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Theoretical Models of Binary and Ternary Quantum Wells Solar Cell Wafer Based in $A_xB_yC_{1-x-y}D$ System.

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Abstract

Two models derived by the direct application of the Schrodinger Hamiltonians are presented. The first model is for binary alloy active region Quantum Well QW, the second is for ternary alloy active region QW. The models are quite rich in parameters that can be tuned to get desired results. The thickness t for the active region of the quantum wells are considered.

Keyword: Solar cell, QW, Alloy, Schrodinger Hamiltonian, Mole fraction

1. INTRODUTION

Energy is the basic need of the world and the world uses energy at the rate of 15 terawatts [1, 2]. The increase in the usage of energy scales exponentially with the increase in the world's population and activities needing energy [3, 4].
Solar energy is the most abundant renewable source of energy available to mankind [5, 6]. The efficient conversion of solar energy to electricity is a critical research problem that is ongoing. Most of the present Photovoltaic (PV)cells are driven by semiconductor and optoelectronic technologies that are bulk-based [7]. PV cells also draw from thin film technologies based on direct band gap materials and have reached conversion efficiency of about 11%[8, 9]. The conversion efficiency of the PV cells is still left to be improved.
The search for technologies that will improve the conversion efficiency and production cost of PV cells lead to the Nanostructure technology where, instead of searching for new materials for new application and for new wavelength ranges, one now uses various combinations of materials to synthesize new material systems or control their composition and thickness. Both lattice-matched and lattice-mismatched pairs are now grown and it is impossible to tell which material combinations has which specific properties and is useful in which applications [3]. The materials may be combined within the same group, or even between different groups to grow binary, ternary, quaternary and even penternary alloys. This articles focus on the Quaternary alloy system $A_xB_yC_{1-x-y}D$, such as Cu_2ZnSnS_4 (CZTS, which is a promising candidate for nano structured PV solar cells and has attracted considerable interest recently)[10, 11, 5]. This is because all the constituents of CZTS are low cost, less toxic and earth abundant [6].The active region is in the nanometric range (ultrathin).
A theoretical model through the use of the Schrodinger Hamiltonian is presented in this article. Section two covers the mathematical formulation which leads to an expression for the thickness, t of the active region shown in Figure 1. And the next concluding section suggests a possible application.

2. Model with binary alloy semiconductor active region.

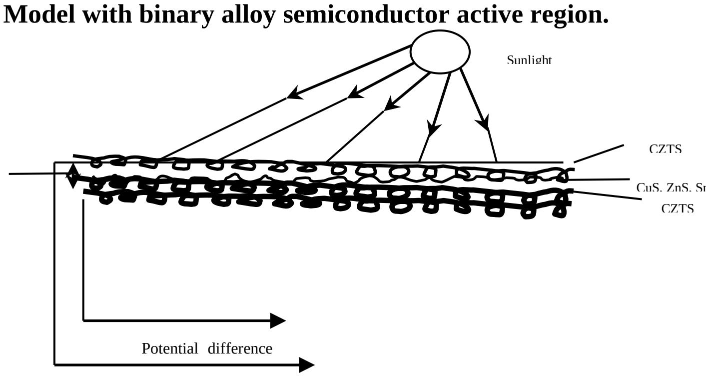

Figure 1: Skecth showing a QW solar cell wafer with three layers. The first and last layers are CZTS. The middle layer (the active region) is either CuS or ZnS or SnS

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Consider a Quaternary alloy $A_xB_yC_{1-x-y}D$, the effective masses of electrons are M_{AD}, M_{BD} and M_{CD} for electrons in CuS, ZnS and SnS respectively see reference [12, 13]

The potential electron experienced in the well is $V(z)$,

$$V(z) = \Delta V_1\, x(z) + \Delta V_2\, y(z) \qquad (1)$$

$$M(z) = M_{AD}\, x(z) + M_{BD}\, y(z) + M_{CD}\,(1-x-y)\,(z)$$

$$M(z) = M_{AD}\, x + M_{BD}\, y + M_{CD} - M_{CD}\, x - M_{CD}\, y$$

$$= (M_{AD} - M_{CD})x + (M_{BD} - M_{CD})y + M_{CD}$$

$$\Rightarrow M(z) = \Delta M_1\, x(z) + \Delta M_2\, y(z) + M_{CD} \qquad (2)$$

From Eq. (2) the mole fraction $x(z)$ obtained is

$$x(z) = \frac{1}{\Delta M_1}\left(M(z) - \Delta M_2\, y(z) - M_{CD}\right)$$

Substitute for x in Eq. (1) and $V(z)$ becomes

$$V(z) = \frac{\Delta V_1}{\Delta M_1}\left(M(z) - \Delta M_2\, y(z) - M_{CD}\right) + \Delta V_2\, y(z)$$

$$= \theta_1\left(M(z) - M_{CD}\right) - \Delta M_2\,\theta_1\, y(z) + \Delta V_2\, y(z)$$

$$V(z) = \theta_1 M(z) + \alpha\, y(z) - \beta \qquad (3)$$

Where

$$\left.\begin{aligned} \theta_1 &= \frac{\Delta V_1}{\Delta M_1} \\ \alpha &= \Delta V_2 - \Delta M_2\,\theta_1 \\ \beta &= \theta_1 M_{CD} \end{aligned}\right\} \qquad (4)$$

