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Effect of Buffer Layer on Cu (In, Ga)Se₂ Solar Cell Performance

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Abstract- Search of sustainable energy resources is continued from the decades. The industrialization growth in various domains and socio-economic developments created huge demand of electrical power while the conventional resources are shrinking. This opens doors for research and developments in renewable energy resources such as, Solar, Wind, Hydro and Geothermal Energy sectors. Among these energy solar energy emerged as one of the sustainable energy resource. This research work targeted to improve the efficiency of thin film flexible Copper Indium Gallium Di-Selenide abbreviated as CIGS cell through optimization of buffer layer parameters. The proposed model used zinc sulphide (ZnS) as a potential buffer layer to make the solar cell free from toxic Cadmium (CdS) sulphide. Further the doping profile and width of buffer layers are investigated along with corresponding change in energy states and electrical permittivity of the material. The complete solar cell model is simulated using MATLAB scripting and SCAPS model. the results are compared with the existing result of CdS-CIGS. The ZnS-CIGS model is simulated with variation in thickness of buffer layer and optimized material parameters are determined.

Keywords- Thin-film, Buffer layer, Efficiency, Simulation

1. INTRODUCTION

Three kinds of solar cells are widely reported, researched and reached to the production level for industrial purpose. The distinguished cells have their own advantages and disadvantages. Silicon solar cell suffers with high cost, wastage of materials and their size, while organic solar cells suffer with efficiency and cost of industrialization. Thin film CIGS solar cell shown better flexibility with comparable efficiency and fulfills the demand of battery powered solar cell for hand held devices, wearable gadgets, and toys industries. The presented paper is motivated through the research work reported by Benmir et. al.[1]. The buffer layer ZnS deposited over kesterite material in order to remove the toxic material CdS from the solar cell.

The wide optical energy gap and similar crystal structure of doped ZnS make it a potential candidate as a buffer layer for thin film solar cell. A solar irradiance AM1.5 model is considered and simulated as shown in figure 1.

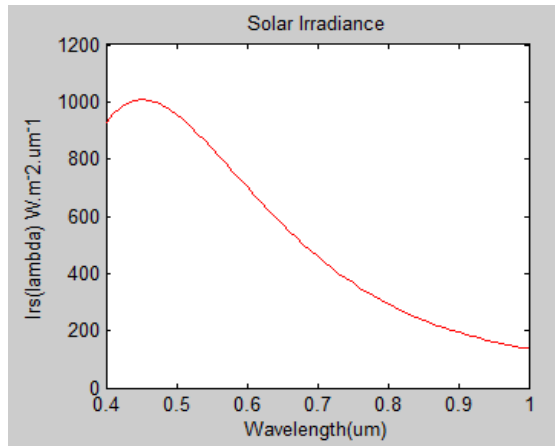


Fig.1. Irradiance Simulation Result

2. BUFFER LAYER

The buffer layer should be as transparent as possible for the visible range of solar spectrum and possesses significant balance of conductivity at interfaces with active layer and trans-conducting oxide. This layer works as n-region also known as electron transport layer or window layer of the photovoltaic pn-junction diode.

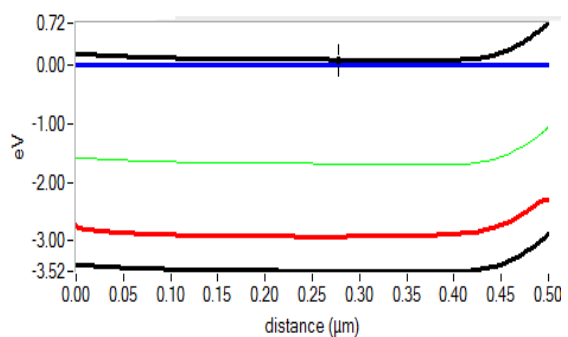


Fig.2. Band Structure of Zn_{1-x}S:Cu_x

The band gap of buffer layer expected to be wider to lower down the absorption of lights into the region. The zinc sulphide with different concentration of copper Zn_{1-x}S:Cu_x reported by Mahdi Hasan and Raoof Ali[2]. This paper preferred 8% of Zn_{1-x}S:Cu_x with band gap 3.61eV and simulated the SCAPS 1-D model. The band structure determines flat band that is highly conductive at conductive oxide layer and curved

band at absorption layer interface. The wide band gap makes it transparent to the light source.

