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Numerical Simulation of Copper Indium Gallium Diselenide Solar Cells Using One Dimensional SCAPS Software

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Abstract

The effect of multivalent defect density, thickness of absorber and buffer layer thickness on the performance of CIGS solar cells were investigated systematically. The study was carried out using Solar Cells Capacitance Simulator (SCAPS) code, which is capable of solving the basic semiconductor equations. Employing numerical modelling, a solar cell with the structure $Al|ZnO:Al|In_2S_3|CIGS|Pt$ was simulated and in it, a double acceptor defect (-2/-1/0) with a density of 10^{14} cm^{-3} was set in the absorber in the first instance. This initial device gave a power conversion efficiency (PCE) of 25.85 %, short circuit current density (Jsc) of 37.9576 $mAcm^{-2}$, Photovoltage (Voc) of 0.7992 V and fill factor (FF) of 85.22 %. When the density of multivalent defect (-2/-1/0) was varied between 10^{10} cm^{-3} and 10^{17} cm^{-3} the solar cells performance dropped from 26.81 % to 16.87 %.The champion device was with multivalent defect of 10^{10} cm^{-3} which shows an enhancement of 3.71 % from the pristine device. On varying the CIGS layer thickness from 0.4 μm to 3.6 μm, an increase in PCE was observed from 0.4 μm to 1.2 μm then the PCE began to decrease beyond a thickness of 1.2 μm. The best PCE was recorded with thickness of 1.2 μm which gave Jsc of 37.7506 $mAcm^{-2}$, Voc of 0.8059 V, FF of 85.2655 %. On varying the In_2S_3 (buffer) layer thickness from 0.01 μm to 0.08 μm, we observed that there was no significant change in photovoltaic parameters of the solar cells as buffer layer thickness increased.

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Keywords: SCAPs, CIGS, Multivalent defect, buffer layer, absorber

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1. Introduction

CIGS is a quaternary compound semiconductor which is an alloy of $CuInSe_2$ (CIS) and $CuGaSe_2$ (CGS) and comprises four elements namely: Copper, Indium, Gallium and Selenium. It is a direct band gap material [1] whose energy band gap could be varied from 1.06 eV – 1.70 eV by changing the Indium to Gallium ratio [2]. According to Hamanche [3], CIGS is the most promising candidate for efficient and low-cost solar cells based on the advantages of the optical and electrical properties of the material [3]. In spite of these attractive features of CIGS material, there are factors which could affect the performance of solar cells whose absorbers are made from this material. Such factors include defect density in semiconductor layers and interfaces of the solar cell, absorber layer and buffer layer thicknesses, bandgap of semiconductor materials, working temperature of the solar cell among others.

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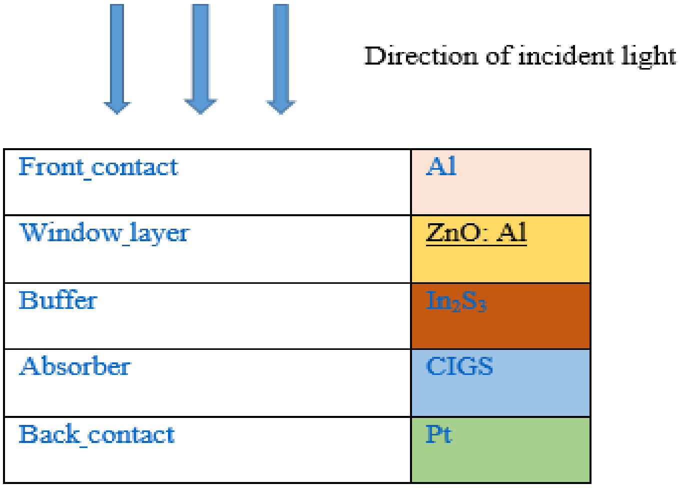
Multivalent defects are defects caused by transition metals which usually occur as impurities or as part of the structure of some semiconductors [4]. Transition metals are metals which have valence electrons in two shells instead of only one. They therefore exhibit multiple oxidation states and can transit from one charge state to another by accommodating a variable number of electrons in their d-orbitals. When multivalent elements occur as impurities in semiconductors, it is not always clear how many of their valence electrons would be used for charge exchange. For example, if tin (Sn) is doped on divalent zinc (Zn) or Magnesium (Mg) site. We are not sure if it will behave as +IV element or a +II element. There is really the possibility that a multivalent impurity would transit from one oxidation state to another and their transition would appear as deep level inside the band gap of the material. Deep levels which are associated with a change in oxidation state tend to deteriorate the electronic properties of semiconductors. As they form recombination centers and carrier traps [4]. We therefore investigate in this work, the effect of multivalent defect density, thickness of absorber and buffer layer on the performance of CIGS solar cells using SCAPS-1D. This software was used to calculate the short circuit current density (Jsc), open circuit voltage (Voc), Fill factor (FF) and efficiency (η) which are photovoltaic parameters used for the assessment of solar cells' performance. The spectral response of the solar cells in the face of varying defect density, absorber layer thickness and buffer layer thickness were also studied.

2. Materials and Methods

2.1. Cell Structure

The solar cells simulated have the structure $Al|ZnO:Al|In_2S_3|CIGS|Pt|$ as shown in figure1. The main parts of the cells are CIGS absorber and the In_2S_3 buffer layers. The CIGS absorber is responsible for trapping light from the sun. It is considered environmental friendly because of the absence of Cadmium in its structure. The material has a direct band gap and high absorption coefficient requiring just a few micrometers to absorb the maximum incident photon. The wide band gap of this material has also been found to be variable depending on the composition of the CIGS material [5]. The In_2S_3 is chosen as the buffer since it is stable, has a wider band gap and is considered nontoxic, when compared with other buffers such as CdS. It is also transparent and photoconductive [6]. A transparent conductive Oxide (TCO) layer (acting as the window) made of ZnO:Al is deposited on top of the buffer layer as it is transparent to most of the solar spectrum because of its wide band gap.Although ZnO:B (Boron doped Zinc Oxide) could be more beneficial for the solar cells because it lowers absorption losses leading to an increase in the quantum efficiency of the solar cells[7], ZnO:Al is used in this research because it is a low cost TCO and it is also highly conductive. Front and back contacts usually made of metallic elements are introduced in the cells' structure for the conduction of photogenerated charge carriers in and out of the solar cells. Al is used as the front contact in this work, because it is lightweight, non-magnetic and corrosion resistant. It is a good conductor of electricity; more conductive than Copper and less expensive than silver. A back contact of Pt is preferred to the commonly used Molybdenum since it is nontoxic when compared with Molybdenum and gives a cell with higher efficiency [8].



