A THEORETICAL MODEL OF QUANTUM WELL SOLARWAFER

BY

ISAAC AITALEGBE

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DEPARTMENT OF PHYSICS

FACULTY OF PHYSICAL SCIENCES

UNIVERSITY OF BENIN

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A PROJECT SUBMITTED TO THE DEPARTMENT OF PHYSICS FACULTY OF PHYSICAL SCIENCES, IN PARTIAL FULFILLMENT FOR THE REQUIREMENT OF BACHELOR SCIENCE (B.Sc.) (INDUSTRIAL PHYSICS) OF THE UNIVERSITY OF BENIN, BENIN CITY, EDO STATE, NIGERIA.

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CERTIFICATION

This is to certify that this project was carried out by ISAAC AIȚALEGBE with Matriculation Number PSC1909141 in partial fulfillment of the requirements the award of the degree of Bachelor of Science (B.Sc.) of the Department Of Physics, Faculty of Physical Sciences, University of Benin under the supervision of

26/11/2025

DR. ARTHUR EJERE — **DATE**

(PROJECT SUPERVISOR)

DEPT. OF PHYSICS HEAD OF DEPT. Date......

8/12/25

PROF C.O AIGBOGUN — **DATE**

(H.O.D PHYSICS)

EXTERNAL EXAMINER — **DATE**

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I give my profound gratitude to GOD ALMIGHTY for granting me divine and understanding not only in carrying out this project work successfully, but also during my days in the University of Benin. Indeed he has been and God and a father to me.

I sincerely appreciate my project supervisor, Dr Authur Ejere for his dedicated guidance which undoubtedly led to the success of this work.

I appreciate my parents Mr And Mrs AITALEGBE for all their guidance, love, provision and support which has gotten me this far in my academics. I also want appreciate every academic staff of the Department of Physics for the knowledge they impacted in me throughout my stay in the department./

TABLE OF CONTENT

DEDICATION

This work is dedicated to god almighty

ABSTRACT

The purpose of this project is to present a theoretical model (by I Hamiltonian for the thickness of the active region of Quantum Well Solar Cell Wafer. The model is quite rich in parameters that can be tuned to get desired results.

CHAPTER ONE

INTRODUCTION

The demand for energy is on the increase by the day as a result of the accelerated level of industrialization, especially in emerging economies. According to International Energy Agency (IEA), the world uses energy at the rate of 4761 020J per year which is equivalent to power consumption of 1 5Tera Watts (Todorov, *et, al.,* 2010). As the world population increases geometrically, the need for energy will also increase in proportion, and by the end of 2030, it is forecasted to double that of today.

With the increasing consumption of conventional energy such as coal andfossil fuel and the serious environment impact, it has become expedient and imperative to explore and exploit clean renewable sources of energy that will replace the conventional sources (Suryawanshi *et. al*, 2012). Amongst various alternative sources of energy known today, solar energy is the most promising because it is abundant, economical, environmentally friendly and effective for mankind. (Wang *et. al.,* 2013; Katagiri, *et. al..* 2009).