3. ACTIVE LAYER

This is main region or layer of the solar cell responsible for generation of charge carriers through absorption of light irradiance. It is p-region of the photovoltaic pn-junction diode. The optically lower band gap material is preferred for this layer. Copper Indium Gallium di-selenide modeled with band gap of 1.2 eV, and relative permittivity 10. When light with photonic energy ($h\nu$) greater than the energy gap ($> E_g$) between valance band and conduction band of solar cell, incidents on the materials, electrons from the valance band jumps to the conduction band with higher momentum and thus cross the upper conduction band layer. These electrons now relaxed by aligned movement through the external load connected to the cell constitute a load current.

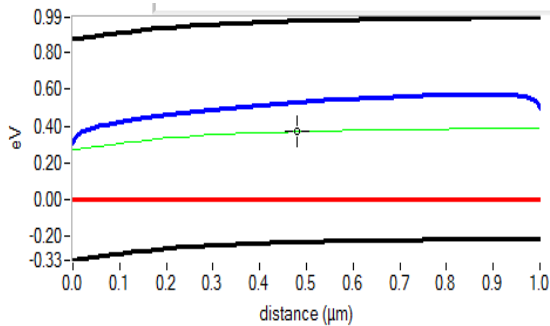


Fig.3. Band Structure of Zn_{1-x}S:Cu_x

The band structure of absorption layer determines flat band at metallic interface while curved band at the pn-junction. The materials having small optical energy gap are preferred so that maximum absorption is possible in the region to improve efficiency.

4. MODELING OF SOLAR CELL

The presented work focused on modeling and simulation of one dimensional thin film solar cell. The simulation is initially done with MATLAB scripting and it is also simulated with SCAPS-1D simulator to verify the model across different platforms. The material parameters are set to compute the various components of diode equation into the solar cell like absorption of light, charge carriers generation and recombination, dark current, open circuit voltage, Short circuit current. The absorption co-efficient is modeled with excitation of electrons from VB to CB considering temperature constant. The transition is approximated for direct band gap materials and so absorption co-efficient determined by [3]

$$\alpha = A \left(\frac{hc}{\lambda} \right)^{r-1} \left(\frac{\lambda_g - \lambda}{\lambda_g} \right)^{r-1} \quad eq. (1)$$

Where $\frac{1}{2} \leq r \leq \frac{3}{2}$; and λ_g is the wavelength corresponding to optical energy gap, for indirect band gap $\frac{3}{2} \leq r \leq \frac{5}{2}$

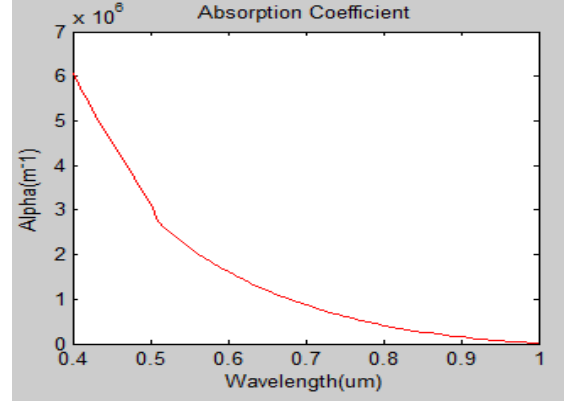


Fig.4. Absorption of CIGS Solar V/S wavelength

The built-in junction potential difference is also given by Einstein

$$V_{bi} = \frac{kT}{q} \ln \left(\frac{N_d N_a}{n_i^2} \right) \quad eq. (2)$$

Equation for rate of generation of charge carries is modeled for solar PV cell

$$G_R(x) = (1 - R) \int 1 - r(\lambda) f(\lambda) \alpha(\lambda) e^{-\alpha(x+W_n)} d\lambda \quad eq. (3)$$