The 1 – D Effective mass Schrodinger Equation is

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right) + V(z)\right]\psi = E\psi \qquad (5a)$$

Substituting for $V(z)$ using Eq. (3) gives

$$\left[-\frac{\hbar^2}{z}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right) + \theta_1\, M(z) + \alpha\, y(z) - \beta\right]\psi = E\psi \qquad (5b)$$

For infinitesimal change $y(z)$ can be written as

$$y(z) = \frac{\gamma M(z)}{\Delta M_2}$$

where γ is a number and $M(z)$ takes value from M_{CD} to M_{AD}, and hence (5b) becomes

$$\left[-\frac{\hbar^2}{z}\left(\frac{1}{M(z)}\frac{d}{dz}\right) + \theta_1\, M(z) + \alpha\,\frac{\gamma M(z)}{\Delta M_2} - \beta\right]\psi = E\psi \qquad (5c)$$

Now, $\dfrac{\alpha\gamma}{\Delta M_2} = \dfrac{\Delta V_2\,\gamma}{\Delta M_2} - \gamma\theta_1 = (\theta_2 - \theta_1)\,\gamma$

Where $\theta_2 = \dfrac{\Delta V_2}{\Delta M_2}$

The Eq. (5c) becomes

$$\left[-\frac{\hbar^2}{z}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right) + \theta_1\, M(z) + \gamma\,(\theta_2 - \theta_1)\, M(z) - \beta\right]\psi = E\psi \qquad (5d)$$

$$\left[-\frac{\hbar^2}{z}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right) + \gamma\left(\theta_2 - \theta_1 + \frac{\theta_1}{\gamma}\right)M(z) - \beta\right]\psi = E\psi$$

$$\left[-\frac{\hbar^2}{z}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right) + \phi M(z) - \beta\right]\psi = E\psi$$

$$\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d\psi}{dz}\right) - \frac{2}{\hbar^2}\left(\phi M(z) - \beta - E\right)\psi = 0$$

Where $\phi = \gamma\left(\theta_2 - \theta_1 + \dfrac{\theta_1}{\gamma}\right)$

$$\frac{-1}{(M(z))^2}\frac{dM(z)}{dz}\frac{d\psi}{dz} + \frac{1}{M(z)}\frac{d^2\psi}{dz^2} - \frac{2}{\hbar^2}\left(\phi M(z) - \beta - E\right) = 0$$

$$\frac{d^2\psi}{dz^2} - \frac{1}{M(z)}\frac{dM(z)}{dz}\frac{d\psi}{dz} - \frac{2M(z)}{\hbar^2}\left(\phi M(z) - \beta - E\right) = 0 \qquad (5)$$

Introduce a new function $u(z)$

$$u(z)=\psi_{(z)}\ \exp\left(-\frac{1}{2}\int_a^b \frac{1}{M(z)}\frac{dM(z)}{dz}\,dz\right)$$

$$u(z)=\psi_{(z)}\ \exp\left(-\frac{1}{2}\int_a^b \frac{dM(z)}{dz}\right)$$

$$=\psi_{(z)}\ \exp\left(-\frac{1}{2}\left[lin\ M(z)\right]_a^b\right)$$

$$=\psi_{(z)}\ \exp\left(lin\left[M(z)\right]^{-\frac{1}{2}}\right)=k\ \psi_{(z)}\left(M(z)\right)^{-\frac{1}{2}}$$

$$u(z)=k\ \psi_{(z)}\ \left(M(z)\right)^{-\frac{1}{2}} \qquad (6)$$

From Eq. (6)

$$\psi(z)=\frac{1}{k}\left(M(z)\right)^{\frac{1}{2}}\ u(z) \qquad (7)$$

Differentiate Eq. (7) once and twice and then substitute into Eq. (5) to get

$$\frac{d\psi_{(z)}}{dz}=k\left(M(z)\right)^{\frac{1}{2}}\frac{du}{dz}+\frac{1}{2}\frac{u(z)}{\left(M(z)\right)^{\frac{1}{2}}}\frac{dM(z)}{dz}$$

and

$$\frac{d^2\psi_{(z)}}{dz^2}=\left[M(z)^{1/2}\frac{d^2u(z)}{dz}+\frac{du}{dz}\frac{1}{2}\frac{1}{\left(M(z)\right)^{1/2}}\frac{dM(z)}{dz}+\frac{1}{2}\left(\frac{1}{M(z)^{1/2}}\frac{du}{dz}\frac{dM(z)}{dz}\right.\right.$$
$$\left.\left.+\frac{u}{\left(M(z)\right)^{1/2}}\frac{d^2u}{dz^2}+\frac{1}{2}\frac{1}{\left(M(z)\right)^{1/2}}\frac{dM(z)}{dz}\right)\right]$$

Eq. (5) becomes

$$\frac{d^2u}{dz^2}+\left[A(z)-\frac{2M(z)}{\hbar^2}\left(\phi M(z)-\beta-E\right)\right]u=0 \qquad (8)$$

Where,

$$A(z)=\frac{1}{2}\frac{d}{dz}\left[\frac{1}{M(z)}\frac{dM(z)}{dz}\right]-\frac{1}{4}\left[\frac{1}{M(z)}\frac{dM(z)}{dz}\right]^2$$