Today in Nigeria in both rural and urban areas consumer constantly suffer power outages due to perpetual power deficits. There seems to be no respite from thesecrippling deficit seen from the figures that are been published from time to time and there appear to be no hope of the shortage syndrome easing-up both in the near and far future. Thus, it has almost become a ritual to insistently and persistentlyclamor for more power generation. Thus, the school of thought which is predominantly majority believes in the endogenous diversification in the energysector, particularly solar technologies, which emphasizes copious and continuous supply of energy to consumers. Polycrystalline silicone is the most commonly used by photovoltaic (PV) industry. However, these technologies rely on an indirect band gap absorber semiconductor, thereby requiring a thick layer to absorb more fractions of the incident solar radiations (Katagriri *et. al,* 2010). Also in order to increase the efficiency, recent PV research has led to the development of thin film PV technologies. Currently, the main thin film solar cells include the amorphous silicon thin film, cadmium telluride (CdTe), Copper Indium Selenium (CIS), Copper Indium Gallium Selenium (CIGS), the gallium arsenide and cadmium telluride contain toxic elements (Cadmium and Arsenic) and copper indium gallium selenide system contains rare indium elements; thus, these two types of solar cells cannot meet the future development of solar technology because of the toxicity of cadmium and selenium and the limitation in supplies for indium and tellurium.With the advancement of growth technologies the Molecular beam Epitaxy (MBE), metal organic chemical vapour deposition (MOCVD), etc, it is now possible to fabricate multilayered semiconductor nanostructure like quantum Wells (QWs) Quantum Wires (QWRs), Quantum Dot (QPs) and Superlattices (SLS), in which the individual layer thickness may be as small as one monolayer of 2 tb 3 Angstrom. These structures have given rise to new devices that are used in all areas of optoelectronics, quantum electronics and photonics. Recently, quaternary compound Cu_2ZnSnS_4 (CZTS) has been intensively examined as an alternative PV material due to its similarity in material properties with CIGS and the relative abundance of the raw materials. CZTS is a compound semiconductor of (12) (II) (IV) (VI) of stannite structure its band gap is about 1.5 ev, which is very close to the best band gap required by serniconductor solar cells (1.3ev) with a high absorption coefficient (>lO4cmj. The search technologies that will improve the conversion of efficiency and production cost of PV 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. The materials may be combined within the same group, oreven between different groups to grow hinar, ternary. quatemary and even penternary alloys. This project focus or the Quanternary Alloy System ABCD such as Cu2ZnSnS4 (CZTS) which is a promising candidate for nanostructured PV solar cells has attracted considerable interest recently (Znao. e. 2D-: Wadia *et al.*, 2009; Wang et. al., 2013). This is because all the constituents CZTZ are low cost, less toxic and earth abundant (Katagiri *et. al.*, 2009). The active region is in the nanometric range (ultrathin) and could be CuS or ZnS or SnS,

BACKGROUND THEORY

The term photovoltaic comes from the Greek word '*photos*' meaning light and the name of the Italian Physicist Alexandra Volta, after whom the Volta and consequently voltage are named. It means literally light and electricity. The Photovoltaic effect was first recognized in 1839 by the French Physicist Alexandre Edmun Becquerel. However, it was Charles Fritts who coated the semiconductor selenium with an extremely thin layer of gold to form the junctions. The device was only 1% efficient at the time. In 1946, Russel Ohi patented the modern solar cell as Sven Ason Bergiund had a prior patent concerning methods of increasing the capacity of photosensitive cells.

In 1888 Russian Physicist Aleksander Stoletov built the first cell based on photoelectric effect discovered by Heinrich Hertz in 1887. The nano structuring of semiconductor materials was first introduced by William Shockely (1951) and later by Kroemer (1957). The first report on the growth and measurement of the optical properties of confined electrons in the Quantum Well (QW) came in 1974 by

Dingle and his collaborators. Almost concurrently Chang and his co-workers in 1974 reported on electrical measurement made (Change *et. al.,* 1974). In order to understand how a solar cell works, a little background theory of semiconductor physics is required for simplicity i.e. the working principle of a single crystalline silicone.

Silicone is a group 4 elements, this means that each "Si" atom has 4-valence electrons in its outermost shell which can covalently bond to other silicone atoms to form a solid. The atoms in a silicone crystal are arranged in order, three dimensional array. There are other terms used to refer to the size of silicone — namely; polycrystalline, microcrystalline and nanocrystalline etc. and they refer to crystal grains which make up the solid. The most commonly used by the PV industry is polycrystalline silicone PC-Si. Silicon is a semiconductor. This means that in a solid silicon crystal, there are certain bands of energies which the electrons are allowed to have and other energies which are disallowed or forbidden. These forbidden energies are called the "band gap." The allowed andthe forbidden bonds of energy are explained by Quantum Mechanics. At room temperature, pure silicone is a poor electrical conductor, in Quantum Mechanics this is explained by the fact that the form energy level lies in 5 the forbidden band gap. To make ifire silicon a better conductor it is doped with very small amounts of impurity atoms from either Group III or V of the periodic table to form P-type or N-type semiconductors.

CHAPTER TWO

PHOTO EFFECT

The term "photo effect" refers to the energy transfer from photons i.e. quantum of electromagnetic radiation) to electrons contained inside material. Photon energy is thereby converted into potential and kinetic energy of electrons. The electron absorbs the entire quantum energy of the photon defined as the product of Planck's quantum and the photon frequency. External and internal photo effect is distinguished.