Only real value is considered against absorption of light. It determines the wavelengths less than wavelength corresponding to energy gap λ_g of the material. The minority current components can be given as

$$J_{p1} = \frac{(e * F(\lambda) * (1 - R) * \alpha_1 * L_{p1})}{(\alpha_1 * L_{p1})^2 - 1} * \left[\frac{S_{p1} * L_{p1}}{D_{p1}} + e^{-\alpha_1 W_n} \left(\frac{S_{p1} * L_{p1}}{D_{p1}} \cosh \left(\frac{La}{L_{p1}} \right) + \sinh \left(\frac{La}{L_{p1}} \right) \right) \right]$$

$$J_{p2} = \frac{S_{p1} * L_{p1}}{D_{p1}} * \sinh \left(\frac{La}{L_{p1}} \right) + \cosh \left(\frac{La}{L_{p1}} \right) - (\alpha_1 * L_{p1} * e^{-\alpha_1 W_n})$$

$$J_p = J_{p1} * J_{p2} \quad eq. (4)$$

$$J_{n1} = \frac{(e * F(\lambda) * (1 - R) * \alpha_2 * L_{n1})}{(\alpha_2 * L_{n1})^2 - 1} * \left[\frac{S_{n1} * L_{n1}}{D_{n1}} + e^{-\alpha_2 W_p} \left(\frac{S_{n1} * L_{n1}}{D_{n1}} \cosh \left(\frac{Lb}{L_{n1}} \right) + \sinh \left(\frac{Lb}{L_{n1}} \right) \right) \right]$$

$$J_{n2} = \frac{S_{n1} * L_{n1}}{D_{n1}} * \sinh \left(\frac{Lb}{L_{n1}} \right) + \cosh \left(\frac{Lb}{L_{n1}} \right) - (\alpha_2 * L_{n1} * e^{-\alpha_2 W_p})$$

$$J_n = J_{n1} * J_{n2} \quad eq. (5)$$

These are diffusion currents into buffer and absorption layer respectively. Here, J_p, J_n represent minority current into n and p-region respectively. R represents total rate of recombination into PV cell.

CIGS thin film solar cell shown in figure 5 is designed with the help of SCAPS-1D software. Here active layer of CIGS is placed at back end and interfaced with back contact while the buffer window is kept at front end below the transparent conducting oxide layer. ZnO layer prevents the

surface contamination of solar cell as well as it provides good conductivity for cathode electrode interconnects.

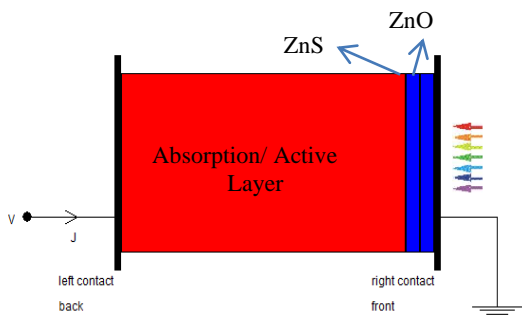


Fig.5. CIGS Solar Cell SCAPS 1-D Model

5. RESULTS

Area of the cell is taken 0.410 cm², thickness of buffer layer is varied from 0.5um to 4um; thickness of active layer is 4um. The simulation also requires fixing of material parameters of the solar cell listed in the table [3].

