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A general theoretical design of semiconductor nanostructures with equispaced energy levels: preliminary report for quantum wells in semiconductor ternary alloys ($A_xB_{1-x}C$)

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Abstract

The purpose of this study is to formulate a general theoretical design of equispaced energy levels for semiconductor nanostructures. Here we present a preliminary report for the design of equispaced energy levels for quantum wells (QWs) in semiconductor ternary alloys ($A_xB_{1-x}C$). The procedure is by mapping the envelope function Schrodinger equation for a realistic QW, with the local conduction-band edges 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 signatures for the equispaced energy levels for QWs in semiconductor ternary alloys.

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

1. Introduction

The need to advance and improve on the applications of nanomaterials has continued to inspire the need for advances in nanofabrication techniques. One area which has received considerable attention is nano-embeddement in one dimention (1D), two dimension (2D) and three dimension (3D) leading to quantum wells, quantum wires and quantum dots respectively. Confinement of electrons in these nanostructures gives rise to quantum effects. (Dingle et al, 1974; Marquezimi et al, 1996; Harrison, 2005). One of these effects is that experimental measurements involving these embedded electrons are influenced by their environment and consequently prone to errors (Taylor et al., 2005; Kumar et al., 2012). One of the manifestations of these errors is decoherence (Schlosshauer, 2004; Golubev and Zaikin, 2008). Consequently many of the applications of these nanomaterials especially those that require emission and absoption are often affected by decoherence which usually affects quantum systems. The nano-structuring of semiconductor materials was first introduced by Shockley (1951) and later by Kroemer (1957). However, the decoherence problem has affected the progress of semiconductor nanofabrication technology (Coish and Loss, 2005; Fischer and Loss, 2009). This has instigated the search for other better hosts which may reduce the decoherence but cannot in principle eliminate it for the obvious reason that there is no physically isolated quantum system in nature (Schlosshauer, 2004; Akpojotor and Akpojotor, 2009). One possible way to reduce the effect of decoherence may be to design semiconductors nanostructures with equispaced energy levels which will lead to coherent emission and absorption in these nanomaterials. The approach to achieve this is to map the Schrodinger equation for the semiconductor nanostructure into the appropriate dimensional simple harmonic oscillator (SHO) by coordinate transformation approach. In general, the SHO is a fundamental problem in physics with equispaced energy levels. Though all its solutions are yet unknown but many of them are already known. One common physical property of the SHO is that its solution yields sub-bands that are equispaced in energy and the eigenfunctions are given by the Hermite polynomials. Since the goal of physics is to account for all physical phenomena, irrespective of their complexities, with the few known ones, the mapping of the semiconductors nanostructures into the SHO will enable us to obtain its appropriate solutions for the effective mass function m(z), potential function V(z), grading function x(z) and the electron wavefunction $U_i(z)$ as signatures for the equispaced energy levels for the semiconductor ternary alloys QWs (Milanovic and Ikonic, 1996; Milanovic et al, 1996; Ejere and Idiodi, 2011; Ejere and Akpojotor, 2011). The reason for calculating the effective masses is because they can be used as inputs for further single band calculations to obtain the electronic structure when the absolute size of the structures is known (Pryor and Pistol, 2005). Further, the carrier effective mass of a QW which is strongly connected to the carrier mobility, is one of the most important device parameters. The reason being that low carrier effective mass means the parent material 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 (Ejere and Akpojotor, 2011; Ejere and Idiodi,

2011) of 1D systems for the semiconductor ternary alloys ($A_xB_{1-x}C$) but also because many of the physical effects in quantum well structures can be seen at room temperature and can be exploited in real devices.

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

2. Theoretical formulation

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

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dz^2}+V(z)=E\psi \tag{2.1}$$

where V(z) is the structural potential (i.e., the "quantum well" potential) seen by the electron along the direction of confinement (z), m is the electron effective mass, and E and ψ are the eigenenergy and eigenfunction associated with the solution to Eq. (2.1).