External

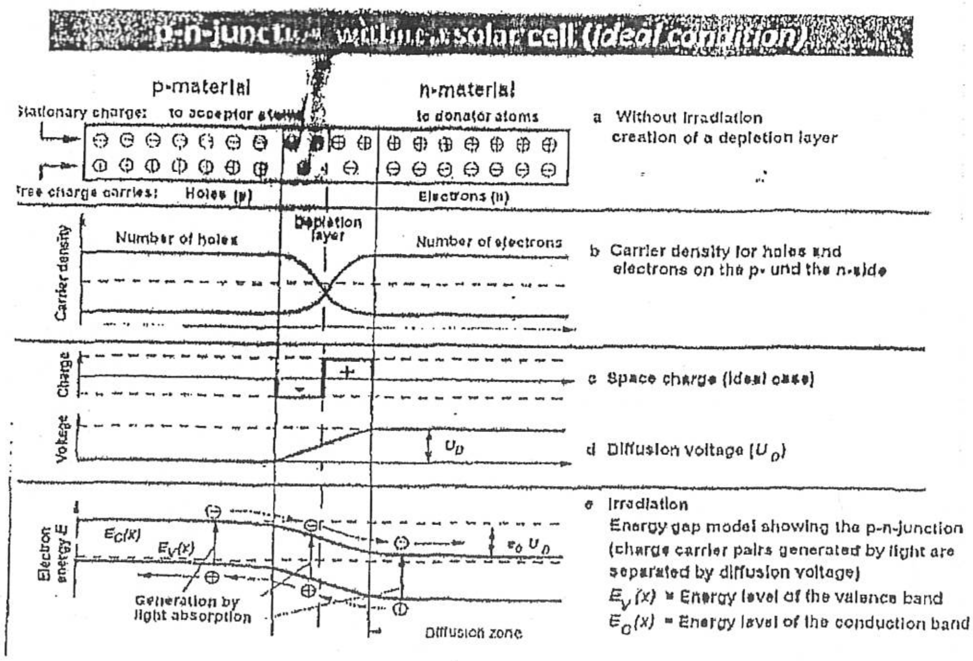
- If electromagnetic radiation hits the surface of a solid body within the ultraviolet range, electrons can absorb energy from the photon.
- Then they are able to surmount the required work function to escape from the solid body, provided that there is sufficient photon energy.

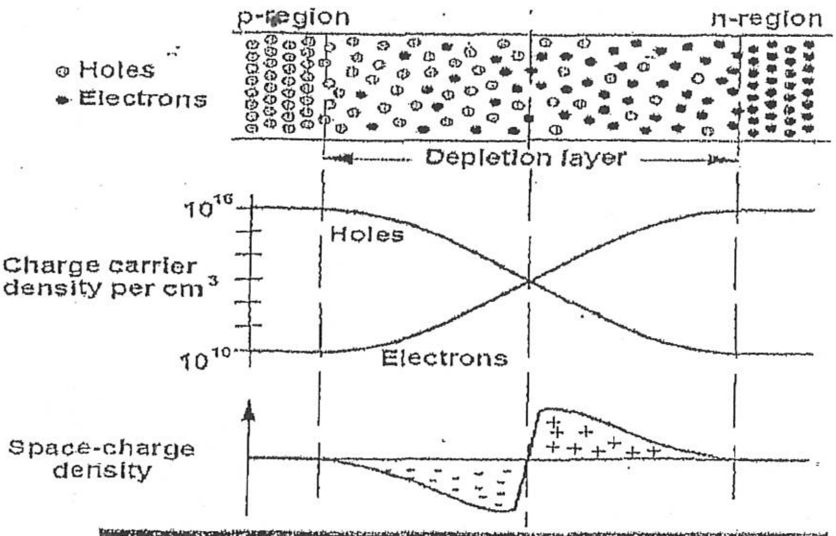
Internal

- The internal photo effect describes also absorption of electromagnetic radiation within a solid body.
- The electrons are in this case not detached from the solid body.
- They are only lifted from the valence band up to the conduction band.

