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The Effects of CIGS Absorber Layer Thickness and Band Gap Energy on

the Performance of CIGS Thin Film Solar Cell: A Numerical Simulation

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Abstract

This work examines the effects of the Copper Indium Gallium Selenide (CIGS) absorber layer on the performance of a CIGS photovoltaic cell through numerical simulation using Analysis of Microelectronic and Photonic Structure – 1Dimensional (AMPS – 1D) software. The band gap energy and thickness of the CIGS absorber layer were varied while keeping the other properties, such as carrier concentration of the CdS buffer and ZnO window layers, constant. The optimum value obtained for the band gap energy of the CIGS absorber layer was 1.2 eV, while the thickness was 2500 nm. These optimum values were used to simulate the optimum CIGS solar cell with 83.2% fill factor, 0.718 V open circuit voltage, 28.8 mA/cm^2 short circuit current density, and conversion efficiency of 17.197%.

Keywords: CIGS PV cell, AMPS - 1D simulation, Band-gap energy, Layer thickness, Conversion efficiency.

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1. Introduction

Copper Indium Gallium Selenide (CIGS) compound semiconductor crystallizes as a tetragonal chalcopyrite structure and is of the material family group I - III - VI₂. $CuIn_xGa_{(1-x)}Se_2$ is the chemical formula for the molecule, which consists of a copper indium selenide (CIS) and copper gallium selenide (CGS), both of solid solution, having x range from 1 for pure CIS to 0 for pure CGS. The collection of the photogenerated carriers can be enhanced by modifying the Ga concentration (x) profile in the CIGS absorber layer. Photons are absorbed if their energy is equal to or greater than the bandgap energy of absorber layers.

Hence higher material bandgap energy means less photons absorbed into the laver and vice versa [1]. Ga content, which is tunable, has been proven to affect the bandgap energy of the CIGS PV cell [2]. Thus, too high Ga content translates to higher bandgap energy which translates to less photons absorbed. The band gap can be varied by switching the value of x, ranging from an approximate value of 1.0 eV (for CIS) to an approximate value of 1.7 eV (for CGS) [3]. When x is adjusted, the band gap can increase from 1.02 eV (CuInSe₂) to 1.68 eV (CuGaSe₂), in the process principally affecting the energy level of the conduction band of the absorber Cu (In, Ga) Se₂ (CIGS) [4]. Cu content of CIGS PV cell affect its conductivity. At $\frac{Cu}{(ln+Ga)}$ < 0.7 (Cu – poor) CIGS cells, shunt paths occur within the cell or at boundaries between cells resulting from low conductivity, while $\frac{Cu}{(ln+Ga)} > 1$ (Cu – rich) CIGS cells have very high conductivity which similarly shunt paths [5].

The selenium content however has effects on grain size, leading to changes in concentration of boundaries around the grain. This will thus affect carrier mobility, recombination and generation of current [6]. CIGS PV cell has been studied for the ability of its band gap to be double-graded. Double-grading is a process by which the Ga content of the two edges of the CIGS absorber layer is graded, thereby giving it different band gap energies at different positions [7]. Intrinsic defects in CIS-based semiconductors regulate their electric characteristics, thus synthesizing a CIS semiconductor in Cu-poor and Se-rich conditions exhibit p-type conductivity, whereas Cu-rich material synthesized in Se-deficient conditions tends to exhibit n-type characteristics [8-10]. CIGS solar cell is a multilayer thin film cell comprising 5 different layers on a glass substrate, as shown in Figure 1. Previous research based on the CdS/CuGaInSe₂ system has obtained an efficiency of 18.8%, 19.2% and 20.3% [11-12]. Nakamura et al. (2019) achieved an efficiency of 23.35% by fabricating CIGS cells using a Cd-free double buffer layer [13]. A 19.8% efficiency large sub-module of CIGS has been fabricated by Avancis, of which the results were confirmed by the National Renewable Energy Laboratory (NREL) [14]. Generally, the CIGS solar cell is regarded as a highly efficient thin film solar cell (~21.7 %) [15].