If the length of the QW is L_z and we assumed for simplicity that the barrier on either sides of the well are infinitely high, then the n'th solution will be

$$E_n=\frac{-\hbar^2}{2m}\left[\frac{n\pi}{L_z}\right]^2 \text{ and } \psi_n=A\sin\left[\frac{n\pi z}{L_z}\right] \tag{2.2}$$

where n = 1, 2, 3, …
The energy levels in Eq. (2.2) are quadratically spaced and the eigenfunctions are sine waves as sketched in Figure 1. Thus it is easy to see that the electron effective mass varies quadratically and that the energy level spacing becomes large for narrow wells (i.e. small Lz) and small effective mass. In other words, lower effective mass can only be realized from smaller wells which will result into increased effect of decoherence. This is one of the reasons that the ideal case of treating the QW as an infinite potential well is not realistic.
In the semiconductor ternary alloy, $A_xB_{1-x}C$, the x is the grading function which linearly depends on the conduction band edge hence the potential *V(z)* experienced by the electron in the QW:

$$x(z)=\frac{V(z)}{\Delta V} \tag{2.3}$$

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

$$x(z)=[m(z)-m_{BC})]/\Delta m\,. \tag{2.4}$$

where $\Delta m=m_{AB}-m_{BC}$ is the difference of effective mass between the materials AB and BC.
It can then be shown that the actual potential experienced by the electron is

$$V(z)\equiv\phi[m(z)-m_{BC}]\,. \tag{2.5}$$

Further, to conserve the electron flux, we have to choose barrier continuous case, $(1/m)d\psi/dz$ which will lead to the envelope function Schrodinger equation for a realistic QW with a position dependent effective mass related to the position dependent potential (Milanovic and Ikonic, 1996; Radovanovic et al., 2000):

$$\frac{-\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_z}\frac{d\psi}{dz}\right)+\phi[m(z)-m_{BC}]\,\psi=E\psi\,. \tag{2.6}$$

We seek the functions m(z), x(z) and V(z) such that the energy spectrum of Eq. (2.6) has equidistant states same as one dimensional SHO (Einevoll et al, 1990; Milanovic and Ikonic, 1996). For convenience the following units are used: Energy in eV, Length in Å and Effective mass in free electron mass.

Taking into account these units, Eq.(2.6) becomes

$$\frac{d}{dz}\left(\frac{1}{m_z}\frac{d\psi}{dz}\right)+q\{E-\phi[m(z)-m_{BC}]\}\psi=0\,. \tag{2.7}$$

Now if we introduce the coordinate transformation $z = g(y)$ and consequently introducing a new function u(y) (Eugene, 1970 and Abramowitz and Stegun, 1972):

$$u(y)=\psi(y)\exp\left[-\frac{1}{2}\int_{y_0}^{y}\frac{1}{mg'}\frac{dmg'}{dy}dy\right]. \tag{2.8}$$

Eq.(2.7) becomes

$$\frac{d^2u}{dy^2}+\left[A(y)+qmg'^2\{E-\phi[m(z)-m_{BC}]\}\right]u=0\,. \tag{2.9}$$

where

$$A(y)=\frac{1}{2}\frac{d}{dy}\left[\frac{1}{mg'}\frac{dmg'}{dy}\right]-\frac{1}{4}\left[\frac{1}{mg'}\frac{dmg'}{dy}\right]^2. \tag{2.10}$$

The potential for the 1DSHO denoting equispaced energy level is given by (Ejere and Akpojotor, 2011; Ejere and Idiodi, 2011; Ejere, 2011)

$$V=\frac{1}{2}m_{1DSHO}\left(\frac{\Delta E}{\hbar}\right)^2y^2+V_0\,. \tag{2.11}$$

Taking Eq. ((2.11) into account Eq. (2.9), it will become

$$\frac{d^2u}{dy^2}+q\left[E-V_0-\frac{q}{4}m_{1DSHO}\left(\frac{\Delta E}{\hbar}\right)^2y^2\right]m_{1DSHO}u=0\,. \tag{2.12}$$

Eqs. (2.7) and (2.12) must coincide and Eqs. (2.9) and (2.12) must also coincide. Then their solutions can be obtained respectively as

$$m(z)=m_{BC}Cosh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\phi}}z\right) \tag{2.13}$$

and

$$V(z)=\phi_{BC}Sinh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\phi}}z\right). \tag{2.14}$$

Now taking into account Eqs. (2.4) and (2.13), the grading function becomes

$$x(z)=\frac{m_{BC}}{\Delta m}Sinh^2\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\phi}}z\right). \tag{2.15}$$

Eqs. (2.13) - (2.15) 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 wavefunction corresponding to the eigenstates is given by

$$\psi_i(z)=\left(\frac{1}{i!2^i}\right)^{1/2}[q\Delta Em]^{1/4}U_i(z)\,. \tag{2.16}$$

where the eigenfunctions U(z) are the well known Hermite functions (Russel, 1998):

$$U_i(z)=\left(\frac{1}{i!2^i}\right)^{1/2}[q\Delta Em(z)]^{1/4}H_i(z)e^{-\frac{1}{2}(z)}\,. \tag{2.17}$$