Front contact	Al
Window layer	ZnO: Al
Buffer	In_2S_3
Absorber	CIGS
Back contact	Pt

Figure 1. Model of the simulated solar cell.

2.2. Numerical Modelling

The method used for this work is numerical simulation. Numerical simulation often gives insight into the interpretation of measurements even as it aids in the assessment of the potential merits of a cell structure [7]. Some softwares among which is SCAPS-1D can be used to analyze the effect of the variation of materials parameters, that is, the presence or absence of particular properties or the varying of all properties in the range of values, for the optimization of solar cells' efficiencies. This helps the producers of solar cells with the needed insight to effect necessary changes in their production methods in order to improve product performance. SCAPS- 1D simulation results have a good agreement with the results of existing experimental works [9] and this is the major motivating factor for its use in this research. SCAPS computes the steady state band diagram, recombination profile and carrier transport in one dimension, based on Poisson's equation (equation 1) together with the continuity equations (equations 2a and 2b) for holes and electrons.

$$\nabla \cdot \epsilon E = q(p - n + N) \tag{1}$$

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n(x,t) - R_n(x,t) \tag{2a}$$

$$\frac{\partial p(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J_p}{\partial x} + G_p(x,t) - R_p(x,t) \tag{2b}$$

where E = electric field; ϵ = permittivity of semiconductor; q = electronic charge; n = concentration of electrons; p = concentration of holes; N = net charge due to dopants and other trapped charges; Jn and Jp = current density of electrons and holes; Gn and Gp = rates of electron and holes generation in

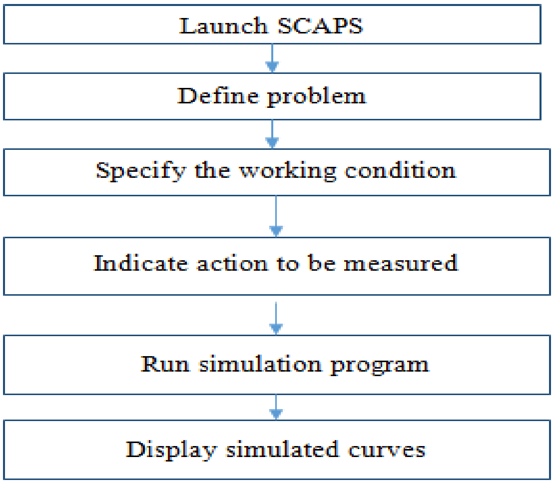


Figure 2. Simulation procedure.

Figure 3. SCAPS solar cell definition panel.

the semiconductor device; *Rn* and *Rp* are rates of electron and hole recombination in the solar cells.

Figure 2 shows the steps that were taken in the simulation, starting with the launch of SCAPS.

2.3. *Simulated Parameters*

The material parameters were selected from experimental results [10,11,12]. Table1 gives a summary of the parameters for each layer in the simulation. Defect parameters in the layers and interfaces were sourced from literatures [1, 13, 14, 15] as shown in table 2. The work functions of the front contact (Al) and back contact (Pt) are 4.26 eV and 5.93 eV, respectively [16]. A working temperature of 300 K, solar spectrum AM1.5 and a Scanning voltage of 0 V- 1.3 V were used for all simulations.

The solar cell definition panel shown in figure 3 is the environment where the physical properties of the various layers of the solar cells were inputted.

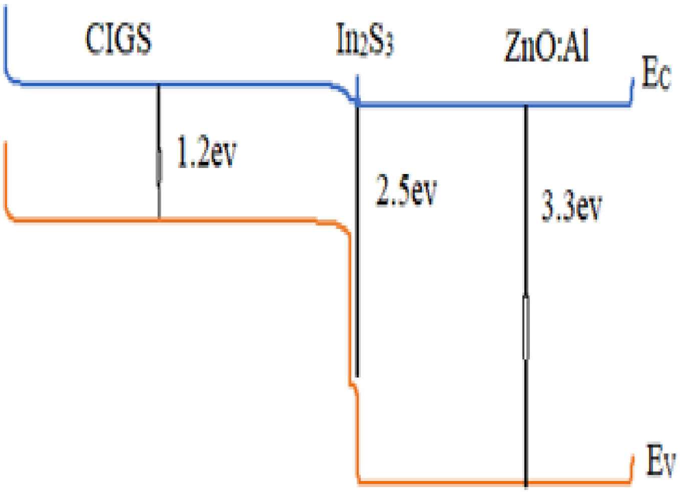


Figure 4. Energy band diagram in the CIGS solar cell.

3. Results and Discussion

3.1. *Performance parameters from initial simulation*

In the initial device set up for this work, a multivalent defect in the form of a double acceptor (-2/-1/0) defect with a Gaussian energy distribution, defect energy level (Et) = $\{0.1, 0.4\}$ eV above E_v and a concentration of 1.0×10^{14} cm^{-3}, was introduced into the CIGS (absorber) layer. This defect which is mainly caused by Cu_{III} (Cu_{III} is a double acceptor and III represents a group 3 element such as Indium or Gallium) defect is common in CIGS absorbers [17]. Details of other defects set in the simulation are given in Table 2; the resulting performance parameters of the open- circuit voltage (V_{OC}), short- circuit current density (J_{SC}), fill factor (FF) and efficiency determined using J-V characteristics are compared with those derived from experimental work [18]. The comparison which is shown in Table 3 reveals that there is a good agreement between data from calculations and those from experiment hence validating parameters used in the simulation. The J-V curve and quantum efficiency curve are also obtained and shown below. The parameters of the different layers used in the simulation are also given in Table 1.

In the quantum efficiency (spectral response) curve shown in Figure 6, there is an observed increase of spectral response in the short wavelength between 350 nm(0.35 μm) and 400 nm(0.4 μm). The curve reveals a maximum efficiency of approximately 100 % occurring between 400 nm(0.4 μm) and 1000 nm(1 μm) but this high efficiency begins to fall off after 1000 nm(1 μm). This fall is very likely due to incomplete absorption of the long wavelength photons. This analysis pertaining to the quantum efficiency, agrees very much with those reported in literatures [1,19].