Developing standard techniques that can guarantee maximum efficiency at the least production cost is a significant issue in the field of solar cell development [16]. Reducing the thickness of the component layers of a thin film solar cell is crucial in managing upscale value active materials, energy input, as well as production costs, all while shortening the deposition time [17]. As Salhi (2022) stated, second-generation solar cells such as CIGS require the thickness to be of just some microns to be able to absorb incident light sufficiently as compared with silicon, which needs approximately 200 microns of thickness [18]. Hence, the current challenge of PV solar technology is to increase cell efficiency and reduce the cost of production. To achieve these, optimizing the manufactural

parameter of these solar cells via simulation for a convenient and cost-effective approach is needed. Numerical simulation has proven to be a crucial tool for solar cell research and optimization [19]. Baig et al. (2020) have used a numerical simulation tool to theoretically enhance the performance of an experimentally fabricated Sb₂Se₃-based solar cell [20]. CIGS solar cells have been modelled using a variety of analytical and computational techniques [21]. Therefore, before the fabrication process begins, the numerical simulation will always provide the chance to evaluate the various PV devices' underlying functioning principles [22]. The present work optimizes the performance of CIGS thin film photovoltaic cells through numerical simulation, utilizing the Analysis of Microelectronic and Photonic Structures (AMPS - 1D) beta version software, by adjusting the energy of the band gap and thickness of the CIGS layer, while maintaining other layers' thicknesses fixed at default values established from literature, and observing some of the variations in the device performance. The device performance is mainly attributed to the conversion efficiency, short circuit current density, fill factor, open circuit voltage, and quantum efficiency. The present work optimizes the performance of CIGS thin film photovoltaic cells through numerical simulation.

2. Materials and methods

This study utilized the numerical simulation software called AMPS – 1D beta 1.00 version, for the simulation procedure. AMPS – 1D is a very general computer simulation code that analyzes, as well as designs two terminal structures, thereby deriving their current-voltage characteristic behavior. Devices of Schottky barrier, homojunction and heterojunction p-i-n devices, structures of homojunction and heterojunction p-n, p-i-p and n-i-n are some of the devices that the AMPS – 1D software can analyze. These devices may have poly-crystalline, amorphous or single crystal layers, or any combination thereof. The device configuration may be in the presence of light or the absence of it; hence, solar cells, photodiodes, and even particle detector characteristics (as long as sufficient absorption coefficients of the required devices are chosen) are included [23].

2.1. Simulation procedure

A PV cell must have three distinct layers in AMPS-1D for modelling. As long as the number of grid points stays within the restriction of 400 grid points, additional layers may be added as required. The three layers used in this modeling are the n-type ZnO, n-type CdS, and p-type CIGS. The band gap energy of the CIGS layer and its thickness is altered, while the characteristics of the ZnO and CdS layers are kept constant. The baseline settings utilized in the simulation throughout the investigation are shown in **Table 1**. The front and back contacts can be distinguished by their work functions and their reflectivity at the contact interface of the semiconductor, where the front contact's work function is 0 eV or at the Fermi level E_F , and its reflectivity is 0.05. Similar to the front contact, the back contact has an above E_F work function of 0.9 eV and 0.8 reflectivities. The AM 1.5 G photon flux was used for the illumination. The number of incident photons was entered for wavelengths between 380 to 900 nm, with a step size of 20 nm.

3. Results and discussion

3.1. Effect of band gap energy

To determine how the absorber layer's band gap energy affects the functionality of the cell, the Ga content of the CIGS layer, defined by $\frac{Ga}{Ga+In}$ or *x* in equations (1) and (2) was varied from x = 0 (CIS) to x = 1 (CGS) with an interval of 0.1. Equations (1) and (2), which define the energy band gap (Eg) and electron affinity (χ_e), respectively, are given as follows:

$$E_{g} = 1.04 + 0.391x + 0.262x^{2}$$
(1)
$$\chi_{e} = 4.61 - 1.162x + 0.034x^{2}$$
(2)