For i = 0, 1, 2:

$$H_0(z) = 1,\ H_1(z) = 2z \text{ and } H_1(z) = 4z^2 - 2 \tag{2.18}$$

Thus the corresponding eigenfunctions are

$$\psi_0(z) = [q\Delta E m_{BC}]^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\phi}}z\right) e^{-\frac{1}{2}(z)^2}. \quad (2.19)$$

$$\psi_1(z) = 2\left[\frac{1}{4}q\Delta E m_{BC})\right]^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\phi}}z\right) z e^{-\frac{1}{2}(z)^2}. \quad (2.20)$$

$$\psi_2(z) = \frac{2}{2}\left[\frac{1}{4}q\Delta E m_{BC})\right]^{1/4} Cosh^{1/2}\left(\frac{\Delta E}{2}\sqrt{\frac{q}{\phi}}z\right)(2z^2-1) e^{-\frac{1}{2}(z)^2}. \quad (2.20)$$

3. Presentation and discussion of results

The calculations of the electron effective mass, grading function, potential and wavefunctions are performed by a method that has been previously described (Ejere and Akpojotor, 2011; Ejere and Idiodi, 2011).The electron effective mass, the potential and the wavefunctions (at i = 0, 1 and 2) are obtained from Eqs. (2.13), (2.14), (2.19), (2.20) and (2.21) respectively using a common value in the literature for $\Delta E = 30\ MeV$ (Qi and Qi, 1999). The values of the materials' effective masses and the minimum band gaps are obtained from David (1991) and band off-set (the last column of Table1) from Milanovic and Ikonic (1996) and Ejere and Idiodi (2011). Graphs of the electron effective mass and potential dependence on the chosen direction of confinement for four ternary semiconductors QWs ($Ga_xAs_{1-x}Sb$, $InxAs1_{-x}Sb$, $Ga_xIn_{1-x}Sb$ and $In_xP_{1-x}As$) are shown in Figures 3a, 4a, 5a and 6a. All these graphs 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 conduction band edge hence the potential also has a linear relation with the electron effective mass (Radovanovic et al., 2000). Since band edges dependence on material composition is indispensible in bandgap engineering (Pryor and Pistol, 2005), the equispaced states electron effective mass will be very useful in obtaining equispaced energy levels in QWs.

The calculated dependence of the normalized wavefunctions $U_i(z)$ of the first three bound states on the direction of confinement provides the expected results as clearly depicted in Figures 3b, 4b, 5b, and 6b which favourably compare with Figure 1 and that of the simple harmonic motion. This is done 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 wavefunction from our formulation implies that our coordinate transformation was successful.

Conclusion

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 wavefunctions respond to the design (Nurmikkor and Gunshor, 1994). The application of the QW has continued 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 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 equispaced 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 (Imam et. al., 2002; Pryor and Pistol, 2005). 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 (Yang et al., 2013) and quantum dots which are three – dimensional confinement (Akpojotor and Akpojotor, 2009). It is expected that the equispaced energy levels 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 (Imam et. al., 2002). Finally, our theoretical design here can be tested not only by experimenting with real materials but also with ultacold atoms in optical lattices (Akpojotor, 2012).

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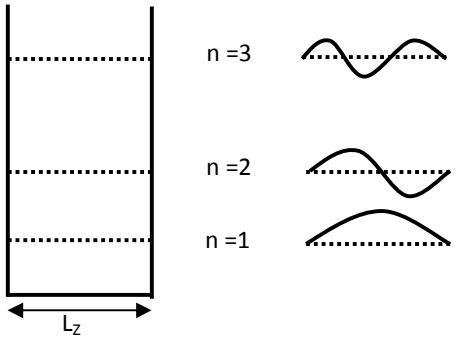

Figure 1: (a) Quadratically spaced energy levels of an 'infinite' quantum well and (b) the corresponding wavefunctions

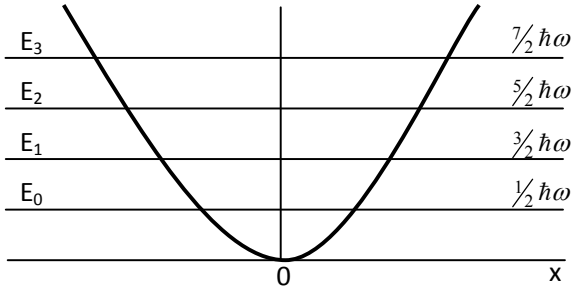

Figure 2: Common representation of the equispaced energy levels of the simple harmonic oscillator