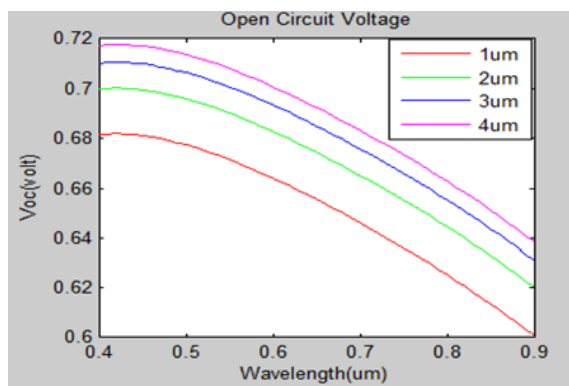


Fig.6. Open circuit voltage of CIGS_CdS solar cell V/S wavelength

Absorption is evaluated for the wavelength from 350nm to 700um the average value is obtained $\alpha = 4.2 \times 10^4 \text{ cm}^{-1} \text{ eV}^{1/2}$. Open circuit voltage increased with thickness of buffer layer but the rate of recombination also tends to increase. The optimum thickness of doped ZnS is observed as 1um for the buffer layer with CIGS cell. While there is very small change in short circuit current densities observed with the limited thickness variations of buffer layer.

Absorption is evaluated for the wavelength from 350nm to 700um the average value is obtained $\alpha = 4.2 \times 10^4 \text{ cm}^{-1} \text{ eV}^{1/2}$. Open circuit voltage increased with thickness of buffer layer but the rate of recombination also tends to increase. The optimum thickness of doped ZnS is observed as 1um for the buffer layer with CIGS cell. While there is very small change in short circuit current densities observed with the limited thickness variations of buffer layer.

Table1. Material parameters used

Parameters	Numerical Values	Unit
Acceptor concentration (Na)	10 ¹⁷	cm ⁻³
Donor concentration (Nd)	10 ¹⁵	cm ⁻³
Relative permittivity CIGS (ϵ_{r1})	10	
Relative permittivity ZnS (ϵ_{r1})	9	eV
Band width CIGS (Eg2)	1.2	eV
Band width ZnS (x1)	3.52	eV
Electronic affinity CIGS (x2)	4.5	eV
Electronic affinity ZnS (x1)	3.9	eV
Effective conduction band density of states (NC1)	2.2 x 10 ¹⁸	cm ⁻³
Effective valence band density of states (NV2)	1.5x 10 ¹⁸	cm ⁻³
Reflectivity(R)	0.1	
Hole mobility (μ_p) (CIGS)	30	cm ² .v.s ⁻¹
Hole mobility (μ_p) (ZnS)	40	cm ² .v.s ⁻¹
Electron mobility (μ_e) (CIGS)	30	cm ² .v.s ⁻¹
Electron mobility (μ_e) (ZnS)	230	cm ² .v.s ⁻¹
Hole capture cross section (σ_p) CIGS	10 ⁻¹⁴	cm ²
Hole capture cross section (σ_p) ZnS	10 ⁻¹¹	cm ²
Electron capture cross section (σ_n) CIGS	10 ⁻¹⁵	cm ²
Electron capture cross section (σ_n) ZnS	10 ⁻¹⁷	cm ²
Thermal speed (vth)	10 ⁷	cm.s ⁻¹
Defect density (Ntp) CIGS	10 ¹⁴	cm ⁻³
Defect density (Ntn) ZnS	10 ¹³	cm ⁻³
Recombination speed of the holes (front surface) ZnS (Sp)	10 ³	cm.s ⁻¹
Recombination rate electrons (rear surface) CIGS (Sn)	10 ⁷	cm.s ⁻¹
Ideal diode factor	1.45	

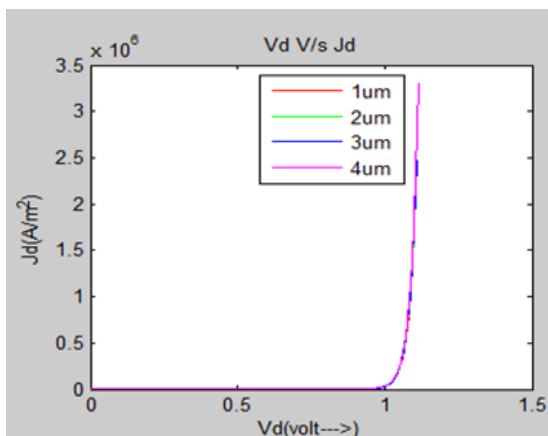


Fig.7. Current density V/S Vd (diode voltage) of CIGS solar cell

6. CONCLUSION

The simulation results from figure 1 to figure 9 except figure 2, 3, and 5 are executed in MATLAB by scripting the derived eq. 1 to eq. 5. The identical model simulated using SCAPS for checking the cross platform performance of the cell.