ΔV_1 and ΔV_2 are percentage partition of ($E_{g1}-Eg_2$) and ($E_{g1}-Eg_3$) respectively

The Hamiltonian of an electron in the well interacting with electromagnetic field is

$$\frac{1}{2M}\left(p-eA\right)^2+V(r)=E$$

That is,

$$\left(\frac{P^2}{2M(z)}-\frac{e}{M(z)}\left(\bar{A}\,.\,\bar{P}\right)+\frac{e^2}{2M(z)}+V(z)\right)u=Eu$$

$$\left[\frac{\hbar^2}{2M(z)}\frac{d^2}{dz^2}-\frac{e}{M(z)}\left(\bar{A}\,.\,\bar{P}\right)+\frac{e^2}{2M(z)}A^2+V(z)-E\right]u=0$$

$$\left[\frac{d^2}{dz^2}-\frac{2e}{\hbar^2}\left(\bar{A}\,.\,\bar{P}\right)+\frac{e^2}{\hbar^2}A^2+\frac{2M(z)\,V(z)}{\hbar^2}-\frac{2M(z)E}{\hbar^2}-E\right]u=0$$

Put $P=\left[2\ m(z)\left(E-W\right)\right]^{1/2},\ W=Work\ \ function$ of the active region

$$\frac{d^2u}{dz^2}-\left[\frac{2e}{\hbar^2}\left(\bar{A}\,.\,\bar{P}+\frac{eA^2}{2}\right)-\frac{2M(z)}{\hbar^2}\left(W-E\right)\right]u=0$$

$$\frac{d^2u}{dz^2}-\left[\frac{2e}{\hbar^2}\left[\left(2M(z)\ \left(E-W\right)\right)^{1/2}\ ACos\ \theta+\frac{eA^2}{\hbar^2}\right]+\frac{2M(z)}{\hbar^2}\left(E-W\right)\right]u=0$$

$$\frac{d^2u}{dz^2}+\left\{-\frac{e^2A^2}{\hbar^2}-\frac{2M(z)}{\hbar^2}\left[\left(E-W\right)+4M(z)\ \left(E-W\right)^{1/2}\ AeCos\,\theta\right]\right\}u=0 \qquad (9)$$

Compare Eqs (8) and (9), they coincide if

$$A(z)=-\frac{e^2A^2}{\hbar^2} \qquad (10)$$

where,

$$A=\frac{e^2\,w_0^2\ \gamma^2}{3\ x\ c^3\ \hbar\ \varepsilon_0}\ |z|^2 \qquad [14]$$

and

$$\phi M(z)-\beta-E=\left(E-W\right)+4\ M(z)\ \left(E-W\right)^{1/2}\ AeCos\ \theta \qquad (11)$$

From Eq. (10

$$\frac{1}{2}\frac{d}{dz}\left[\frac{1}{M(z)}\frac{dM(z)}{dz}\right]-\frac{1}{4}\left[\frac{1}{M(z)}\frac{dM(z)}{dz}\right]^2=-\frac{e^2A^2}{\hbar^2}$$

$$M(z)\ \frac{d^2M(z)}{dz^2} - \frac{5}{4}\left(\frac{dM(z)}{dz}\right)^2 + \frac{(M(z))^2 e^2 A^2}{\hbar^2} = 0$$

$$m(z)\ \frac{d^2M(z)}{dz^2} - \frac{5}{4}\left(\frac{dM(z)}{dz}\right)^2 + \frac{(M(z))^2 e^2 Q^2 z^4}{\hbar^2} = 0 \qquad - \quad - \quad - \quad - \qquad (12)$$

Where,

$$Q = \frac{e^2\ \omega_0^2\ \gamma^2}{3\ \pi\ C^3\ \hbar\, \varepsilon_0} \text{ and } A = Q\ |\ Z\ |^2$$

From Eq. (11)

$$\left(\phi - 4\ (E-W)^{1/2}\ e\ Q\ Z^2\ Cos\,\theta\right) M(z) = 2E - W + \beta$$

$$M(z) = \frac{2E - W + \beta}{\phi - 4\ (E-W)^{1/2}\ e\ Q\ Cos\,\theta\ Z^2}$$

$$M(z) = \frac{C}{a + bz^2} = y \qquad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (13)$$

$$\frac{dy}{dz} = -\frac{C}{(a + bz^2)^2}\ .\ 2bz = -\frac{2bcZ}{(a + bz^2)^2} \qquad - \quad - \quad - \quad - \quad - \quad - \qquad (14)$$

$$\frac{d^2y}{dz^2} = \frac{(a + bz^2)^2\ .\ 2bc - \dfrac{2bcz\ .\ (-2)\ 2bz}{(a + bz^2)^3}}{(a + bz^2)^4}$$

$$\frac{d^2y}{dz^2} = \frac{2bc\ (a + bz^2)^2}{(a + bz^2)^4} - \frac{2(zb)^2\ c\ Z^2}{(a + bz^2)^7} \qquad - \quad - \quad - \quad - \quad - \quad - \qquad (15)$$

Eq. (12) can be re written as

$$y\frac{d^2y}{dz^2} - \frac{5}{4}\left(\frac{dy}{dz}\right)^2 + q\ y^2\ z^4 = 0 \qquad - \quad - \quad - \quad - \quad - \quad - \qquad (16)$$