Table 1: Some semiconducting properties of selected ternary alloys (David, 1991)

Semiconductor ternary alloy systems $A_x B_{1-x} C$	**Effective Mass (M_0) and Minimum band gap (eV)**		**Band off set (meV)**
	M_{BC}	**M_{AC}**	
Ga_xAs_{1-x} Sb	GaSb 0.050 m_0 0.67 eV	GaAs 0.067 m_0 1.35 eV	578
In_xAs_{1-x} Sb	InSb 0.013 m_0 0.165 eV	InAs 0.027 m_0 0.36 eV	168
$Ga_xIn_{1-x}Sb$	InSb 0.013 m_0 0.165 eV	GaSb 0.050 m_0 0.67 eV	430
$In_xP_{1-x}As$	InAs 0.027 m_0 0.36 eV	InP 0.077 m_0 1.27 eV	792

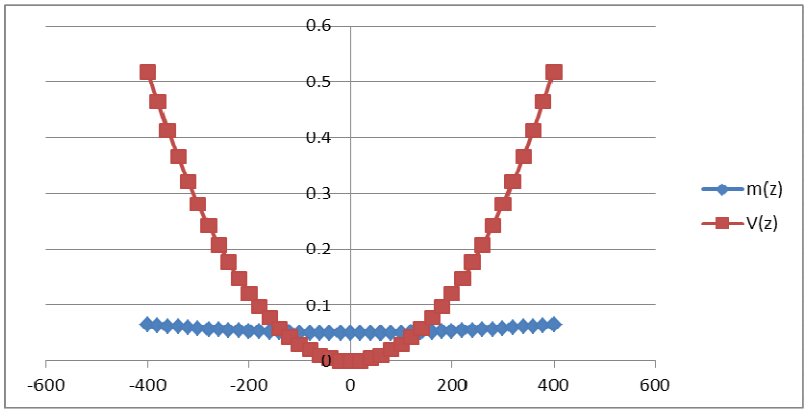

Figure 3a (Colour online): The effective mass m (z) and, the potential V(z) for $Ga_xAs_{1-x}Sb$

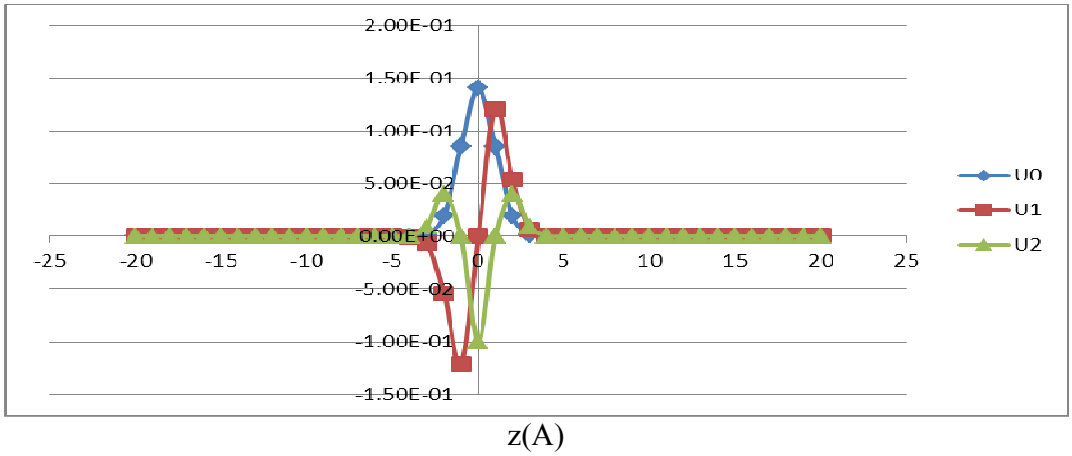

Figure 3b (Colour online): The normalized wave functions $U_i(z)$ of the first three bound state for $Ga_xAs_{1-x}Sb$

