Equispaced level in the quantum well calculated for two semiconductor ternary alloys conduction band.

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ABSTRACT

A model of equispaced-level in the conduction band of semiconductor quantum well (QW) nanostructures is applied to two ternary alloys - $Ga_xIn_{1-x}P$ and $Ga_xP_{1-x}As$ with achievable results. The model addresses the case of confining potential that may be realized by appropriate grading of the semiconductor alloy and the case of non-confining potential where the electron effective-mass tends to zero as z tends to infinity [m ($z \to \pm\infty$)$\to 0$]. This latter case is not realizable.

1.0 Introduction

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).

This paper is organized as follows. In section 2, we present the theoretical background. Section 3- analytical solution procidure, section 4- results and discussion. And a brief conclusion is given in section 5.

Controlled confinement of electrons in one dimension in semiconductor heterostructures such that a well with width of the order of the de Broglie wave length of electron between barriers is formed, constitutes a QW. An electron in this well displays quantum phenomena (Dingle et al, 1974; Basu, 1997; Marquezimi et al, 1996).

The focus in this article is on presenting the calculated effective mass function m(z), potential function V(z) and the electron wave function $U_i(z)$, for two ternary alloy QWs (Milanovic and Ikonic, 1996; Milanovic et al, 1996; Ejere and Idiodi, 2011).

2.0 Theoretical background

The governing equation of equispaced-level in the conduction band of a semiconductor Quantum well nanostructure is the 1-D time-independent Schrodinger equation given by:

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

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

Energy in eV units,

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

Effective mass in free electron mass units, then Eq.(1) becomes

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

3.0 Analytical solution procedure

The interest is in introducing a new coordinate by putting $z=g(y)$ into Eq.(1) and 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,

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

where,

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

The potential V for denoting 1-DHO equispaced level is given by

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

Substituting for V in the schrodinger equation

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

Equations (2) and (6) must coincide and equations (3) and (6) must also coincide. Solving to give

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

$$V(z)=\theta\, m_{BC}\ Sinh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\ \ z\right)$$
(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 (Lee et al, 1996) will be seriously affected by truncation therefore the influence of truncation is negligible for all practical purposes (Milanovic and Ikonic, 1989; Paul, 2005; Reeno et al., 2007; James et al, 2010; Arthur, 2011).

The wave function corresponding to eigenstates is given by

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

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

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

For $i=0,1,2$

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

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

$$U0(z) = \psi_0(z) = (q\,\Delta E m_{BC})^{1/4}\, Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\; z\right).e^{-\frac{1}{2}(z)^2}$$

$$U1(z) = \psi_1(z) = 2\left(\frac{1}{4}q\,\Delta E m_{BC}\right)^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\; z\right).\; z\, e^{-\frac{1}{2}(z)^2}$$

$$U2(z) = \psi_2(z) = \frac{2}{2}\left(\frac{1}{4}q\,\Delta E m_{BC}\right)^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\theta}}\; z\right).(2z^2 - 1)e^{-\frac{1}{2}(z)^2}$$

(12)