3.2. *Effect of multivalent defect concentration in CIGS (absorber) layer*

The density of absorber layer defect has a direct effect on photovoltaic cell performance because as the concentration of

Table 1. Materials parameters for $CIGS|In_2S_3|ZnO:Al|$ solar cell [10,11,12].

Layer parameter	CIGS	In_2S_3	$ZnO:Al$
Thickness (μm)	2	0.04	1.6
Band gap, $E_g(eV)$	1.2	2.5	3.3
Electron affinity, $\chi_e(eV)$	4.25	4.25	4.6
Relative permitivity ϵ_e	13.6	13.5	9
N_c, effective density of states $(1/cm^3)$	2.2×10^{18}	1.8×10^{19}	2.2×10^{18}
N_v, effective density of states $(1/cm^3)$	1.8×10^{19}	4.0×10^{13}	1.8×10^{19}
Electron mobility, $\mu_n(cm^2/V_s$	100	400	100
Hole mobility, $\mu_p(cm^2/V_s$	25	210	25
Acceptor concentration $N_A(1/cm^3)$	1.0×10^{16}	0	0
Donor concentration $N_D(1/cm^3)$	0	1.0×10^{18}	1.0×10^{18}

Table 2. Defect parameters of buffer, window and interfaces [1, 13, 14, 15].

Parameters	In_2S_3	ZnO:Al	CIGS/In_2S_3 Interface	In_2S_3/ZnO:Al Interface
Defect Type	Acceptor	0.04	1.6	
Capture cross section for electrons $\sigma_n(cm^2)$	1.0×10^{-15}	1.0×10^{-12}	1.0×10^{-14}	1.0×10^{-12}
Capture cross section for holes $\sigma_h(cm^2)$	5.0×10^{-13}	1.0×10^{-12}	1.0×10^{-14}	1.0×10^{-15}
Energetic Distribution	Gaussian	Gaussian	Single	Single
Energy level with respect to reference (eV)	0.6 above E_v	0.6 above E_v	0.6 above E_v	0.6 above E_v
Characteristic Energy level (eV)	0.1	0.1	0.1	0.1
Total density (cm^{-3})	1.0×10^{14}	1.772×10^{16}		
Concentration (cm^{-2})			1.0×10^{10}	1.0×10^{10}

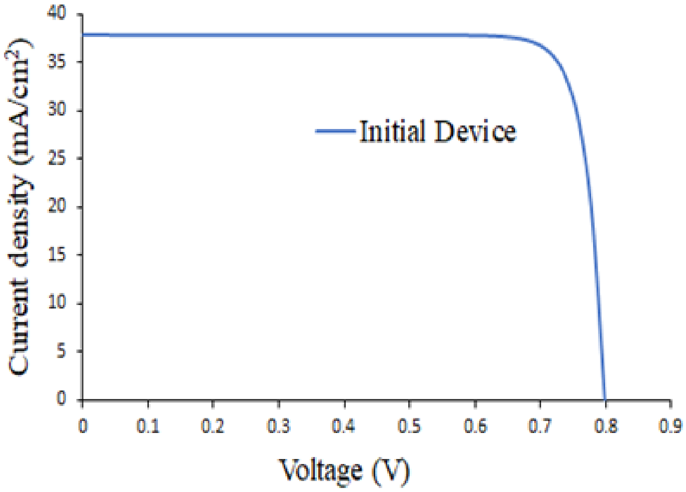


Figure 5. J-V curve of CIGS solar cell with initial parameters.

Table 3. Results from initial simulation compared with experimental data.

	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	Efficiency (%)
Experimental [18]	0.7410	37.8000	80.60	22.60
Simulation	0.7992	37.9576	85.22	25.85

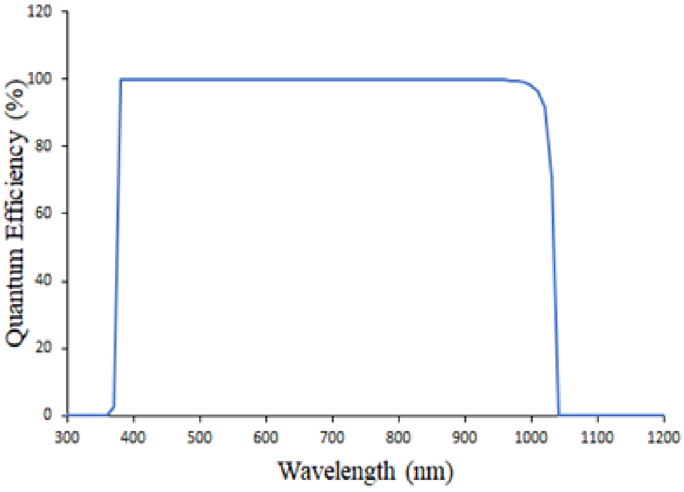


Figure 6. Quantum efficiency curve with initial parameters.

defects increase, the minority charge lifetime reduces. This is evident from

$$\tau = \frac{1}{\sigma V_{th} N_t} \tag{3}$$

Equation 3 above where τ is the minority charge lifetime, σ is electron/hole capture cross section, V_{th} is thermal velocity of electron/holes and N_t is total density of defects but $\sigma V_{th} = c$ and c is the capture constant of electron/holes so $\tau = \frac{1}{cN_t}$ meaning that the life time τ is inversely proportional to the product of defect density and capture constant of the charge carrier. With reduction in life time, the diffusion length of electrons and holes reduces. Diffusion length is the average distance a charge carrier can travel in a semiconductor material before it recombines.

$$Diffusion\ length,\ L = \sqrt{D_\tau} \tag{4}$$

meaning that if defect density increases, τ reduces and diffusion length reduces also. In Equation 4, D is the diffusion coefficient for electrons/holes With a reduction in diffusion length, the probability of collection of photogenerated charge carriers at the terminals reduces; this in turn lowers the photocurrent for the solar cell, and increase the chances of recombination hence increasing the recombination loss in the absorber [20].