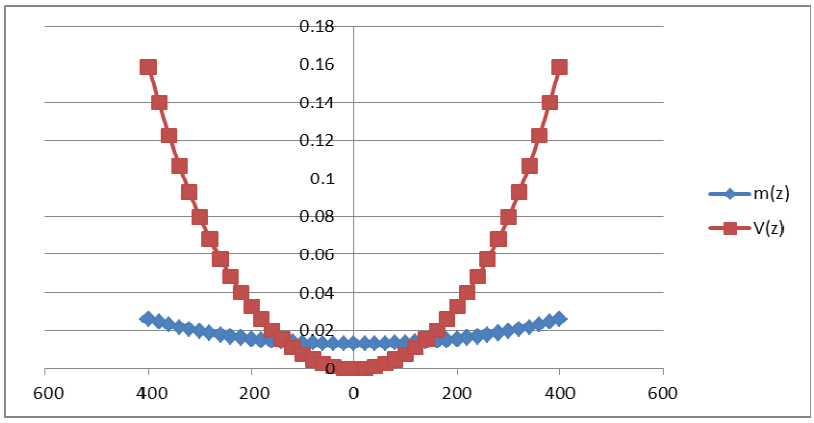

Figure 4a: (Colour online): The effective mass m (z) and the potential v(z) for $In_xAs_{1-x}Sb$

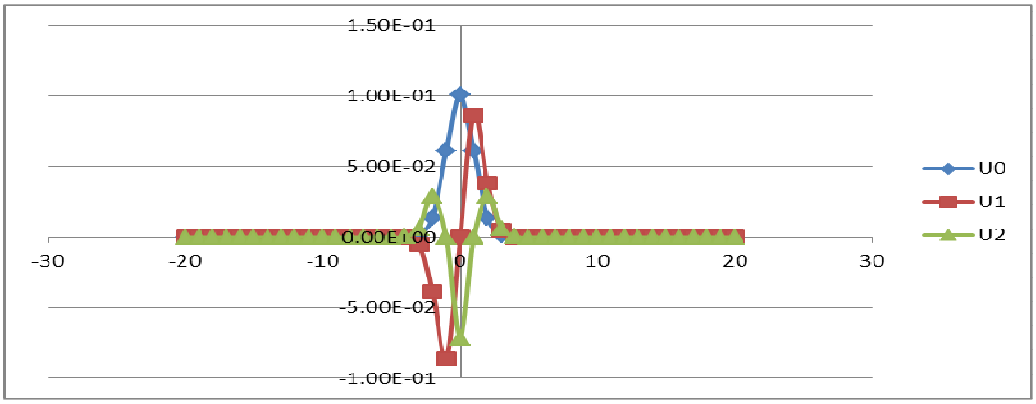

Figure 4b (Colour online): The normalized wave functions $U_i(z)$ of the first three bound state for $In_xAs_{1-x}Sb$

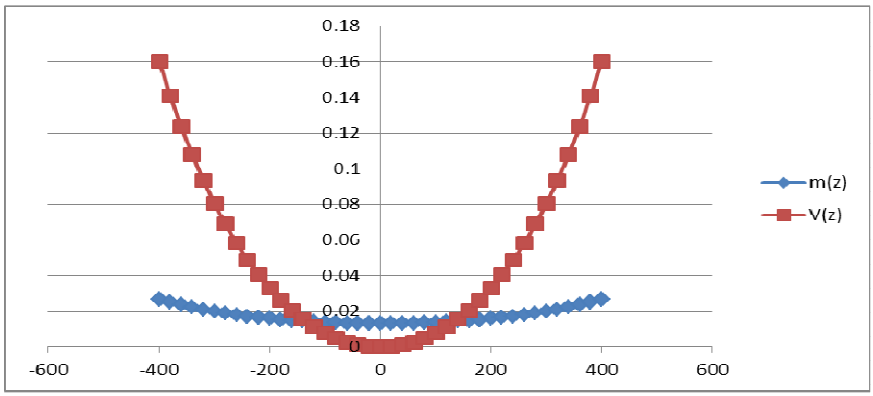

Figure 5a (Colour online): The effective mass m (z) and the potential V(z) for $Ga_xIn_{1-x}Sb$