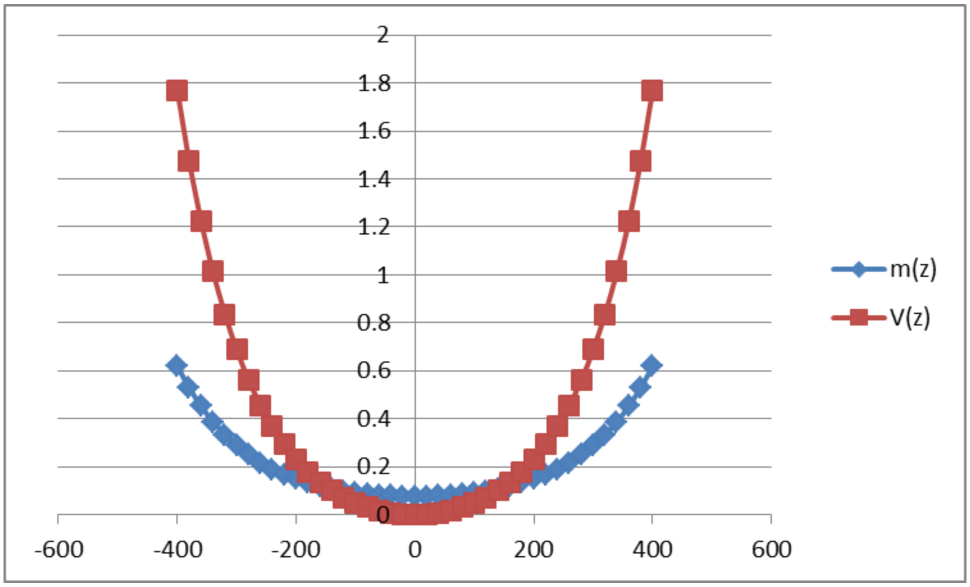
4.0 Results and Discussion

The variation of the effective mass and the potential functions, required to obtain equispaced levels with ΔE= 30meV are obtained. It enable 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)

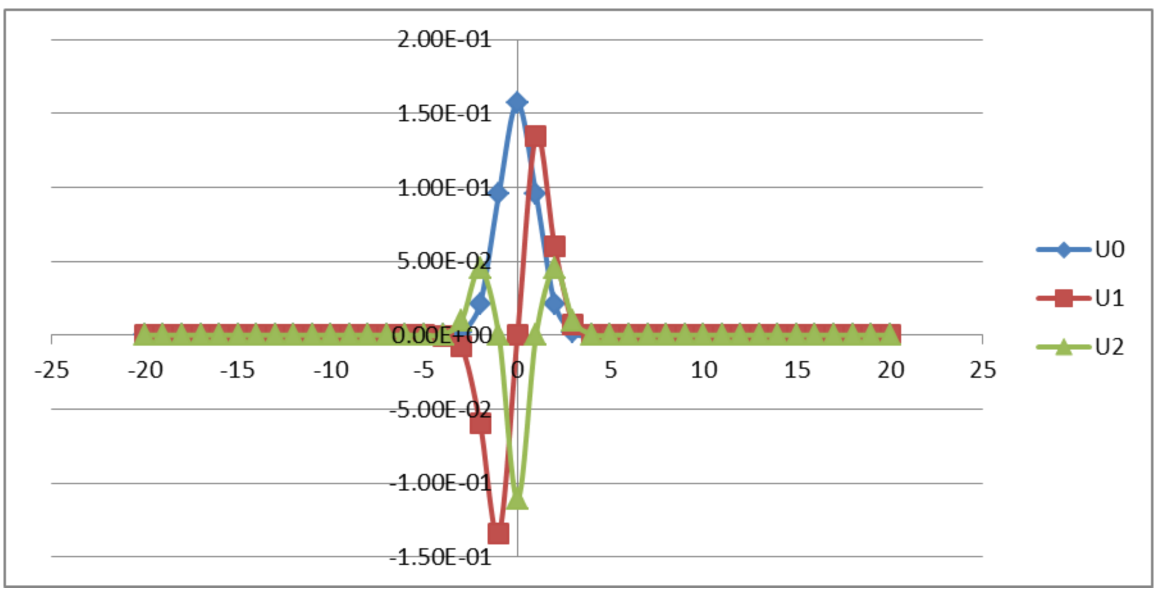
	Semiconductor Alloy system (Ternary Alloy) **$A_x\ B_{1-x}\ C$**	**Electron Effective Mass (M_0) and Minimum band Gap (eV)**		**Band off Set (meV)**
		M_{BC}	**M_{AC}**	
1	In P/Ga P ($Ga_x\ In_{1-x}\ P$)	In P 0.077 m_0 1.27 eV	Ga P 0.35 m_0 2.24 eV	825meV
2	Ga $P_x\ As_{1-x}$	Ga As 0.067 m_0 1.35 Ev	Ga P 0.35 2.24 eV	770meV

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. See Ejere and Idiodi, 2011 and Milanovic and Ikonic, 1989.