Where,

$$y = M(z)$$

And $q = \dfrac{e^2Q^2}{\hbar^2}$

Substitute Eqs. (13), (14) and (15) in Eq. (16)

$$\left(\frac{C}{a + bz^2}\right)\left[-\frac{2bc}{(a + bz^2)^2} - \frac{2(2b)^2\ cZ^2}{(a + bz^2)^7}\right] - \frac{5}{4}\left[\frac{-2bcz}{(a + bz^2)}\right]^2 + q\left(\frac{C}{a + bz^2}\right)^2 Z^2 4 = 0$$

Factor out $\dfrac{c}{b + bz^2}$

That is $\dfrac{c}{b + bz^2} = 0 \qquad$ -- - - - - - - (17)

$$-\frac{2b}{a + bz^2} - \frac{2(2b)^2 z^2}{(a + bz^2)^6} - \frac{5}{4}\left[-\frac{2bz}{a + bz^2}\right]^2 + qz^4 = 0$$

$$-1 - \frac{4bz^2}{(a + bz^2)^5} - \frac{5}{4}\ (-z)^2 + q\ (a + bz^2)\ z^4 = 0$$

$$\frac{q(a + bz^2)z^4}{2b} - \frac{4bz^2}{(a + bz^2)^5} - \frac{5z^2}{4} - 1 = 0 \qquad - \quad - \quad - \quad - \quad - \qquad (18)$$

$$q = \frac{e^2Q^2}{\hbar^2}\ ,\quad Q = \frac{e^2\omega_0^2\ \eta^2}{3\pi\, c^3\ \hbar\, \varepsilon_0}$$

$$a = \phi = \gamma\ \left(\theta_2 - \theta_1 + \frac{\theta_1}{\gamma}\right),$$

$b = 4\ (E-W)^{1/2}\ \ Q\ Cos\theta$, θ is the angle between the Electromagnetic vector potential and the momentum vector.

$c = 2E - W + \beta$

$\theta_1 = \dfrac{\Delta V_1}{\Delta M_1}$, $\theta_2 = \dfrac{\Delta V_2}{\Delta M_2}$ $\qquad \theta \neq \theta_1$ or θ_2

$$y = M(z) \neq y(z)$$

$\beta = \theta_1\ M_{CD}$

Look for z from Eq. (18)

$$\frac{q\left(a+bz^2\right)z^4\left(a+bz^2\right)^5}{\left(a+bz^2\right)^5}-\frac{4bz^2}{\left(a+bz^2\right)^5}-\frac{5z^2\left(a+bz^2\right)^5}{\left(a+bz^2\right)^5}-\frac{\left(a+bz^2\right)^5}{\left(a+bz^2\right)^5}=0$$

$$q\left(a+bz^2\right)^6z^4-4bz^2-5z^2\left(a+bz^2\right)^5-\left(a+bz^2\right)^5=0$$

$$\left(a+bz^2\right)^5\left[q\left(a+bz^2\right)z^4-5z^2-1\right]-4bz^2=0$$

$$\left(a+bz^2\right)^5\left(aqz^4+bqz^6-5z^2-1\right)-4bz^2=0$$

$$\left(a^5+5a^4bz^2+10a^3b^2z^4+10a^2b^3z^6+5ab^4z^8+b^5z^{10}\right)\times\left(aqz^4+bqz^6-5z^2-1\right)-4bz^2=0$$

$$a^6qz^4+5a^5bqz^6+10a^4b^2qz^8+10a^3b^3qz^{10}+5a^2b^4qz^{12}+ab^5qz^{14}$$
$$+a^5bqz^6+5a^4b^2qz^8+10a^3b^3qz^{10}+10a^2b^4qz^{12}+5ab^5qz^{14}+b^6qz^{16}$$
$$-5a^5z^2-25a^4bz^4+50a^3b^2z^6-50a^3b^3z^8-25ab^4z^{10}-5b^5z^{12}$$
$$-a^5-5a^4bz^2-10a^3b^2z^4-10a^3b^3z^6-5ab^4z^8-b^5z^{10}-4bz^2=0$$

Re-arranging, and switching off power z^6 and above to give

$$+\left(a^6q-25a^4b-10a^3b^2\right)z^4$$
$$+\left(-5a^2-5a^4b-4b\right)z^2$$
$$+\left(-a^5\right)=0$$

Put $P=z^2$ $\left(\therefore\ z=\sqrt{P}\right)$ Eq. (18) gives

$$\left(a^6q-25a^4b-10a^3b^2\right)P^2+\left(-5a^2-5a^4b-4b\right)P-\left(-a^5\right)=0 \qquad - \quad - \quad - \qquad (19)$$

$$R=\left(a^6q-25a^4b-10a^3b^2\right)$$
$$S=\left(-5a^2-5a^4b-4b\right)$$
$$T=\left(-a^5\right)$$

i.e $RP^2+SP+T=0$ -   -   -   -   -   -   -   (20)

$$\Rightarrow p=\frac{-S\pm\sqrt{S^2-4RT}}{2R}$$

$$\sqrt{S^2-4RT}=\left(-5a^2-5a^4b-4b\right)^2-4\left(a^6q-25a^4b-10a^3b^2\right)\left(-a^5\right)$$
$$=25a^4+25a^6b+20a^2b+25a^8b^2+25a^6b+20a^4b^2+20a^2b+20a^4b^2+16b^2+4a^{16}q$$
$$-100a^9b-40a^8b^2$$