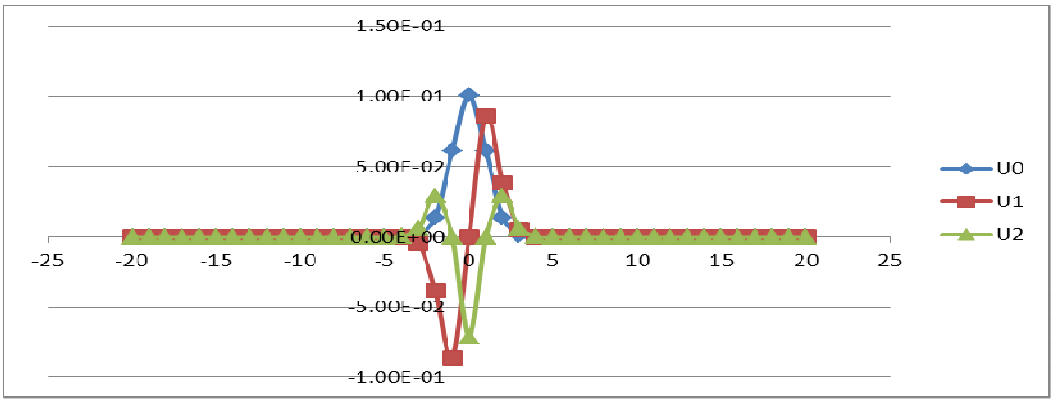

Figure 5b (Colour online): The normalized wave functions $U_i(z)$ of the first three bound state for $Ga_xIn_{1-x}Sb$

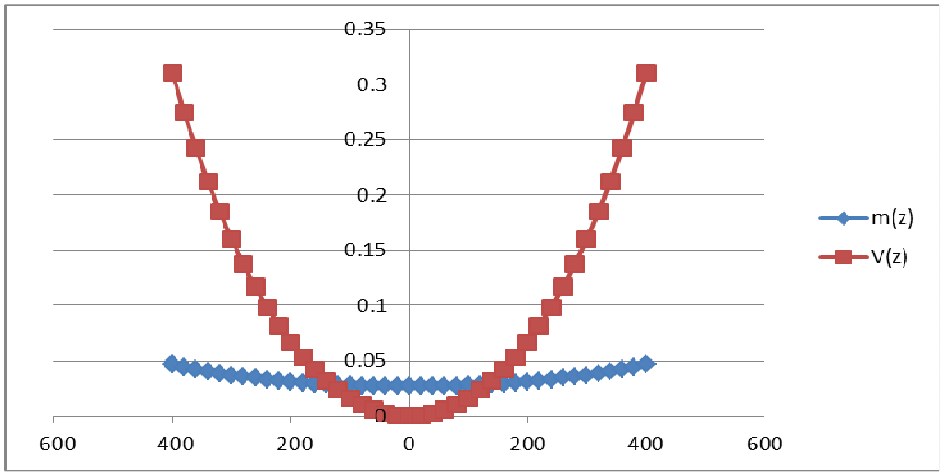

Figure 6a (Colour online): The effective mass m (z) and the potential V(z) for $In_xP_{1-x}As$

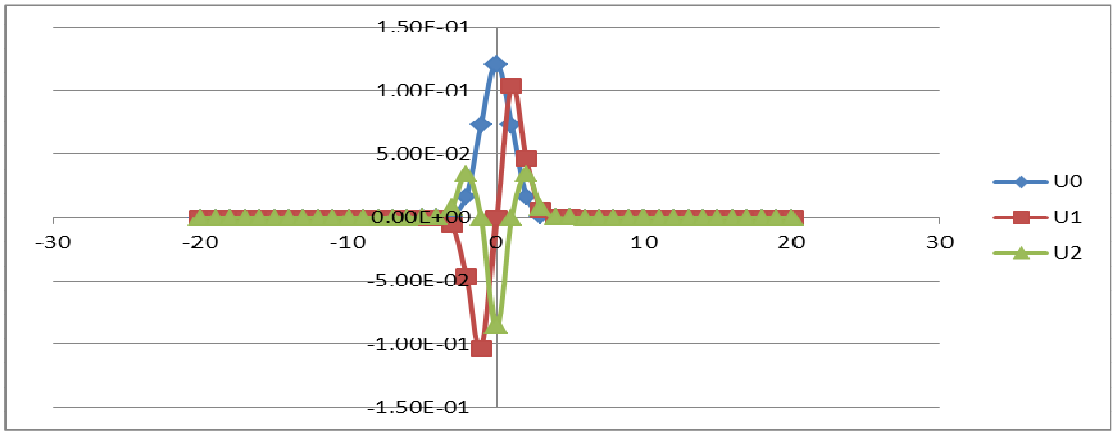

Figure 6b (Colour online): The normalized wave functions $U_i(z)$ of the first three bound state for $In_xP_{1-x}As$

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