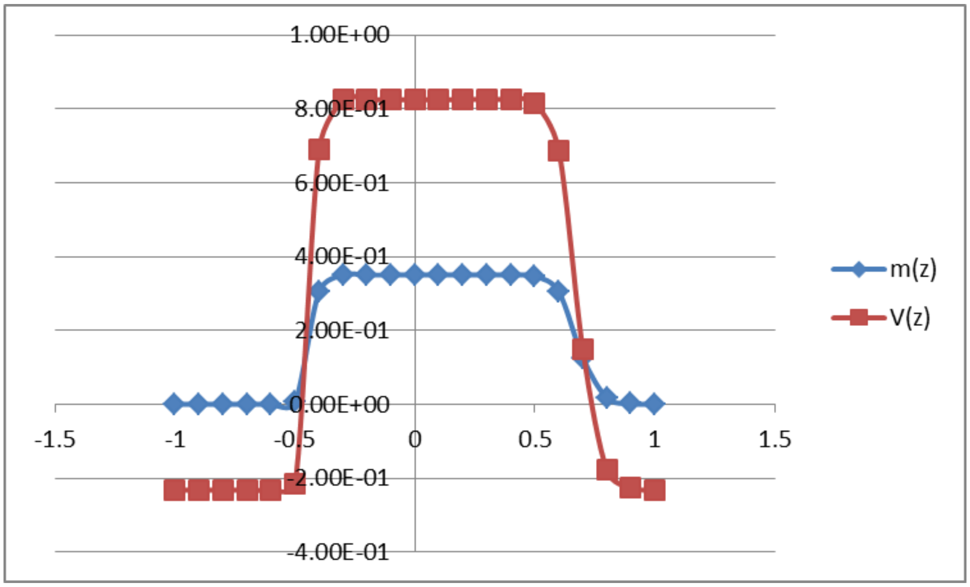
z(A)

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



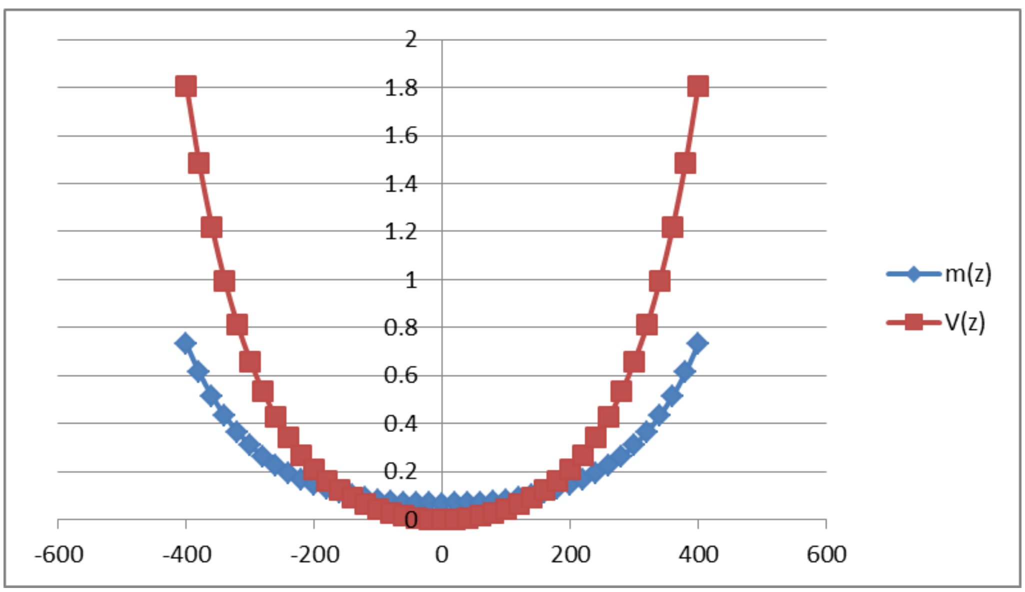
z(A)