Using the above equations (1) and (2), the E_g significantly increased from the value of 1.04 eV (pure CIS) to the value of 1.69 eV (pure CGS) while χ_e decreased from 4.61 eV to 3.4 eV as Ga content varied from x = 0 to x = 1 respectively. Table 2 shows the changes in output parameters with band gap energy variation. Table 2 demonstrates a rise in the fill factor as the band gap energy increases, reaching a maximum FF of about 84% at a band gap energy of 1.30 eV. A sharp decrease occurs after 1.30 eV because increasing Ga content is known to cause defects that affect electron and hole affinities [26]. The increase in the open circuit voltage (Voc) with an increase in band gap energy is in agreement with the work of Green (1992), which posits an increase in open circuit voltage when the energy of the band gap of the CIGS absorber layer of a solar cell increases [27]. In contrast, short circuit current density decreases with increasing band gap energy from 28.907 to 28.606 mA/cm² for band gap energy of 1.04 to 1.69 eV, respectively. This decrease is in agreement with the work of Parisi et al. (2015) which explains that more photon absorption on the absorption layer at lower band gap energy leads to short circuit current density increased and vice versa [28].

However, conversion efficiency reaches its maximum at about 21% with a band gap energy of 1.37 eV. This energy band gap value is approximately the optimum band gap energy of 1.4 eV, as Green (1982) reported [29]. The conversion efficiency begins to drop with further increases above 1.37 eV. This decrease arises from the band gap energy being too high for the photon energy to excite electrons to attain adequate energy that is sufficient enough to enable its transition from the energy level of the valence band to the conduction band. However, of important note is that augmenting the energy of the band gap anywhere above 1.2 eV is not an ideal technological solution as there is a tendency for it to cause an increase in the defect density of the areas with high Ga content [30]. Therefore, the

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high efficiency reported in the simulations cannot be achieved in a real device; hence 1.2 eV is the optimum band gap energy for a CIGS PV cell [31].

3.2. Effect of layer thickness

The thickness of the CIGS absorber layer was initially varied from a thickness of 500 to 5500 nm, with an interval of 500 nm to observe its effect on the solar cell performance, while the layer thickness of CdS and ZnO was kept constant at a default value. Table 3 presents solar cell performance results as the CIGS layer thickness is varied. The fill factor increases with an increase in CIGS layer thickness and reaches a peak value of 83.2% at 2500 nm thickness. The fill factor value starts to level off at 83.2% as the thickness of the CIGS layer reaches 2500 nm. The V_{oc} also follows a similar trend reaching a maximum value of 0.720 V when CIGS layer thickness increases up to 4500 nm. This increase might be due to the reduction of recombination loss between the CIGS layer and back contact as the CIGS layer thickness increases. This maximum value is maintained even with a further increase in thickness to above 4500 nm. The J_{sc} increases to a peak value of 28.914 mA/cm² at 4000 nm but decreases with a further increase in thickness above 4000 nm. This increment is due to the reduced recombination of photogenerated carriers at the back contact. A thicker absorber layer locates the back contact further away from the depletion region. Thus, incoming photons are absorbed deep into the absorber layer, and an increase in the thickness of the absorber layer results in more photogenerated carriers collected before the recombination process, which directly improves J_{sc} [32].

The sudden decrease in J_{sc} at a thickness above 4000 nm could be due to incoming photons being absorbed deep into the absorber layer, which is farther from the depletion region. Reaching the space charge region during the lifetime of the carriers is near impossible at this point and hence will be recombined in the absorber bulk [33]. This change in J_{sc} influences the change in efficiency. The efficiency is observed to rise as the thickness increase from 500 nm to a maximum value of 17.340% at 4000 nm and slowly decreases above 4000 nm. This increase in efficiency results from the absorption of more photon energy from solar radiation, which produces higher current density since more electron-hole pair is produced, resulting in more electricity. In addition, the possibility of photogenerated carriers recombining at the back contact decreases since recombination depends mainly on the junction depth. With the increase in absorber layer thickness, the junction depth is increased, which in turn ensures the efficient collection of photogenerated carriers in a thicker absorber layer [34-35]. The sudden decrease in efficiency with a thickness less than 4000 nm may be due to the carriers going through a recombination process around the region of the back contact. After all, the back contact is having a greater distance from the depletion area makes it more difficult for the back



contact to capture electrons for collection. Hence, 2500 nm was considered the optimum CIGS thickness.