Defects could be introduced either intentionally or unintentionally into semiconductors during the growth process, during processing of the device or from the working environment [21]. Theoretical studies which are confirmed by results of measurement show that most of the existing defects in chalcopyrite solar cells, are multivalent in nature [22, 23]. In this study, the impact of varying multivalent defect concentration is observed by choosing the values of the defect density in the range of 10^{10} cm^{-3}–10^{17} cm^{-3}. Table 4 gives the performance parameters of the CIGS solar cells with various values of multivalent defect density in the absorber. It would be observed that the solar cells' performance does not change much when the defect density is below 10^{14} cm^{-3}. This result tallies with the finding of similar study [24] in this regard. Figure 7 shows that all electrical performance parameters start degrading at a defect density of $\approx 10^{15}$ cm^{-3}. V_{OC} goes down from 0.82086 V to 0.67284 V, representing a decrease of 22.38 %. J_{SC} falls from 37.96297 mA/cm^2 to 33.33359 mA/cm^2 corresponding to a decrease of 13.89 %. These drops may be attributed to recombination within localized energy levels created by defects which cause current leakage [25]. As a result, the conversion efficiency goes down from 26.8116 % to 16.8716 % representing a decrease of 58.92 %. Since solar cell efficiency is the amount of energy in the form of sunlight that can be converted into electricity by a solar cell, this 58.92 % decrease in conversion efficiency brought about by an increase in concentration of multivalent defect in the absorber layer poses a disadvantage to the functioning of the solar cell. According to a study [26], an efficient solar cell will have a high short circuit current density J_{sc}, a high open circuit V_{oc} and a fill factor as close as possible to 1 (or 100 %). The fill factor is a measure of the ideality of a solar cell. In Figure 7, the fill factor is observed to depart more from its ideal value of 100 % with an increase in the density of multivalent defect in the absorber leading to less efficiency and ideality of the solar cells.

Table 4. Dependence of cells performance on multivalent defect density in CIGS absorber layer.

Multivalent defect density (cm^{-3})	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	η (%)
10^{10}	0.82086	37.96297	86.0388	26.8116
10^{11}	0.82083	37.96297	86.0371	26.8102
10^{12}	0.82059	37.96292	86.0196	26.7967
10^{13}	0.81785	37.96244	85.8998	26.6700
10^{14}	0.79924	37.95760	85.2210	25.8537
10^{15}	0.74993	37.90711	83.6588	23.7824
10^{16}	0.70338	37.29294	80.0979	21.0106
10^{17}	0.67284	33.33359	75.2251	16.8716

The multivalent defect density which produces an optimum performance of the solar cells is $10^{10}/cm^3$ at an open circuit voltage V_{oc} of 0.8209 V, short circuit current density J_{sc} of 37.96300 mA/cm^2, fill factor FF of 86.0388 % and conversion efficiency η of 26.8116 % (as shown in Figure 8). This implies that multivalent defect densities (double acceptors, in this case) in CIGS solar cells should be controlled in such a way that they do not exceed this value.

Figure 9 shows the quantum efficiency (QE) as a function of wavelength for different values of defect density in the CIGS layer. When the wavelength is in the range of 300 nm(0.3 μm) – 1200 nm(1.2 μm) the absorption efficiency decreases with increased multivalent defect density in the CIGS layer. This is because as defect density increases the recombination (which causes loss of charge carriers) phenomena becomes more pronounced and since quantum efficiency is the ratio of the number of carriers collected by the solar cell to the number of incident photons [19], quantum efficiency drops.

3.3. Effect of varying In_2S_3 (buffer) layer thickness

The influence of the thickness of In_2S_3 buffer layer on performance of the photovoltaic cell is shown in Figure 10. The thickness of the buffer was varied from 0.01 μm through 0.08 μm. Although the variation of all photovoltaic parameters with increasing buffer thickness is not very significant, a reduction in the efficiency of the solar cells with increasing thickness of the buffer was noticed, in line with the findings in literatures [27, 28, 29]. This is caused by absorption of some photons in this layer [27] as a large number of short-wave length photons are absorbed before reaching the absorber layer while photons having wavelengths greater than that associated with the band gap of the buffer cannot generate electron-hole pairs and are therefore lost as heat. Whereas a thin buffer layer means majority of photons can pass through the buffer into the absorber without being absorbed, increasing the buffer layer thickness causes a drop in efficiency of the solar cells. This is due to photon loss occurring inside the buffer layer.

When a smaller number of photons make it through the buffer, less electron-hole pairs are created and this means less electricity is generated. This agrees with the findings [29]. The observed reduction in J_{SC} is caused by less production of electron-hole pair as a smaller number of electron- hole pairs can reach the absorber layer with increase in buffer layer thickness. A decreased short circuit current means that less photogenerated carriers are produced and this lowers the efficiency of the solar cells. Apart from the very little initial decrease in V_{oc} when buffer layer thickness is increased from 0.01 μm to 0.02 μm, the open circuit voltage remains constant showing that the buffer layer thickness has little or no effect on V_{oc}. From Figure 10, there is a slight increment in fill factor when buffer layer thickness is increased from 0.02 μm to 0.03 μm thereafter, FF begins to drop again. These changes must have resulted from valence band discontinuities at the interfaces that appear as spikes [14]. The best efficiency of the solar cells after variation of the buffer thickness is 25.9813 % and this is achieved