$$=\left(25a^4+50a^6b+40a^2b+65a^8b^2+40a^4b^2+16b^2+4a^{11}q-100a^9b\right)^{1/2}$$

$$P=\frac{\left(5a^2+5a^4b+4b\right)\pm\left(25a^4+50a^6b+40a^2b+65a^8b^2+40a^4b^2+16b^2+4a^{11}q-100a^9b\right)^{1/2}}{2\left(a^6q-25a^4b-10a^3b^2\right)}$$

$$P=\frac{S\pm D}{2R}\ \ i.e\ \ \frac{S}{2R}\pm\frac{D}{2R} \qquad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (21)$$

$$P_1=\frac{S}{2R}-\frac{D}{2R}\ \ and\ \ P_2=\frac{S}{2R}+\frac{D}{2R}$$

$$Z_1=\left(\frac{S}{2R}-\frac{D}{2R}\right)^{1/2}\ \ and\ \ Z_2=\left(\frac{S}{2R}-\frac{D}{2R}\right)^{1/2} \qquad - \quad - \quad - \quad - \quad - \qquad (22)$$

The thickness, *t* of the well, the active region is

$$t=Z_2-Z_1 \qquad - \quad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (23)$$

3. Model with ternary alloy semiconductor active region.

How about making the active layer a ternary alloy $A_x B_{1-x} C$? That is $A_x B_{1-x} C$ sandwich between $A_x B_y C_{1-x-y}D$
For the active layer (and ternary alloy)

$$\overline{M}(z)=\Delta\overline{M}\ \overline{x}(z)+M_{BC} \qquad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (24)$$

Where $\Delta\overline{m}=\left(M_{AC}-M_{BC}\right)$

Modification on the CZTS put $M_{CD}=\overline{M}(z)$ in $M(z)=M_{AD}x(z)+M_{BD}\,y(z)+M_{CD}(1-x-y)(z)$ to give

$$M(z)=M_{AD}x(z)+M_{BD}\,y(z)+\overline{M}(z)\,(1-x-y)(z)$$
$$=M_{AD}x(z)+M_{BD}\,y(z)+\left(\Delta\overline{m}\ \overline{x}(z)+M_{BC}\right)(1-x-y)(z)$$
$$=M_{AD}x(z)+M_{BD}\,y(z)+\Delta\overline{m}\ \overline{x}(z)+M_{BC}-\Delta\overline{m}\ \overline{x}(z)\ x(z)$$
$$M_{BC}x(z)-\Delta\overline{m}\ \overline{x}(z)\,y(z)-M_{BC}\,y(z)$$
$$=\left(M_{AD}-M_{BC}\right)x(z)+\left(M_{BD}-M_{BC}\right)y(z)-\left(x(z)+y(z)\right)\Delta\overline{m}\ \overline{x}(z)+\Delta\overline{m}\ \overline{x}(z)+M_{BC}$$
$$=\Delta m_3\ x(z)+\Delta m_4\ y(z)-\left(x(z)+y(z)-1\right)\Delta\overline{m}\ \overline{x}(z)+M_{BC}$$
$$M(z)=\Delta m_3\ x(z)+\Delta m_4\ y(z)-\left(x(z)+y(z)-1\right)\Delta\overline{m}\ \overline{x}(z)+M_{BC} \qquad - \qquad (25)$$

Where

$$\Delta M_3 = M_{AD} - M_{BC}$$
$$\Delta M_4 = M_{BD} - M_{BC}$$
$$\Delta \overline{M} = M_{AC} - M_{BC}$$
$$\bar{x}(z) \neq x(z)$$

From Eq (1)

$$V(z) = \Delta V_3\, x(z) + \Delta V_4\, y(z) + \Delta \overline{V}\, \bar{x}(z) \qquad (26)$$

$$\bar{x}(z) = \frac{1}{\Delta \overline{m}} \left(\overline{m}(z) - m_{BC}\right) \text{ from Eq. (24)} \qquad (27)$$

From eq. (25)

$$M(z) = \left(\Delta m_3 - \Delta \overline{m}\, \bar{x}(z)\right) x(z) + \left(\Delta m_4 - \Delta \overline{m}\, \bar{x}(z)\right) y(z) + \Delta \overline{m}\, \bar{x}(z) + M_{BC}$$

$$\Rightarrow x(z) = \frac{1}{\left(\Delta m_3 - \Delta \overline{m}\, \bar{x}(z)\right)} \left[M(z) - \left(\Delta m_4 - \Delta \overline{m}\, \bar{x}(z)\right) y(z) - \Delta\, \overline{m}\, \bar{x}(z) - M_{BC}\right]$$

Some transforms, put

$$\Delta \overline{m} = \beta_1\, \Delta m_3 = \beta_2\, \Delta m_4 \qquad (28)$$

$$\Rightarrow x(z) = \frac{1}{\Delta m_3 \left(1 - \beta_1\, \bar{x}\right)} \left[M(z) - \Delta m_4 \left(1 - \beta_2\, \bar{x}(z)\right) y(z) - \beta_2 \Delta m_4 - M_{BC}\right]$$

$$x(z) = \frac{1}{\Delta m_3 \left(1 - \beta_1\, \bar{x}(z)\right)} \left[M(z) - \Delta m_4 \left(1 - \beta_2\, \bar{x}(z)\right) y(z) - \beta_2 \Delta m_4 - \bar{x}(z) - M_{BC}\right] \qquad (29)$$