Figure 1: Schematic diagram of a CIGS solar cell showing baseline thickness

General Device Properties							
	Front contact Layer		Back Contact Layer				
	$(x=0\mu m)$		$(x=3.05\mu m)$				
$\Phi_{\rm b0/L} = E_{\rm c} - E_{\rm F} (\rm eV)$	0.0		0.9				
Surface recombination electrons (cm/s)	107		2×10 ⁷				
Surface recombination holes (cm/s)	107		2×10 ⁷				
Reflectivity	0.05		0.8				
Layer Properties							
	ZnO	CdS	5	CIGS			
Width (nm)	500	50		2500*			
Dielectric constant	9.0	10.0		13.6			
Electron mobility (cm ² v ⁻¹ s ⁻¹)	100	100		100			
Hole mobility (cm ² v ⁻¹ s ⁻¹)	25	25		25			
Doping concentration (cm ⁻³)	1.0×10 ²⁰ ND	5.0×10 ¹⁷ ND		3.0×10 ¹⁶ NA			
Bandgap energy (eV)	3.30	2.40		1.20*			
Effective density NC (cm ⁻³)	2.22×10 ¹⁸	2.22×10 ¹⁸		2.22×10 ¹⁸			
Effective density NV (cm ⁻³)	1.78×10 ¹⁹	1.78×10 ¹⁹		1.78×10^{19}			
Electron affinity (eV)	4.00	4.20		4.10			
Defect States							
Gaussian Defects	ZnO	CdS	5	CIGS			
Defect density (cm ⁻³)	1.0×10 ¹⁷	1.0×10^{18}		1.0×10^{14}			
Peak energy (eV)	1.65	1.20		1.20			
Standard deviation (eV)	0.10	0.10		0.10			
Cross-section electrons (cm ²)	1.2×10 ⁻¹²	1.0×10 ⁻¹⁷		1.0×10 ⁻¹³			
Cross-section holes (cm ²)	1.0×10 ⁻¹⁵	4.8×10 ⁻¹²		1.0×10 ⁻¹⁵			

Table 1: Parameters utilized for the baseline CIGS solar cell simulation [24-25].

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* Varied properties while keeping all others constant

Band gap energy (eV)	Fill Factor (%)	Open circuit voltage (V)	Short circuit current density (mA/cm ²)	Efficiency (%)
1.04	80.7	0.560	28.907	13.076
1.08	81.5	0.599	28.859	14.094
1.13	82.4	0.648	28.843	15.406
1.18	83.1	0.698	28.833	16.736
1.24	83.9	0.758	28.820	18.315
1.30	84.2	0.817	28.805	19.814
1.37	83.7	0.881	28.781	21.212
1.44	81.0	0.911	28.758	21.207
1.52	75.3	0.915	28.719	19.788
1.60	66.3	0.916	28.669	17.419
1.69	56.6	0.916	28.307	14.842

Table 2: Effect of band gap energy variation on fill factor, open circuit voltage, short circuit current density, and efficiency.

Table 3: Effect of CIGS layer thickness on fill factor, open circuit voltage, short circuit current density and efficiency.

Thickness (nm)	Fill factor (%)	Open circuit voltage (v)	Short circuit current density (mA/cm ²)	Efficiency (%)
500	80.6	0.679	27.577	15.080
1000	82.4	0.702	28.411	16.420
1500	82.9	0.711	28.697	16.907
2000	83.1	0.716	28.763	17.098
2500	83.2	0.718	28.800	17.197
3000	83.2	0.719	28.851	17.268
3500	83.2	0.720	28.855	17.293
4000	83.2	0.720	28.914	17.348
4500	83.2	0.721	28.901	17.338
5000	83.2	0.721	28.890	17.334

4. Conclusion

AMPS – 1D has been used to study the effects of the band gap energy and thickness of the CIGS absorber layer on the CIGS PV cell performance. It has been shown that conversion efficiency increased with an increase in the band gap energy of the CIGS absorber layer to a certain extent, and further increase showed a decrease in conversion efficiency. Similarly, variation in the thickness of the CIGS absorber layer affects the short circuit current density and consequently influences the conversion efficiency. These observations lead to the conclusion that for an improved CIG PV cell performance, the band gap energy as well as the thickness of the CIGS absorber layer, are of significant importance in the production of a costeffective CIGS PV cell.

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