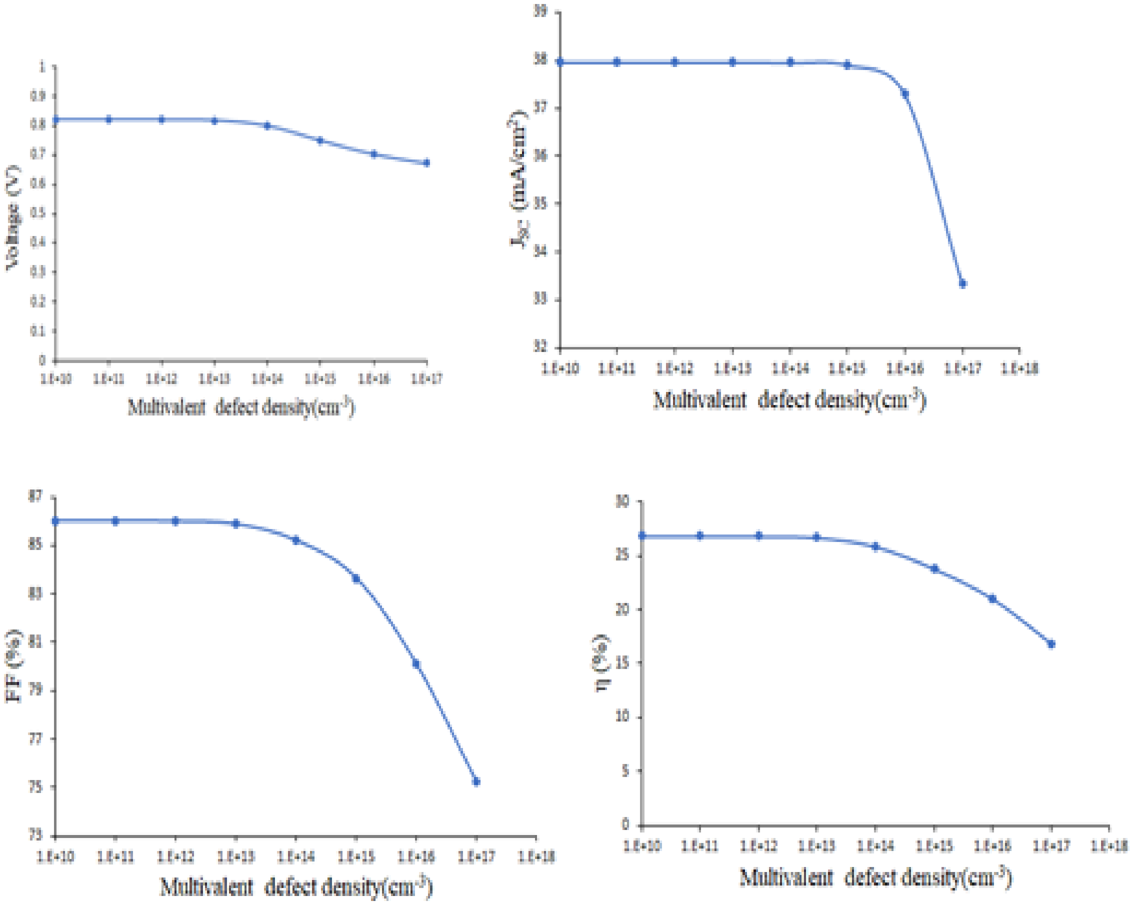


Figure 7. Variation in performance of CIGS solar cells with multivalent defect density.

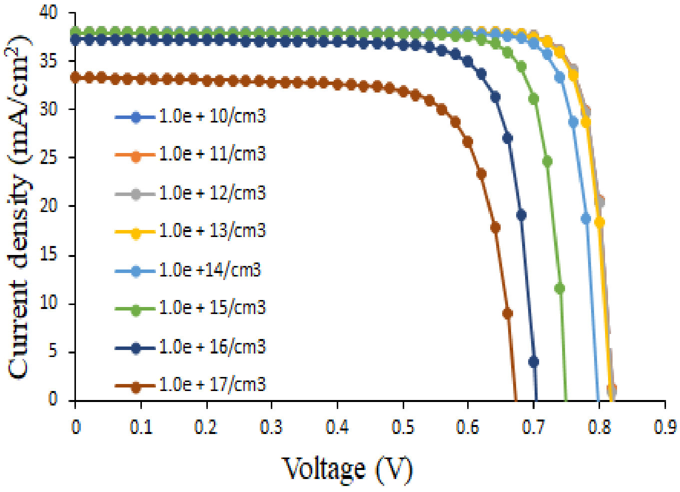


Figure 8. J-V curves of CIGS solar cells with various values of multivalent defect density.

Table 5. Dependence of solar cells' performance on buffer layer thickness.

Thickness of buffer (μm)	**V_{OC} (V)**	**J_{sc} (mA/cm^2)**	**FF %**	**η %**
0.01	0.8030	37.9591	85.2329	25.9813
0.02	0.7997	37.9586	85.2183	25.8698
0.03	0.7993	37.9582	85.2211	25.8556
0.04	0.7992	37.9576	85.2210	25.8537
0.05	0.7992	37.9569	85.2206	25.8529
0.06	0.7992	37.9560	85.2202	25.8521
0.07	0.7992	37.9549	85.2198	25.8512
0.08	0.7992	37.9536	85.2193	25.8502

for a thickness of 0.01 μm at an open circuit voltage V_{oc} of 0.8030 V, J_{sc} of 37.9591 mA/cm^2 and fill factor of 85.2329 % (as shown in Figure 11).

Figure 12 shows the quantum efficiency (QE) as a function of wavelength for different values of buffer (In_2S_3) layer

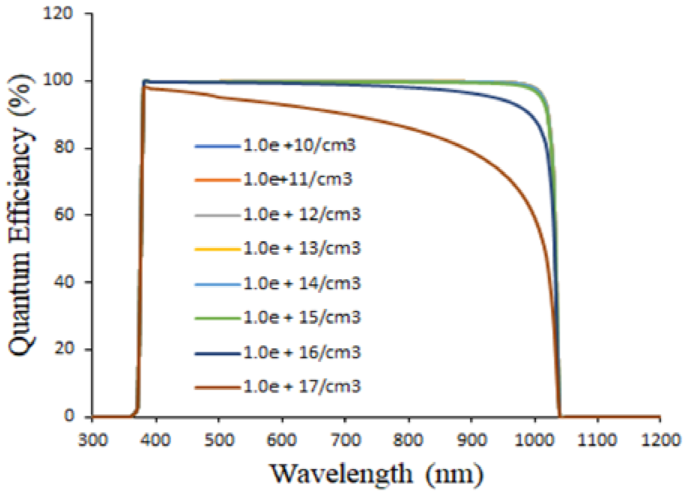


Figure 9. Quantum efficiency as a function of wavelength for different values of defect density in CIGS layer.

thickness. When the wavelength is in the range of 300 *nm* (0.3 *μm*) – 1200 *nm* (1.2 *μm*), we observed that the spectral response curves overlap because the absorption efficiency remains constant for all values of buffer layer thickness. This spectral response in relation to varying buffer layer thickness further proves that buffer layer thickness has little or no effect on CIGS solar cells investigated.