Substitute Eqs (27) and (29) into Eq (26)

$$V(z) = \frac{\Delta V_3}{\Delta m_3 \left(1 - \beta_1\, x(z)\right)} \left[M(z) - \Delta M_4 \left(1 - \beta_z\, \bar{x}(z)\right) y(z) - \beta_2\, \Delta m_4\, \bar{x}(z) - M_{BC}\right]$$
$$+ \Delta V_4\, y(z) + \frac{\Delta \overline{V}}{\Delta \overline{m}} \left(\overline{M}(z) - M_{BC}\right)$$

$$V(z) = \frac{\theta_3}{\left(1 - \beta_1\, \bar{x}(z)\right)} \left[M(z) - \Delta M_4 \left(1 - \beta_z\, \bar{x}(z)\right) y(z) - \beta_2\, \Delta m_4\, \bar{x}(z) - M_{BC}\right]$$
$$+ \Delta V_4\, y(z) + \bar{\theta} \left(\overline{M}(z) - M_{BC}\right) \qquad (30)$$

$$V(z) = \frac{\theta_3}{\left(1 - \beta_1\, \bar{x}(z)\right)} \left[M(z) - \Delta M_4 \left(1 - \beta_z\, \bar{x}(z)\right) y(z) - \Delta M_4 \beta_2\, \bar{x}(z) \approx 1\right]$$

Put $\left(1 - \beta_1 \bar{x}(z)\right) \approx \left(1 - \beta_2\, \bar{x}(z)\right) \approx 1$

$$V(z) = \theta_3 \left[M(z) - \Delta M_4\, y(z) - \Delta M_4\, \beta_2\, \bar{x}(z) - M_{BC}\right] + \Delta V_4\, y(z) + \bar{\theta} \left(\overline{M}(z) - M_{BC}\right)$$
$$V(z) = \theta_3 \left[M(z) - \Delta M_4 \left(y(z) + \beta_2\, \bar{x}(z)\right) - M_{BC}\right] + \Delta V_4\, y(z) + \bar{\theta} \left(\overline{M}(z) - M_{BC}\right)$$
$$V(z) = \theta_3 \left[M(z) - \Delta M_4 \left(y(z) + \beta_2\, \bar{x}(z)\right) - M_{BC}\right] + \Delta V_4\, y(z) + \bar{\theta} \left(\overline{M}(z) - M_{BC}\right)$$
$$V(z) = \theta_3\, M(z) + \left(\Delta V_4 - \theta_3 \Delta M_4\right) y(z) - \theta_3 \Delta M_4\, \beta_2 \bar{x}(z) - \theta_3 M_{BC} + \bar{\theta} \left(\overline{M}(z) - M_{BC}\right)$$

Note that $\bar{\theta} = \frac{\Delta \overline{V}}{\Delta \overline{M}}$

$$V(z) = \theta_3\, M(z) + \left(\Delta V_4 - \theta_3 \Delta M_4\right) y(z) - \theta_3 \Delta M_4\, \beta_2 \bar{x}(z) + \bar{\theta} \left(\overline{M}(z) - \left(\theta_3 + \bar{\theta}\right) M_{BC}\right)$$

Using Eq. (24).

$$V(z) = \theta_3\, M(z) + \left(\Delta V_4 - \theta_3 \Delta M_4\right) y(z) - \left(\theta_3 \Delta M_4\, \beta_2 - \bar{\theta} \overline{M}\right) \bar{x}(z) - \theta_3 M_{BC}$$

Where

$$\left.\begin{aligned} \alpha' &= \left(\Delta V_4 - \theta_3\, \Delta M_4\right) \\ \alpha'' &= \theta_3\, \Delta M_4\, \beta_2 - \bar{\theta}\, \Delta \overline{M} \\ \beta' &= \theta_3\, M_{BC} \\ \bar{\theta} &= \frac{\Delta \overline{V}}{\Delta \overline{M}} \end{aligned}\right\} \qquad (31)$$

Gives $V(z) = \theta_3 M(z) + \alpha'\, y(z) - \alpha''\, \bar{x}(z) - \beta'$ (32)

The I-D Effective Schrodinger Eq. is

$$\left[-\frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{M(z)} \frac{d}{dz}\right) + V(z)\right] \psi = E\psi$$

Substitute for $V(z)$ using Eq. (32)

$$\left[-\frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{M(z)} \frac{d}{dz}\right) + \theta_3 m(z) + \alpha' y(z) - \alpha'' \bar{x}(z) - \beta'\right] \psi = E\psi \qquad (33)$$

For infinitesimal change

$$y(z)=\frac{\gamma_1 M(z)}{\Delta M_4} \text{ and } \bar{x}(z)=\frac{\gamma_1 M(z)}{\Delta M_4} \qquad (34)$$

Substitute Eq (34) into Eq (33) gives

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right)+\theta_3 m(z)+\frac{\alpha'\gamma_1 M(z)}{\Delta M_4}-\alpha''\frac{\gamma_1 M(z)}{\Delta M_4}-\beta'\right]\psi = E\psi$$