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



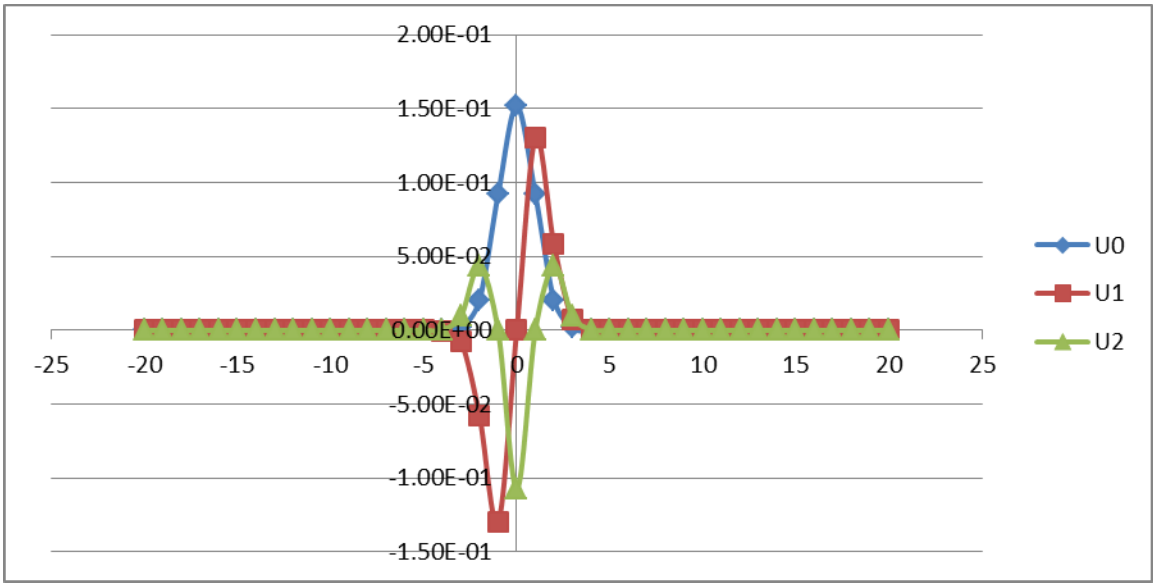
z(A)

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



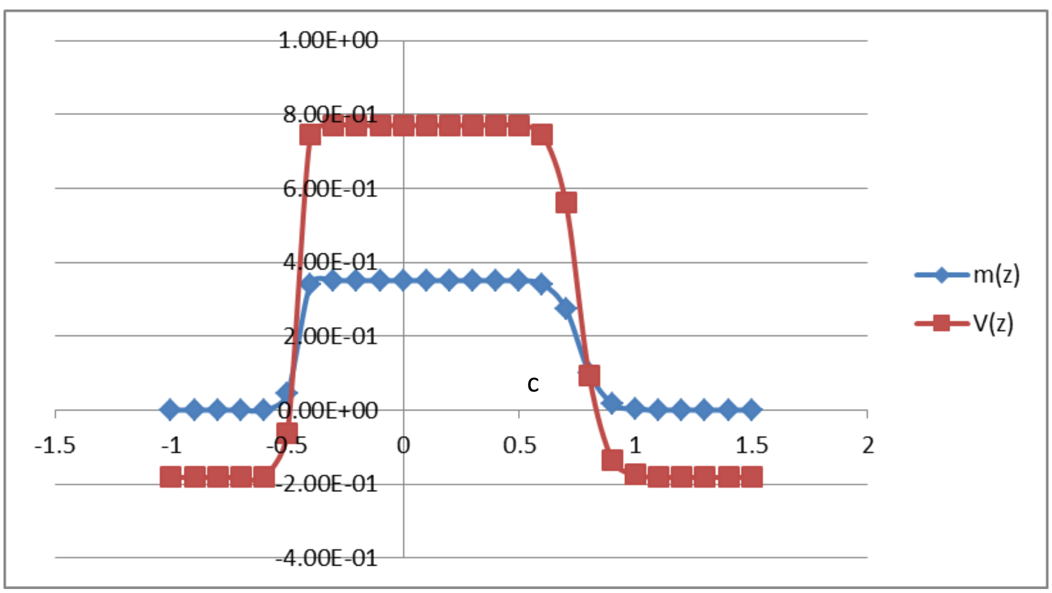
z(A)

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



z(A)

Fig. 2b: The normalized wave functions $Ui(z)$ ***of the first three bound state with*** $\in = 0$ ***$Ga_xP_{1-x}As$***



z(A)

Fig.2c: The Effective mass m (z) and the potential v(z) for $Ga_xP_{1-x}As$

Figures 1a to 2c, shows 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 seven 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.

5.0 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 equispacd level design are achievable with these alloys .

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