3.4. Effect of varying CIGS (absorber) layer thickness

An important parameter which also affects the performance of CIGS solar cells is the thickness of the absorber layer. The effect of thickness of the absorber layer on the solar cell's performance parameters V_{OC}, J_{SC}, FF, PCE is seen in Figure 13. When the thickness of CIGS absorber layer was varied from 0.4 *μm* to 3.6*μm*, the solar cell's efficiency was seen to increase from 23.96 % to 25.94 % for an increase in thickness, of 0.4 *μm* – 1.2*μm* respectively. This increase is attributable to absorption of more photons as absorber layer thickness increases. This translates to the production of a significant number of electron-hole pairs which then leads to an improvement in efficiency of the solar cells [12]. This is good for the performance of the solar cells since it means that more of the sun's energy would be converted to electricity in the solar cells. Beyond an absorber thickness of 1.2*μm*, the efficiency begins to drop due to decreased collection of photo-generated charge carriers which is caused by charge recombination. This tallies with similar finding [24] J_{SC} increases with increasing absorber thickness since longer wavelength photons are absorbed in thicker layers of the absorber and they enhance the amount of photo-generated carriers which in turn boosts efficiency and therefore produces solar cells which perform better.

Fill factor FF remains nearly constant but V_{OC} kept decreasing as a result of recombination of charge carriers [20] which increases in thicker layers of the absorber. this is not good for the performance of the solar cell as the efficiency of the solar cell has a direct dependence on open circuit voltage Voc. For optimum performance, the absorber thickness of the CIGS solar cells should be kept at 1.2 *μm*. The photovoltaic cell parameters corresponding to this optimum value are Voc of 0.8059 V, J_{sc} of 37.7506 mA/cm^2, FF of 85.2655 % and conversion efficiency of 25.9403 % (as shown in Figure 14).

Table 6. Dependence of solar cells' performance on absorber layer thickness.

Thickness of absorber (μm)	**V_{OC} (V)**	**J_{sc} (mA/cm^2)**	**FF %**	**η %**
0.4	0.8126	34.5688	85.2896	23.9577
0.8	0.8097	37.2321	85.2886	25.7114
1.2	0.8059	37.7506	85.2655	25.9403
1.6	0.8024	37.9045	85.2379	25.9258
2.0	0.7992	37.9576	85.2210	25.8537
2.4	0.7961	37.9805	85.2398	25.7724
2.8	0.7933	37.9930	85.2467	25.6934
3.2	0.7909	38.9921	85.2450	25.6128
3.6	0.7887	38.0000	85.2375	25.5452

Figure 15 shows the quantum efficiency (QE) as a function of wavelength for different values of absorber (CIGS) layer thickness. When the wavelength is in the range of 300 *nm* (0.3 *μm*) – 1200 *nm* (1.2 *μm*) the absorption efficiency increases with increased absorber (CIGS) layer thickness. This is because as absorber (CIGS) layer thickness increases the number of absorbed photons increases consequently, a higher number of electron-hole pairs are produced and the quantum efficiency increases [1]. For all values of absorber (CIGS) layer thickness, it is observed that the spectral response curves show a decrease of the long wave length collection. This is most likely due to incomplete absorption of the long wavelength photons [30].

3.5. Performance of optimized parameters

Based on the optimized multivalent defect density, absorber layer thickness and buffer layer thickness, an efficiency of 27 %, current density of 37.75 mA/cm^3, voltage of 0.829 V and fill factor of 86.26 % were obtained as depicted in Figure 16. Compared with the experimental data obtained by Jackson *et al.*[18] were an efficiency of 22.6 % was reported, the optimized cell in this work shows an improvement of 16.30 % in efficiency. Aside the alkali Post Deposition Treatment (PDT) done on CIGS absorbers which were used in the experimental solar cells referred to in Table 8 their efficiencies could be improved upon by carefully controlling the concentration of multivalent defect in their absorbers as this form of defect is prevalent in chalcopyrite materials.

Table 7. Optimized parameters of the device.

Optimized Parameters	**Absorber**	**Buffer**
Thickness (μm)	1.2	0.01
Multivalent defect density (cm^3)	10^{10}	–

