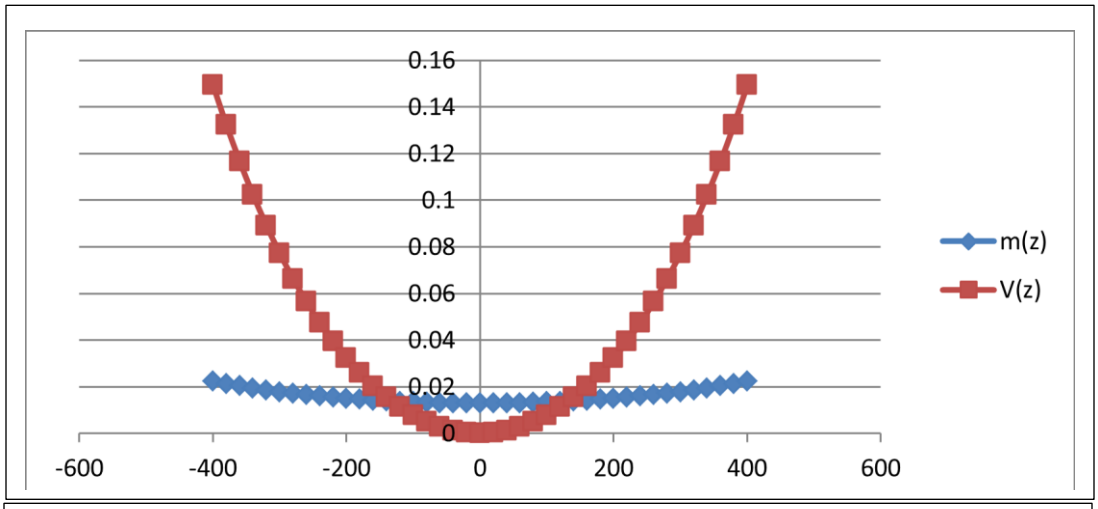

Fig 2a: The Effective mass m (z) and the potential V(z) for $Al_xIn_{1-x}Sb$

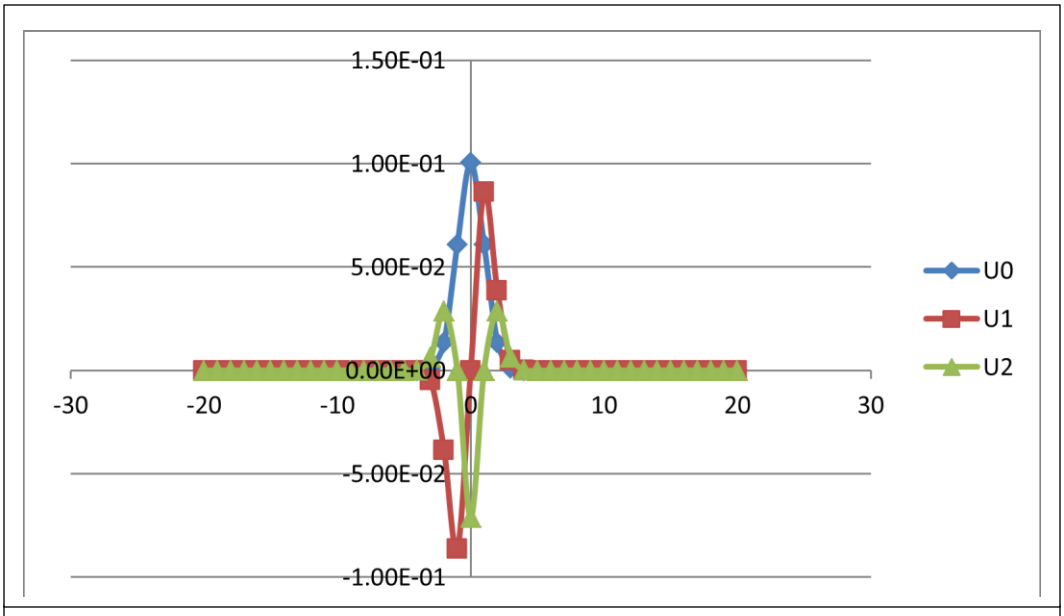

Fig 2b: The normalized wave function $U_l(z)$ of the first three bound states with $\in = 0$ for $Al_xIn_{1-x}Sb$

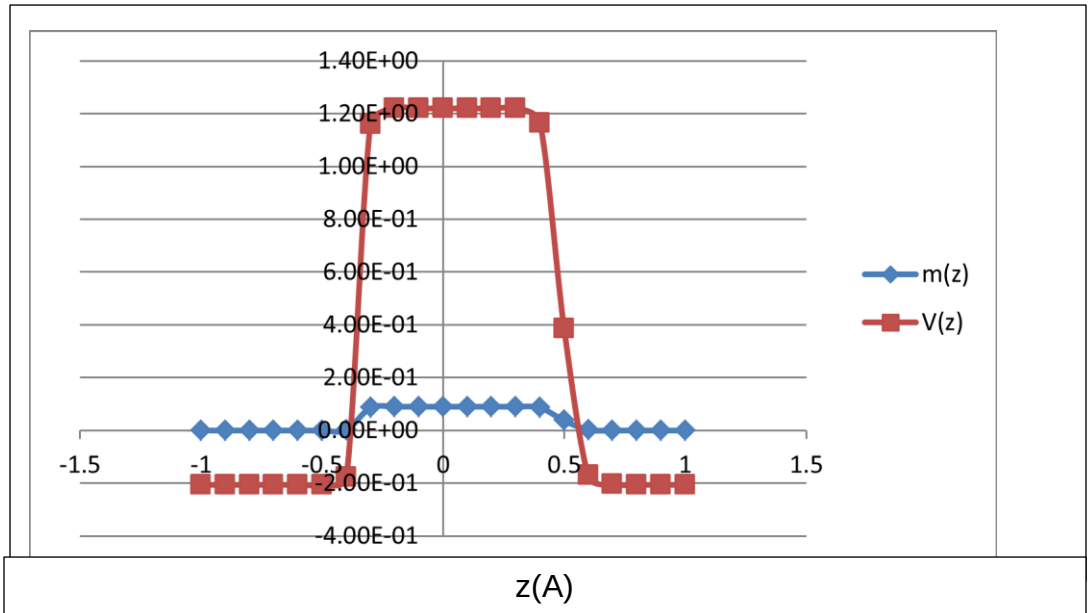

Fig 2c : The Effective mass m (z) and the potential V(z) for $Al_xIn_{1-x}Sb$

4. CONCLUSION

In an ideal world, all experiment would be interpreted using the results of ab initio solutions of the many electrons Schrodinger equation. These results as shown in the figures shows that equispaced level design are achievable with these alloys. The method can be extended to other semiconductor ternary alloys (A_x B_{1-x} C) with appropriate grading. Further, the coordinate transformation procedure can also be used to theoretically design equispaced quantum wells which are two-dimensional confinement and quantum dots which are three – dimensional confinement (Akpojotor and Akpojotor, 2008).

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