- Therefore, electron-hole-pairs are created which enhance the electric conductivity of the solid body.
- **P-N Junction**
- If p- and n-doped materials brought into contact, holes from the p-doped side diffuse into the n-type region and vice versa.
- First, a strong concentration gradient is formed at the p-n- junction, consisting ofelectrons inside the conduction band and holes inside the valence band.
- Due to this concentration, gradient holes from the p-region diffuse into the ii-region while electrons diffuse from the n- to the p area.
- Due to the diffusion, the number of majority carriers are reduced on both sides of the p-n junction.
- The charge attached to the stationary donors or acceptors then creates a negativespace charge on the p-side of the transition area and a positive space charge on then-side.
- As a result of the equilibrated concentration of free charge carriers an electricalfield is built up across the border interface (p-n-junction).
- The described process creates a depletion layer in which diffusion flow andreverse current compensate each other.

- The no longer compensated stationary charges of donors and acceptors define a depletion layer whose width is dependent on the doping concentration.





Creation of a depletion layer within the p-n-junction.

PHOTO VOLTAIC EFFECT

If photons, the quantum's of light energy, hit and penetrate into a semiconductor, they can transfer their energy to an electron from the valance band. If such a photon is absorbed within the depletion layer, the region's electrical field directly separates the created charge carrier pair. The electron moves towards the n-region, whereas the hole moves to the p-region.

If, during such light absorption, electron-hole-pairs are created outside of the depletion region within the p- or n-region (i.e. outside of the electrical field), they may also reach the space-charge region by diffusion due to thermal movements i.e. without the direction being predetermined by an electrical field).At this point, the respective minority carriers (i.e. the electrons within the p-region and the holes in the n-region) are collected by the electrical field of the space-charge region and are transferred to the opposite side. The potential barrier of the depletion layer, in contrast, reflects the respective majority carriers.

Finally, the p-side becomes charged positively while the n-side is charged negatively, both, photons absorbed within, and outside, of the depletion layer contribute to this charging. This process of light-induced charged separation is referred to as p-n-photo effect or as photovoltaic effect.

Thus, the photovoltaic effect only occurs if one of the two charge carriers created during light absorption passes the p-n junction. This is only likely to occur when the electron-hole-pair are generated within the depletion layer. Outside of this electrical field there is an increasing likelihood that charge carrier pairs created by light get lost by recombination. This is more likely the greater the distance is between the location of the generation of the electron-hole-pair and the depletion layer, this is quantified by the "diffusion length" of the charge carriers inside the semiconductor material. The term "diffusion length" refers to the average path lengths to be overcome by electrons or holes within the area without an electrical field before recombination takes place.

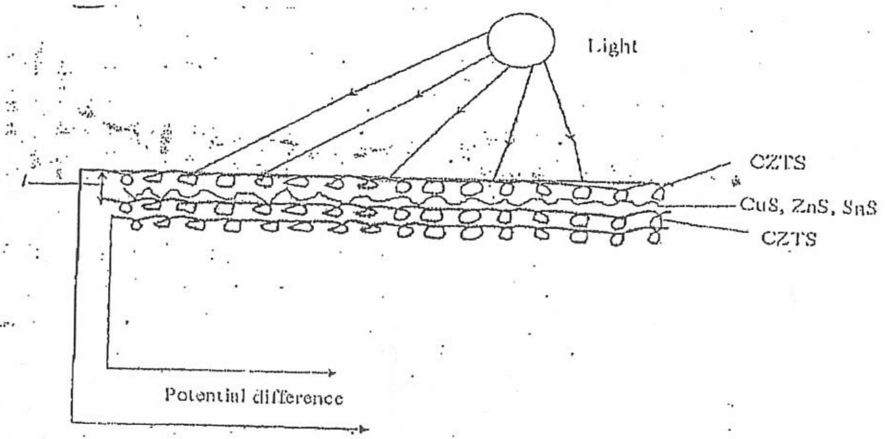
This diffusion length is determined by the semiconductor material and, in case of the identical material, highly depends on the impurity content — and thus also on doping (the more doping the lower the diffusion length) — and on crystal perfection. For silicon the diffusion length varies from approximately 10 up to several 100um. If the diffusion length is less than the charge carriers' distance to the p-n junction most electrons or holes recombine. To achieve an effective charge carrier separation the diffusion length should be a multiple of the absorption of the solar radiation incident on a photovoltaic cell. Due to the charge separation during irradiation, electrons accumulate within the n-region, whereas holes accumulate inthe p-region. Electrons and holes will accumulate until the repelling forces of theaccumulated charges start to impede additional accumulation, i.e. until the electrical potential created by the accumulation of electrons and holes is balanced by the diffusion potential of the p-n junction. Then the open-circuit voltage of the solar cell is reached. The time to achieve these conditions is almost immeasurably short.