Now, $\frac{\alpha'\gamma_1}{\Delta M_4}=\left(\frac{\Delta V_4}{\Delta V_4}-\theta_3\right)\gamma_1=(\theta_4-\theta_3)\gamma_1$

Where $\theta_4=\frac{\Delta V_4}{\Delta M_4}$

And $\frac{\alpha''\gamma_2}{\Delta M_4}=\left(\theta_3\beta_2-\bar{\theta}\beta_2\right)\gamma_2=\left(\theta_3-\bar{\theta}\right)\beta_2\gamma_2$

Using Eq. (28)

Eq. (35) becomes

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right)+\theta_3 m(z)+\gamma_1(\theta_4-\theta_3)m(z)-\beta_2\gamma_2\left(\theta_3-\bar{\theta}\right)m(z)-\beta'\right]\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right)+\left(\theta_3+\gamma_1\theta_4-\gamma_1\theta_3-\beta_2\gamma_2+\beta_2\gamma_2\bar{\theta}\right)m(z)-\beta'\right]\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{M(z)}\frac{d}{dz}\right)+\phi' m(z)-\beta'\right]\psi = E\psi$$

Where $\phi'=\theta_3+\gamma_1\theta_4-y_1\theta_3-\beta_2\gamma_2\theta_3+\beta_2\gamma_2\bar{\theta}$

$$\frac{d}{dz}\left(\frac{1}{m(z)}\frac{d\psi}{dz}-\frac{z}{\hbar^2}\left(\phi' m(z)-\beta'-E\right)\right)\psi=0$$

$$\frac{d^2\psi}{dz^2}-\frac{1}{M(z)}\frac{dM(z)}{dz}\frac{d\psi}{dz}-\frac{2M(z)}{\lambda^2}\left(\phi' M(z)-\beta-E\right)=0 \qquad (36)$$

Using Eq. (7) and Eq (36) gives

$$\frac{d^2u}{dz^2}+\left[A(z)-\frac{2m(z)}{\lambda^2}\left(\phi' m(z)-\beta'-E\right)\right]u=0 \qquad (37)$$

Where $A(z)=\frac{1}{2}\frac{d}{dz}\left[\frac{1}{m(z)}\frac{dm(z)}{dz}\right]-\frac{1}{4}\left[\frac{1}{m(z)}\frac{dm(z)}{dz}\right]^2$

Compare Eqs (8) and (37). They coincide if

$$A(z)=-\frac{e^2A^2}{\hbar^2} \qquad (38)$$

And $\phi' M(z)-\beta'-E=(E-W)+4M(z)(E-W)^{1/2} Ae\,Cos\theta$

$$\phi' M(z)-\beta'-E=(E-W)+4m(z)(E-W)^{1/2} A\,e\,Cos\,\theta \qquad (39)$$

Eq. (38) becomes

$$M(z)\frac{d^2M(z)}{dz^2}-\frac{5}{4}\left(\frac{dm(z)}{dz}\right)^2+\frac{(m(z))^2 e^2 Q^2 z^4}{\hbar^2}=0 \qquad (40)$$

Eq. (39) becomes

$$M(z)=\frac{2E-W+\beta'}{\phi'-4(E-W)^{1/2}e\,Q\,Cos\,\theta\,z^2} \qquad (41)$$

$y=\frac{C}{a+bz^2}$ that is Eq. (13)

Where $y=m(z)$

$a=\phi'$

$b=4(E-W)^{1/2}\,e\,Q\,Cos\,\theta$

$c=2E-W+\beta'$

Using Eqs. (14) and (15). Eq (40) becomes

$$y\frac{d^2y}{dz^2}-\frac{5}{4}\left(\frac{dy}{dz}\right)^2+q\,y^2z^4=0 \qquad (42)$$

Where

$$q=\frac{e^2Q^2}{\hbar^2}$$

The thickness *t* of the well is gotten from Eq. (21)

$$t = z_2 - z_1$$
$$a = \phi'$$
$$= \theta_3 + \gamma_1\theta_4 - \gamma_1\theta_3 - \beta_2\gamma_2\theta_3 + \beta_2\gamma_2\bar{\theta}$$
$$= \frac{\Delta V_3}{\Delta M_3} + \gamma_1\frac{\Delta V_4}{\Delta M_4} - \gamma_1\frac{\Delta V_3}{\Delta M_3} - \beta_2\gamma_2\gamma_1\frac{\Delta V_3}{\Delta M_3} + \beta_2\gamma_2\frac{\Delta\bar{V}}{\Delta\bar{M}}$$

From Eq. (34)

$$\gamma_1 = \frac{\Delta M_4\, y(z)}{M(z)} \quad \text{and} \quad \gamma_2 = \frac{\Delta M_4\, \bar{x}(z)}{M(z)}$$

From Eq. (28)

$$\beta_2 = \frac{\Delta\bar{M}}{\Delta M_4} \ \therefore\ \beta_2\gamma_2 = \frac{\Delta\bar{M}\ \bar{x}(z)}{M(z)}$$

