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# A Theoretical model of a Quatum well Solar cell wafer.

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**ABSTRACT**

A theoretical model (by direct application of the Schrodinger Hamiltonian) for a Quantum well solar cell wafer is presented. The model is quite rich in parameters that can be tuned to get desired results, one of which is the thickness of the active region of the quantum well .

## 1. INTRODUCTION

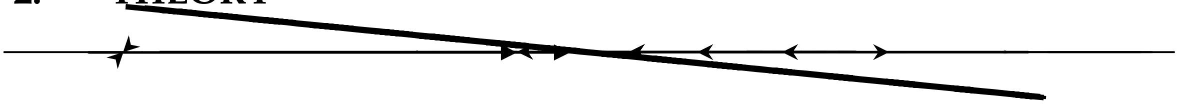
Energy is the basic need of the world and the world uses energy at the rate of 15 terawatts [1, 2]. The increase in the usage of energy scales exponentially with the increase in the world's population and activities needing energy [3].

Assessing energy especially in the form of electricity from renewable and environmentally friendly sources that can replace Fossil fuels is a very active field of research [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]. The conversion efficiencies of PV cells can be improved by the use of perfect crystals, but PV cells made of perfect crystal are expensive. PV cells also draw from thin film technologies based on direct band gap materials such as Copper Indium Sulphide ($CuInS_2$), Copper Indium Gallium Sulphide Sselenide (CIGSSe), Copper Indium Gallium di-Selenide (CIGS), Copper Indium di-Selenide (CIS) and Cadmium Telluride (CdTe). CdTe and CIGS have reached the commercialization stage with highest reported conversion efficiency of 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 nanostructured 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) and could be CuS or ZnS or SnS.

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. And the next concluding section suggests a possible application.

## 2. THEORY



CuS, ZnS, SnS

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]

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

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

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

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

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

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

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

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

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

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

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

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

Where

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

The 1 – D Effective mass Schrodinger Equation is

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

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

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

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

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

Where $\gamma$ is a number. $M(z)$ Takes value from $M_{CD}$ to $M_{AD}$

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

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 Equation becomes

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

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

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

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

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

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

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

Introduce a new function $u(z)$

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

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

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

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

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

From Eq. (6)

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

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

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

and

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

$$\left.\left. -\frac{1}{2}\frac{1}{(M(z))^{1/2}}\frac{dM(z)}{dz}\right)\right]$$

Eq. (5) becomes

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

Where,

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

$\Delta V_1$ and $\Delta V_2$ 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,

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

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

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

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

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

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

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

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

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

where,

$$A = \frac{e^2\,w_0^2\,\gamma^2}{3\,x\,c^3\,\eta\,\varepsilon_0}\,|z|^2 \qquad [13]$$

and

$$\phi M(z) - \beta - E = (E-W) + 4\,M(z)\,(E-W)^{1/2}\,A\,e\,Cos\,\theta \quad - \quad - \qquad (11)$$

From Eq. (10

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

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

$$\frac{1}{4M(z)}\frac{d^2M(z)}{dz^2} - \frac{5}{4\times 4(M(z))^2}\left(\frac{dM(z)}{dz}\right)^2 + \frac{e^2A^2}{\eta^2} = 0$$

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

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

Where,

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

From Eq. (11)

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

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

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

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

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

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

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 $q = \dfrac{e^2Q^2}{\eta^2}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Look for z from Eq. (18)

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

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

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

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

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

$$a^6qz^4 + 5a^5bqz^6 + 10a^4b^2qz^8 + 10a^3b^3qz^{10} + 5a^2b^4qz^{12} + ab^5qz^{14}$$

$$+ a^5bqz^6 + 5a^4b^2qz^8 + 10a^3b^3qz^{10} + 10a^2b^4qz^{12} + 5ab^5qz^{14} + b^6qz^{16}$$

$$-5a^5z^2 - 25a^4bz^4 + 50a^3b^2z^6 - 50a^3b^3z^8 - 25ab^4z^{10} - 5b^5z^{12}$$

$$-a^5 - 5a^4bz^2 - 10a^3b^2z^4 - 10a^3b^3z^6 - 5ab^4z^8 - b^5z^{10} - 4bz^2 = 0$$