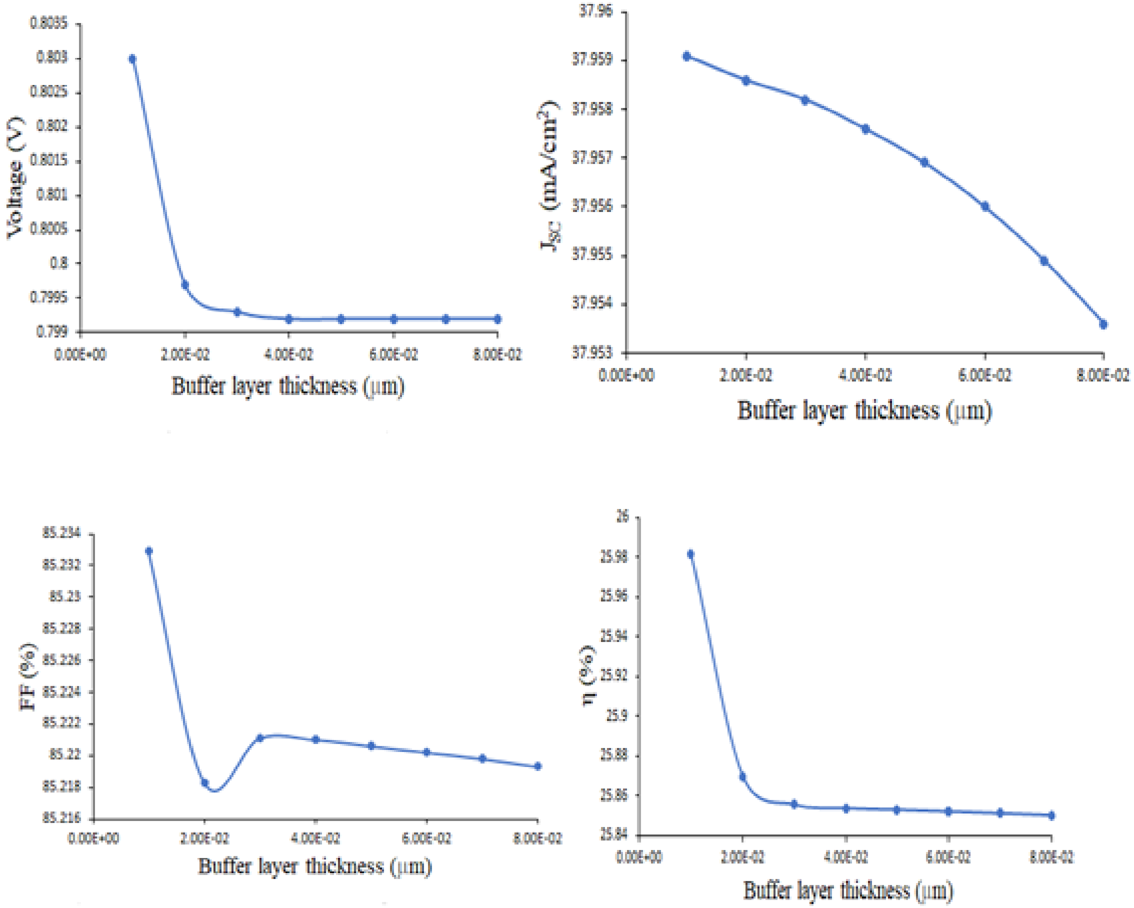


Figure 10. Variation in performance of CIGS solar cell with buffer layer thickness.

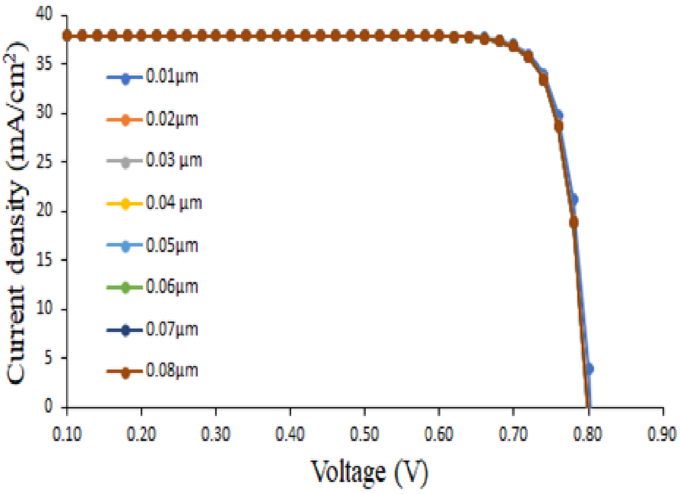


Figure 11. J-V curves of CIGS solar cells with various values of buffer layer thickness.

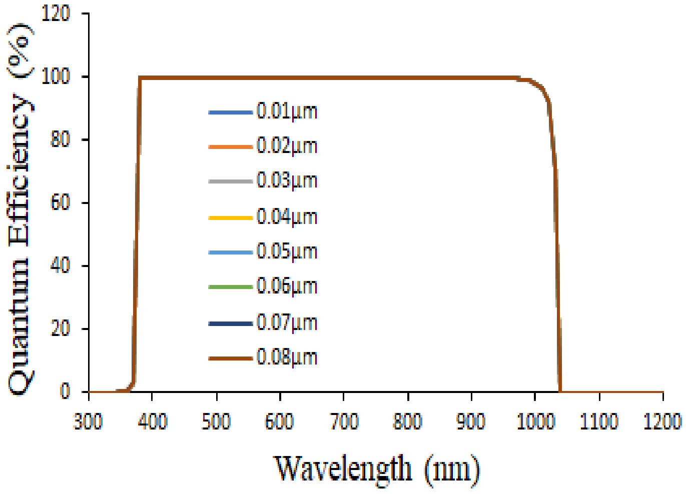


Figure 12. Quantum efficiency as a function of wavelength for different values of buffer (In_2S_3) layer thickness.

4. Conclusion

In this work, we undertook numerical simulation to investigate multivalent defects and the influence of absorber layer thickness and buffer layer thickness on $Al|ZnO:Al|In_2S_3|CIGS$ $|Pt|$ structured solar cells using SCAPS code. The efficiency of the initial device which was found to be 25.85 % with a multivalent defect density of 10^{14} cm^{-3} experienced a boost to 27 % when the solar cell was optimized with an absorber layer thickness of 1.2 μm, buffer layer thickness of 0.01 μm and a