If p- and n-sides are short-circuited by an external connection, the short- circuit current is measured. In this operating mode the diffusion voltage at the p-n junction is restored, According to the operating principle of a solar cell, short circuit current increase is proportional and almost linear to solar irradiance.

CHAPTER THREE

METHODOLOGY

A theoretical model through the use of the Schrodinger Hamiltonian is presented in this chapter, it covers the mathematical formulation which end in deriving anexpression for the thickness of the active region of the quantum well.



Consider a Quaternary alloy ABC1 D, the effective masses of electrons are MAD, MBD, MCD for electrons in CuS, ZnS and SnS respectively.

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

$$v(z) = \Delta v_1 xz + \Delta V_2 y(z) ------------------ (1)$$

$$m(z) = Mx(z) + M_{BD}y(z) + M_{CD} - M_{CD}x - M_{CD}y =$$

$$m(z) = M_{AD}^{(z)}x + M_{AD}^{(z)}y + M_{CD} - M_{CD}x - M_{CD}x - M_{CD}y$$

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

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

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

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

Substitute for x in Eq (1) $v(z)$ becomes

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

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

$$v(z) = \theta_1 M(z) + a y(z) - \beta - - - - - - - - - - - - - - (3)$$

Where

$$\theta_1 = \frac{\Delta V_1}{\Delta M_1}$$

$$a = \Delta V_2 - \Delta M_2 \theta_1$$

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

The 1-D Effective mass Schrodinger Equation is

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

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

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

For infinitesimal change y(z) can be written as

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

Where y is a number, M(z) takes a value from M_{CD} *to* M_{AD}

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

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

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

The Equation becomes

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

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

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

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

Where $\phi=\gamma(\theta_2-\theta_1+\frac{\theta_1}{\gamma})$

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

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

Introducing a new function *u(z)*

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

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

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

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

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

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

From Eq. (6)

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

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

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

And

$$\frac{d^2\psi}{dz^2}\left[M(z)^{\frac{1}{2}}\frac{d^2u(z)}{dz} + \frac{du}{dz}\frac{1}{2}\frac{1}{(m(z))^{1/2}}\frac{dm(z)}{dz} + \frac{1}{2}\left(\frac{1}{(m(z))^{1/2}}\frac{du}{dz}\frac{dm(z)}{dz} + \frac{u}{(m(z))^{1/2}}\frac{d^2u}{dz^2} - \frac{1}{2}\frac{1}{(m(z))^{1/2}}\frac{dM(z)}{dz}\right)\right]$$

Eq. (5) becomes

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

Where

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

ΔV_1 and ΔV_2 are percentage partition of ($Eg_1 - Eg_2$) and ($Eg_1 - Eg_3$)

Respectively

$$\Delta V_1 = (Eg_1 - Eg_2)\frac{75}{100}$$

$$\Delta V_2 = (Eg_1 - Eg_3)$$

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

$$\frac{1}{2m_0}(p - eA)^2 + V(r) = E$$

That is,

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

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

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

Put $P = [2M(Z)(E-W)]^{1/2}$ W= Work Function of the active region

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

$$\frac{d^2u}{dz^2} - \left[\frac{2e}{\hbar^e}(2m(z)(E-W))\,{}^1/_2\,A\cos\theta + \frac{eA^2}{\hbar^2}\right] + \frac{2m(z)}{\hbar^2}(E-W)u = 0$$

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

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

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

Where

$$A = \frac{e^2w_0^2\gamma^2}{3xc^3n\varepsilon_0}|z|^2$$

and

$$\phi m(z) - \beta - E = (E-W) + 4m(z)(E-W)^{\frac{1}{2}}Ae\cos\theta$$

From Eq. (10)