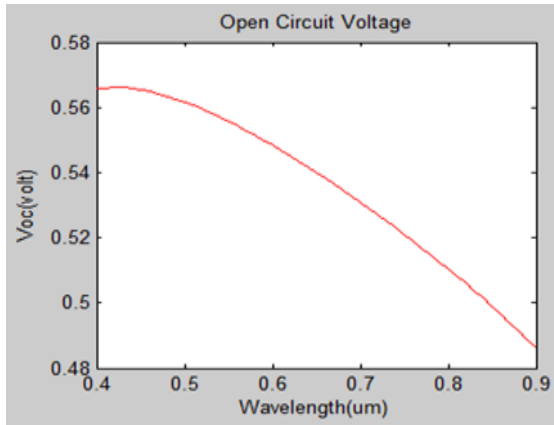


Fig.8. Open circuit voltage of CIGS_ZnS solar cell V/S wavelength at 1um

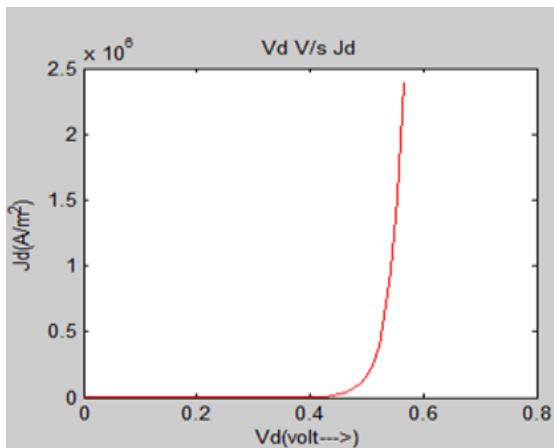


Fig.9. Current density V/S Vd of CIGS_ZnS Solar cell at 1um

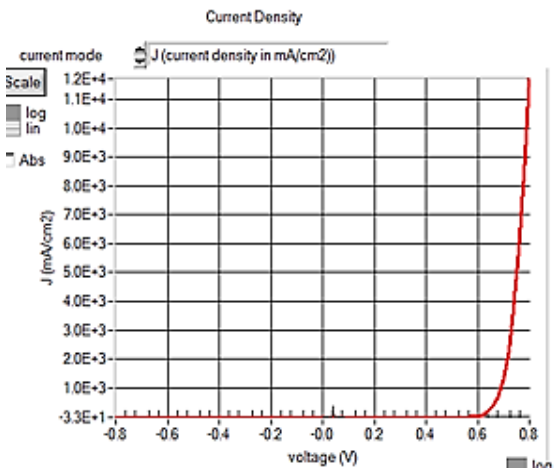


Fig.10. Current density V/S Vd of thin film CIGS Solar cell with ZnS as buffer layer simulated at 1um (SCAPS-1D)

Table1. Performance parameters observed

Parameters/ Materials	CdS_CIGS	ZnS_CIGS
V _{oc} (V)	0.5832	0.5861
J _{sc} (A/m ⁻²)	81.4196	104.7456
FF	0.7403	0.7863
Efficiency	0.1650	0.1963

The observations of simulated results are summarized into table2. All the four parameters open circuit voltage, short circuit current, fill factor and efficiency are found to be increased. Most importantly it provides a way to replace toxic material CdS which were causes hazardous effect to the living species. The results are promising and open new hope for the thin film flexible solar cell.

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