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Numerical Modeling and Analysis of Ultra Thin Film Cu(In,Ga)Se₂ Solar Cell using SCAPS-1D

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Abstract—This paper exhibits a numerical analysis of ultra thin film Cu(In,Ga)Se₂ (CIGS) solar cell which has been performed by using SCAPS-1D simulator. In this paper, the performances of CIGS solar cell is observed by varying absorber layer, buffer layer and window layer thickness. Also the effect of temperature has been carried out. The aim of this work is optimization of CIGS solar cell thickness as well as the efficiency. Results represent that solar cell performances have enhanced with rise in thickness of CIGS absorber layer. Meanwhile opposite scenario is found with the rise in buffer layer and window layer thickness. The highest cell efficiency achieved is 22.67% with 0.7862 V open circuit voltage (V_{oc}), 34.130 mA/cm² short circuit current density (J_{sc}) and 84.49% Fill Factor (FF) on 2000 nm CIGS absorber layer.

Keywords—CIGS; SCAPS-1D; thickness; efficiency.

I. INTRODUCTION

Thin-film solar cells (TFSCs) are the latest development in the field of photovoltaic cells and there is considerable hope for wide spread use of it in the production of electricity. It is a microstructure created by the individual layers of material on the surface of a solid material. TFSCs are more preferable due to its low manufacturing cost, flexibility, reliability, availability and being lightweight. Cadmium Telluride (CdTe), Amorphous-Si and Copper Indium Gallium Di-Selenide (CIGS) are the most promising TFSCs. Among them CIGS based solar cells attracted a lot of interest as a marketable PV technology [1] and now leading the thin film market due to its high efficiency. Most attractive feature of this solar cell is adjustable band gap [2] and it has high absorption coefficient (10^5cm^{-1}) [3]. In spite of its high efficiency, the loss mechanism and inaccessibility of some materials makes it a matter of concern. With the increasing possibility of TFSCs have to keep in mind that materials used for CIGS solar cell should be lessen in a way that it doesn't affect the efficiency. Though it has some limits, it has non-toxic absorber in contrast with CdTe absorber.

The highest efficiency in laboratory is 22.3% achieved by “Solar frontier” [4] (also confirmed by NREL) and 21.7% by “Solar Energy and Hydrogen Research (ZSW)” [5] whereas crystalline Si efficiency is 25% [6]. CIGS solar have caught attention of researchers due its high efficiency. Although it has reached the maximum efficiency, still its parameter needs to

be optimized to get better efficiency in industrial production. Mostefaoui *et al.* showed in their comparative buffer layer study that optimal thickness of CIGS is 2500 nm [7]. While other reports depicted that the thickness of CIGS absorber layer would be optimal at around 3000 nm [8][9]. Besides, Sharmin *et al.* found optimum value of the CIGS absorber layer at 2000 nm [10]. Due to the scarcity of indium, its thickness needs to be thinner in order to reduce the material cost [11]. However, maximum numerical study based only on optimization of absorber and buffer layer. Window layer optimization needs to be taken into consideration for further study.

The purpose of this study is to observe performance of CIGS solar cells, optimize its results with best possible way and minimize different layer thickness to reduce its manufacturing cost. In this study the effect of the absorber and buffer layer thickness as well as window layer thickness and temperature effect on the electrical output parameters of CIGS solar cell has been demonstrated.

II. METHODOLOGY

A. CIGS solar cell structure

The structure of the CIGS cell is as follows ZnO:Al/i-ZnO/CdS/CIGS/Mo/substrate. Fig. 1 illustrates the schematic structure of simulated CIGS solar cell.

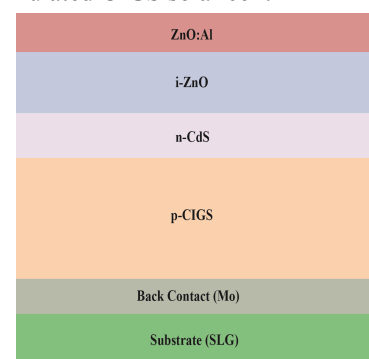


Fig. 1. Simplified layer diagram of simulated CIGS solar cell.