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

$$\frac{1}{4m(z)}\frac{d^2m(z)}{dz^2} - \frac{1}{4(m(z))^2}\left(\frac{dm(z)}{dz}\right)^2 - \frac{1}{16(m(z))^2}\left(\frac{dm(z)}{dz}\right)^2 + \frac{e^2A^2}{\hbar^2} = 0$$

$$m(z) = \frac{C}{a+bz^2} = \gamma -------------------(13)$$

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

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

$$\frac{d^2y}{dz^2} = \frac{2bc(a+bz^2)^2}{(a+bz^2)^4} - \frac{2(zb)^2 cz^2}{(a+bz^2)^7} \text{-----------------}(15)$$

Eq. (12) can be written as

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

Where

$y = m(z)$

and $q = \frac{e^2Q^2}{n^2}$

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

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

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

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

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

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

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

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

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

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

$c = 2E - W + \beta$

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

$$y = m(z) \neq y(Z)$$

$\beta = \theta_1 m_{CD}$

Look for z from Eq. (18)

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

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

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

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

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

Re-arranging, this gives

b^6qz^{16}

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

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

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

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

$+(5a^5bq + a^2bq - 5a^3b^2 - 10a^2b^3)z^6 = 0$

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

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

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

$+(-a^5) = 0$

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

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

$$R = (a^6q - 25a^2b - 10a^3b^2)$$

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

$$T = (-a^5)$$

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

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

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

$$= 25a^4 + 25a^6b + 20a^2b + 25a^8b^2 + 25a^6b + 20a^4b^2 + 20a^2b + 16b^2 + 4a^{16}q - 100a^9b - 40a^8b^2$$

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

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

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

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

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

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

$$= \gamma\frac{\Delta V_2}{\Delta m_1} - \frac{\gamma \Delta V_1}{\Delta m_1} + \frac{\Delta V_1}{\Delta M_1} = \boxed{a = \gamma\frac{\Delta V_2}{\Delta m_2} - \frac{\gamma \Delta V_1}{\Delta M_1} + \frac{\Delta V_1}{\gamma \Delta m_1}}$$

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

$$= 4(E - W)^{\frac{1}{2}} \frac{e^2 w_0^2 \eta^4}{3\pi c^3 \hbar \varepsilon_0} Cos\theta = \boxed{b = \frac{4e^2\omega_0^2\eta^2}{3\pi c^3 \hbar \mathcal{E}_0}(E - W)^{1/2} Cos\theta}$$

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

$$\frac{e^2}{\hbar^2} \frac{e^2 \omega_0^4 \eta^4}{3^2 \pi^2 c^6 h^2 \varepsilon_0^2}$$

$$\frac{e^6 \omega_0^4 \eta^4}{9\pi^2 c^6 \varepsilon_0^2 \hbar^4} = q$$

$$a = \gamma \left(\frac{\Delta V_2}{\Delta m_2} - \frac{\Delta V_1}{\Delta m_1} + \frac{\Delta V_1}{\gamma \Delta M_1} \right)$$

$$\Delta V_2 = (Eg_1 - Eg_3) \frac{j_R}{100}$$

Variables for a

γ, j_1, j_2

$$\Delta V_1 = (Eg_1 - Eg_3) \frac{j_1}{100}$$

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

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

$$M_{CD} = Z\,n\,S$$

$$M_{AD} = C\,u\,S$$

$$M_{CD} = S\,n\,S$$

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

Condition

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

$\omega_0(w) =$ Standing wave (frequency pattern in the well

η =Refractive Index

Variables for b

$\omega, \eta, E, w, \varepsilon, \theta$

$\varepsilon_0(\varepsilon) =$ Permitivity

$$q = \frac{e^6}{9\pi^2 c^6 \hbar^4} \frac{\omega_0^4 \eta^4}{\varepsilon_0^2}$$

Variables for q

$\omega, \eta, \varepsilon$

Consider

$$\left(\frac{c}{a+bz^2}\right)^2 = 0$$

$$\Rightarrow= 0, i.e\ ZE - W + \beta = 0$$

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

The thickness, t, of the well is which active region is or layer is

$$t = Z_2 - Z_1 --------------------------(23)$$

CHAPTER FOUR

CONCLUSION

From Eqs. (22) and (23)