For a possible application, assume

$$M(z) = \frac{1}{2}\Delta M_4$$
$$\gamma_1 = 2y(z), \qquad \gamma_2 = 2\bar{x}(z) \text{ and}$$
$$\beta_2\gamma_2 = 2\bar{x}(z).\ \frac{\Delta\bar{m}}{\Delta m_4}$$
$$\Delta V_3 = \frac{750}{100}\left(Eg_3 - Eg_{BC}\right)$$
$$\Delta V_4 = \frac{750}{100}\left(Eg_4 - Eg_{BC}\right)$$
$$\Delta\bar{V} = \frac{750}{100}\left(Eg_{AC} - Eg_{BC}\right)$$
$$b = 4\left(E - W\right)^{\frac{1}{2}}\ e\ Q\ Cos\theta$$
$$c = 2E - W + \beta'$$

$\bar{M}_{AB}$, $\bar{M}_{BC}$ and $\bar{M}_{AC}$ are the effective masses associated with $\bar{E}g_{AB}$, $\bar{E}g_{BC}$ and $\bar{E}g_{AC}$ energy gaps respectively in the ternary active region.

4. Conclusion

From Eqs. (22) and (23)

$$t = z_2 - z_1$$
$$t = \left(\frac{S}{2R} + \frac{D}{2R}\right)^{1/2} - \left(\frac{S}{2R} - \frac{D}{2R}\right)^{1/2} \qquad - \quad - \quad - \quad - \qquad (43)$$
$$\frac{S}{2R} = \frac{5a^2 + 5a^4b + 4b}{2\left(a^6q - 25a^4b - 10a^3b^2\right)}$$
$$\frac{D}{2R} = \frac{\left(25a^4 + 50a^6b + 40a^2b + 65a^8b^2 + 40a^4b^2 + 16b^2 + 4a^{11}q - 100a^9b\right)^{1/2}}{2\left(a^6q - 25a^4b - 10a^3b^2\right)}$$
$$a = \gamma\left(\theta_2 - \theta_1 + \frac{\theta_1}{\gamma}\right) = \gamma\theta_2 - \gamma\theta_1 + \theta_1$$
$$a = \gamma.\frac{\Delta V_2}{\Delta M_2} - \gamma.\frac{\Delta V_1}{\Delta M_1} + \frac{\Delta V_1}{\Delta M_1}$$
$$\Delta M_1 = M_{AD} - M_{CD}$$
$$\Delta M_2 = M_{BD} - M_{CD}$$
$$\Delta V_1 = \frac{75}{100}\left(Eg_1 - Eg_3\right)$$

using Dingle's partition proposal [13]

$$\Delta V_2 = \frac{75}{100}\left(Eg_2 - Eg_3\right)$$

Where $M_{AD} M_{BD}$ *and* M_{CD} are the effective masses of electron in CuS, ZnS and SnS respectively and Eg_1, Eg_2 and $Eg_3$are the band gap of CuS, ZnS and SnS respectively.

If $\gamma$is chosen at $M(z)$ midpoint between M_{CD} and M_{AD} for a particular mole fraction $y(z)$.

Then

$$\gamma = \frac{\Delta M_2 \ . \ y(z)}{M(z)}$$

$$y' = \frac{\Delta M_2 \ . \ y(z)}{\frac{1}{2}\Delta M_2}$$

$$y' = 2y(z)$$

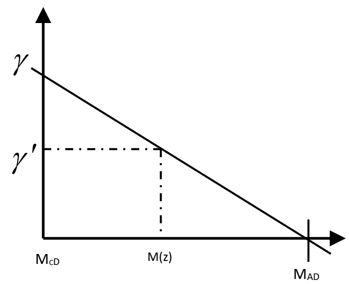

Figure 2:γ considered at midpoint between M_{CD} and M_{AD} on the M(z) axis

$$\therefore \ a = \gamma' \ . \ \frac{\Delta V_2}{\Delta M_2} - \frac{\gamma \Delta V_1}{\Delta M_1} - \frac{\Delta V_1}{\Delta M_1} \quad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (44a)$$

$b = 4\,(E-W)^{1/2}\ Q\ \ Cos\theta$ Put $\theta = 0$

$$b = 4(E-W)^{1/2}\,Q$$

$$b = 4\,(E-W)^{1/2}\ \frac{e^2\ \omega_0^2\ \eta^4}{3\pi c^3\ \hbar\ \varepsilon_0}$$

$$b = \frac{4e^2\ \omega_0^2\ \eta^4}{3\ \pi\ c^3\ \hbar\ \varepsilon_0}\ (E-W)^{1/2} \quad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (44b)$$

$$q = \frac{e^2 Q^2}{\hbar^2}$$

$$q = \frac{e^6\ \omega_0^4\ \ \eta^4}{9\ \pi^2\ c^6\ \hbar^4\ \varepsilon_0^2} \quad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (44c)$$

From Eqs. (44a), (44b) and (44c), the variables to consider taking $CuZnSnS_4$ as an example are the effective masses of electron and band gap in CuS, ZnS and SnS, the mole fraction $y(z)$, the energy of photon $E = \hbar\omega$, the work function *w*, refractive index η, permittivity ε_0 (ε for the material of active region).

Eq (43) can satisfy varied situation as the variable changes. This model is based on the fact that the active region is a diatomic molecular semiconductor. For the case where the active region is a ternary alloy semiconductor the model in section 3 apply.

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