Re-arranging, this gives

$$b^6qz^{16}$$

$$+\left(ab^5q + 5ab^5q\right)z^{14}$$

$$+\left(5a^2b^4q + 10a^2b^4q - 5b^5\right)z^{12}$$

$$+\left(10a^3b^3q + 10a^3b^3q - 25ab^4 - b^5\right)z^{10}$$

$$+\left(10a^4b^2q + 5a^4b^2q - 50a^2b^3 - 5ab^4\right)z^8$$

$$+\left(5a^5bq + a^5bq - 5a^3b^2 - 10a^2b^3\right)z^6$$

Switch off power $z^6$ and above to give

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

$$+ \left(-5a^2 - 5a^4 b - 4b\right) z^2$$

$$+ \left(-a^5\right) = 0$$

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

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

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

$$S = \left(-5a^2 - 5a^4 b - 4b\right)$$

$$T = \left(-a^5\right)$$

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

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

$$\sqrt{S^2 - 4RT} = \left(-5a^2 - 5a^4 b - 4b\right)^2 - 4\left(a^6 q - 25a^4 b - 10a^3 b^2\right)\left(-a^5\right)$$

$$= 25a^4 + 25a^6 b + 20a^2 b + 25a^8 b^2 + 25a^6 b + 20a^4 b^2 + 20a^2 b + 20a^4 b^2 + 16b^2 + 4a^{16} q$$

$$- 100a^9 b - 40a^8 b^2$$

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

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

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

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

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

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

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

## 3. CONCLUSION

From Eqs. (22) and (23)

$$t = z_2 - z_1$$

$$t = \left(\frac{S}{2R} + \frac{D}{2R}\right)^{1/2} - \left(\frac{S}{2R} - \frac{D}{2R}\right)^{1/2} \quad - \quad - \quad - \quad - \qquad (24)$$

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

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

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

$$a = \gamma.\frac{\Delta V_2}{\Delta M_2} - \gamma.\frac{\Delta V_1}{\Delta M_1} + \frac{\Delta V_1}{\Delta M_1}$$

$$\Delta M_1 = M_{AD} - M_{CD}$$

$$\Delta M_2 = M_{BD} - M_{CD}$$

$\Delta V_1 = \frac{75}{100}\left(Eg_1 - Eg_3\right)$ 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 CuS, ZnS and SnS respectively.

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

$$\gamma = \frac{\Delta M_2 \; . \; y(z)}{M(z)} \qquad \gamma' \longleftrightarrow$$

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

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

$$\therefore \; a = \gamma' \; . \; \frac{\Delta V_2}{\Delta M_2} - \frac{\gamma \Delta V_1}{\Delta M_1} - \frac{\Delta V_1}{\Delta M_1} \qquad - \; - \; - \; - \; - \qquad (25a)$$

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

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

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

$$b = \frac{4e^2 \; \omega_0^2 \; \eta^4}{3 \; \pi \; c^3 \; \eta \; \varepsilon_0}\left(E - W\right)^{1/2} \; - \; - \; - \; - \; - \; - \; - \qquad (25b)$$

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

$$q = \frac{e^6 \omega_0^4 \eta^4}{9 \pi^2 c^6 \hbar^4 \varepsilon_0^2} \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad - \qquad (25c)$$

From Eqs. (25a), (25b) and (25c), the variables to consider taken $CuZnSnS_4$ as 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 $\varepsilon_0$ (ε for the material of active region).

Eq (24) can satisfy varied situation as the variable changes. This model is base on the fact that the active region is a diatonic molecular semiconductor. For case where the active region is a ternary alloy semiconductor this model does not apply. Model with ternary alloy semiconductor active region will be presented later.

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