$$t = Z_2 - Z_1$$

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

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

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

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

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

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

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

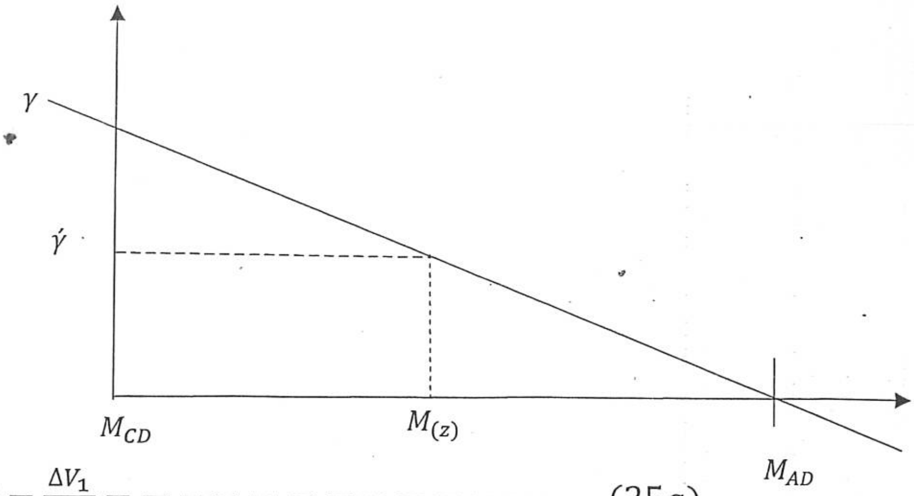
$\Delta V_1 = \frac{75}{100}(Eg_1 - Eg_3)$ using Dingle's partitions proposal [14]

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

Where M_{BD} and M_{CD} are the effective masses of electron in CuS, ZnS and SnS respectively and E_{g1}, E_{g2} and E_{g3} are the band gap CuS, ZnS and SnS respectively.

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

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



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

$$\acute{y} = 2y(z)$$

$$\therefore a = \gamma^! \frac{\Delta V_1}{\Delta M_2} - \frac{\gamma \Delta V_1}{\Delta M_1} - \frac{\Delta V_1}{\Delta M_1} - - - - - - - - - - - - - - - - - (25a)$$

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

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

$$b = 4(E - W)^{1/2} \frac{\ell^2 \omega_0^2 \eta^4}{3\pi c^3 \hbar \mathcal{E}_0}$$

That is

$$b = \frac{4\ell \omega_0^2 \eta^4}{3\pi c^3 \hbar \mathcal{E}_0} (E - W)^{1/2} - (25b)$$

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

$$q = \frac{\ell^6 \omega_0^4 \eta^4}{9\pi c^6 \hbar^4 \mathcal{E}_0^2} - (25C)$$

From Equation (25a),(25b) and (25c), the variables to consider taken Cu, Zn, Sn, S4 as example are the effective masses of electron and band gap in CuS, ZnS and SnS. The mole fraction 'y(z0, the energy of photon E=HW, the work function w, refractive index, permittivity (for the material of active region).

Equation (24) can satisfy varied situation as the variable changes. The model is based 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.

REFERENCES

Fthenakis, V. (2009). "Sustainability of photovoltaic: the case for thin-film solar cells." Renewable and Sustainable energy review 13(9):2746-2750

Ito, K., Nakazawa, T. (1988). "Electrical and optical properties of stannite-Type quaternary semiconductor thin films" Japanese Journal of Applied Physics 27; 2094

Katagiri, Hironori; Jimbo, Kazuo; Maw, Win Shwe; Oishi, Koichhiro; Yarnazaki, Makoto; Araki, Hideaki; Takeuchi, Akiko (2009).

Suryawanshi, M.O.; Agawane, G.L., Agawane, S.M.; Bhosale, S.W. Shin, P.S.; Patil, (2013). "Optical designs that improve the efficiency of Cu2ZnSn (5 , Se) 4-Solar cells." Energy of Materials Science 40(8): 2003,

Todorov, T.K., Reuter, KB., Mitzi, D.B. (2010). "High-efficiency solar cell with earth-abundant liquid-processed absorber. Advanced Materials. 22(20): E156.

Wang, W.; Winkler, M.T.; Gunawan, 0.; Gokrnen, T.; Todorov, T.K.; Zhu, Mitzi, D.B, (2013), "A 12.6% Cu2ZnSnSxSe4-x (CZTSSe) solar cell is presented with detailed device characteristics." Advanced Materials.