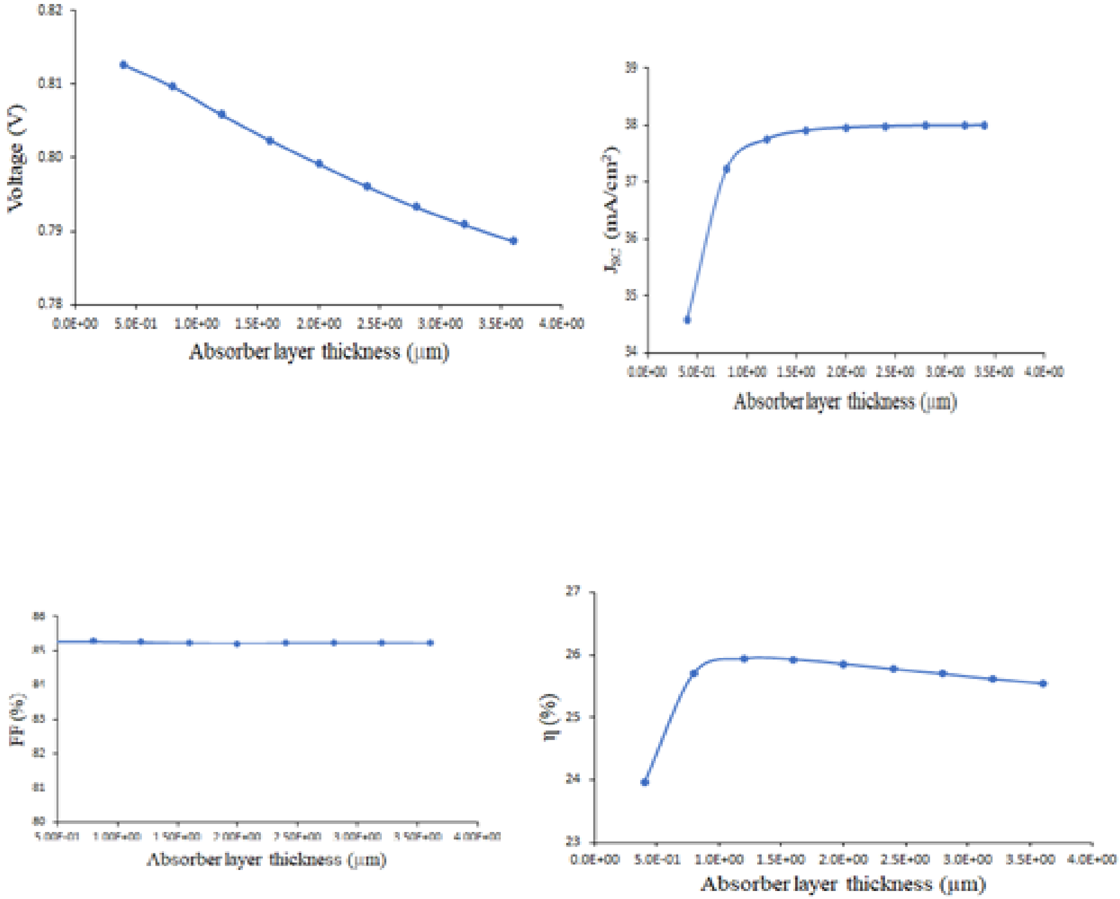


Figure 13. Variation in performance of CIGS solar cells with absorber layer thickness.

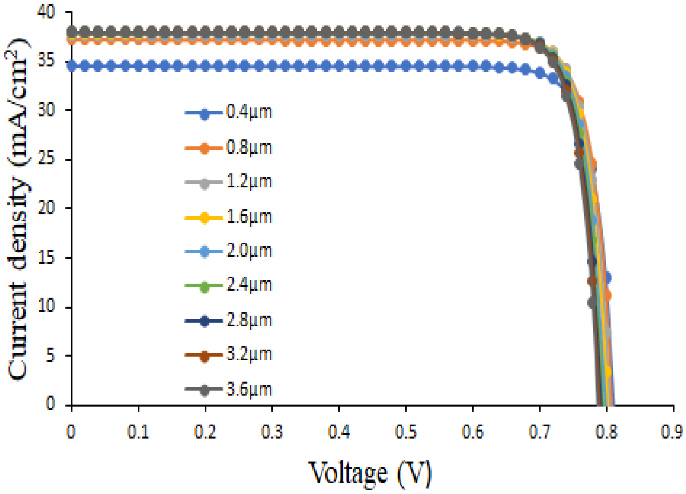


Figure 14. J-V curves of CIGS solar cell with various values of absorber layer thickness.

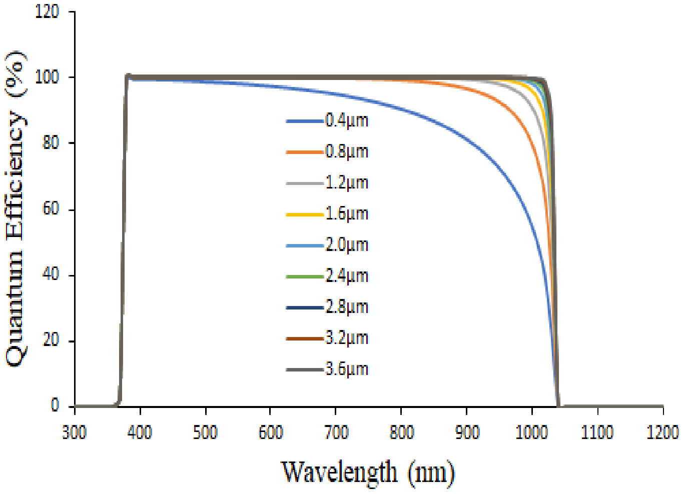


Figure 15. Quantum efficiency as a function of wavelength for different values of absorber (CIGS) layer thickness.

multivalent defect density of 10^{10} cm^{-3} in the CIGS absorber layer. The results obtained revealed that when the density of multivalent defect in the absorber was varied from 10^{10} cm^{-3} through 10^{17} cm^{-3}, the efficiency of the CIGS photovoltaic cells dropped from 26.81 % to 16.87 % representing a decrease of 58.92 %. This result clearly shows how detrimentally multivalent defects can affect the performance of CIGS solar cells. As expected, increasing the absorber layer thickness caused an increase in efficiency until an optimal thickness of 1.2 μm was achieved while increase in buffer layer thickness from 0.01 μm

Table 8. Photovoltaic parameters corresponding to optimized parameters of the CIGS solar cells compared with those of experimental researches.

Simulation	**V_{OC} (V)**	**J_{sc} (mA/cm^2)**	**FF %**	**η %**
Initial	0.7992	37.9576	85.2200	25.8500
Optimized absorber layer thickness (μm)	0.8059	37.7506	85.2655	25.9403
Optimized buffer layer thickness (μm)	0.8030	37.9591	85.2329	25.9813
Optimized multivalent defect density (cm^3)	0.8209	37.9630	86.0388	26.8116
Final Optimization	0.8290	37.7541	86.2600	27.0000
Experimental data	0.7570	34.8000	79.1000	20.8000 [31]
Experimental data	0.7440	36.7000	80.5000	22.0000 [32]
Experimental data	0.7410	37.8000	80.6000	22.6000 [18]

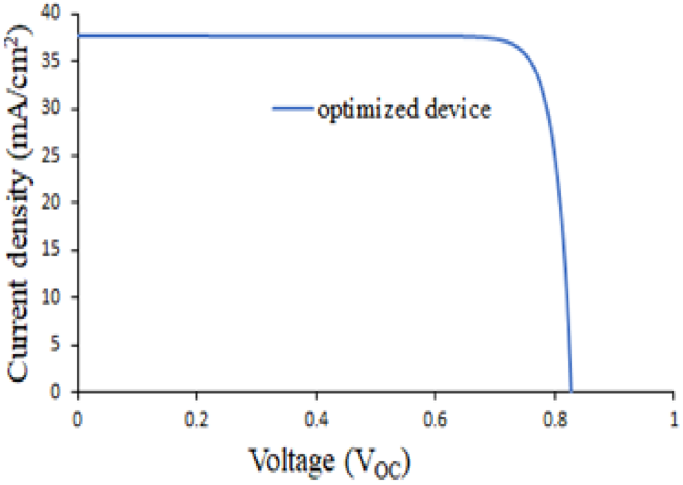


Figure 16. J-V curve of CIGS solar cell with optimized parameters.

through 0.08 μm caused a slight decrease of 0.51 % in efficiency.

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