In this solar cell, Transparent Conductive Oxide (TCO) which is a bi-layer of ZnO having a band gap of 3.3 eV is used as window layer. The first layer is intrinsic Zinc-Oxide (i-ZnO) and the second layer is Aluminum (Al) doped ZnO

(ZnO:Al). Its transmission is 90% [12] which can be deposited through various processing techniques such as CVD, sputtering etc. CIGS absorber layer band gap can be tuned with variation of In:Ga ratio[2]. This results maximum incident sunlight absorption near to the p-n hetero-junction and allows the CIGS absorber layer to have lower thickness compared to traditional Si cells. Cadmium Sulfide (CdS) is mostly used buffer layer in CIGS solar cell to establish p-n junction with absorber layer and yielded high- efficiency cells [13]. It is fabricated between TCO window layer and CIGS absorber layer. It is a direct band gap semiconductor has a band gap of 2.4 eV that utilizes most energy carrying photons to pass through. Molybdenum (Mo) showed constancy with processing temperature, hence consider as a most suitable back contact [13]. It has a metal work function of 4.95 eV [14]. The purpose of this layer is to collect the carriers from the absorber layer. Thickness of back contact varies with the requirement of resistance of the solar cell. Substrate is the starting point of the solar cell where it is fabricated and which determines the flexibility and rigidity of the cell. Glass as substrate is widely used in production as because of its expense is low and it is able to withstand corrosion. Solar cells are mostly fabricated on soda-lime glass (SLG) substrate [4].

B. Numerical modelling and cell parameters

Numerical method helps to examine the results and optimize the process parameters of the cell without fabrication. The semiconductor parameters used for CIGS are band gap E_g , electron affinity χ_e , relative permittivity ϵ_r , density of states in the conduction band N_c , density states in valence band N_v , electron band mobility μ_e , hole band mobility μ_h , donor density N_D and acceptor density N_A . Gaussian defects are also used in this simulation as it has a role in efficiency change. All those parameters of the cell are given in TABLE I. ZnO which is used as front contact has a long range of photon transmission capacity compared to others and Mo is used as back contact has a very high metal work function and those parameters are given in TABLE II. The Interface properties between CIGS/CdS and CdS/i-ZnO are also presented in TABLE III.

In our study, we numerically modeled and simulated CIGS solar cells by using SCAPS (Solar Cell Capacitance Simulator) version of 3.0.0.2 which is a 1D simulator, programmed by the University of Gent [15]. Its motive is to simulate especially the CIGS and CdTe solar cells to observe its AC and DC characteristics before fabrication [16] and observe the numerical data through this. The numerical CIGS solar cell performed on two conditions, i.e. under the dark and under the light. While solar spectrum is AM 1.5G and power density is 100mW/cm². Temperature was kept 300 K in order to observe theoretical structure CIGS cell. The function of current density versus voltage (J-V) characteristic curve is used for extraction of electrical parameters such as V_{oc} , J_{sc} , FF and efficiency. The function of current density versus voltage (J-V) characteristic curve is used for extraction of electrical parameters such as V_{oc} , J_{sc} , FF and efficiency. In this analysis, CIGS layer thickness varied between 500 nm and 2000 nm, CdS and i-ZnO layer thickness varied between 50 nm and 200

nm and ZnO:Al layer thickness was kept constant at 100 nm and all other semiconductor parameters were fixed value as shown in TABLE I, TABLE II and TABLE III aiming to high efficient and thinner CdS/CIGS solar cell.

TABLE I
Material properties for basic CIGS materials

Parameter	ZnO:Al	i-ZnO	CdS	CIGS
Layer (nm)	100	50-200	50-200	500-2000
E_g (eV)	3.3	3.3	2.4	1.15
χ_e (eV)	4.45	4.45	4.2	4.1
ϵ_r	9	9	10	13.6
N_c (cm ⁻³)	2.20×10^{18}	2.20×10^{18}	2.20×10^{18}	2.20×10^{18}
N_v (cm ⁻³)	1.80×10^{19}	1.80×10^{19}	1.80×10^{19}	1.80×10^{19}
v_e (cm/s)	1.00×10^7	1.00×10^7	1.00×10^7	1.00×10^7
v_h (cm/s)	1.00×10^7	1.00×10^7	1.00×10^7	1.00×10^7
μ_e (cm ² /Vs)	100	100	100	100
μ_h (cm ² /Vs)	31	31	25	25
N_D (cm ⁻³)	1.00×10^{20}	1.00×10^{18}	5.00×10^{17}	0
N_A (cm ⁻³)	0	0	0	2.00×10^{18}
Defects properties				
Defect type	Donor	Donor	Acceptor	Donor
Energetic distribution	Gaussian	Gaussian	Gaussian	Gaussian
Energy level (eV)	1.65	1.65	1.2	0.6
σ_n	1.00×10^{-15}	1.00×10^{-15}	1.00×10^{-15}	5.00×10^{-17}
σ_p	5.00×10^{-13}	5.00×10^{-13}	5.00×10^{-13}	1.00×10^{-13}
N_t	1.00×10^{17}	1.00×10^{17}	1.00×10^{18}	1.00×10^{14}

TABLE II
Contact properties

Parameter	Back contact (Mo)	Front contact (ZnO:Al)
SN_0 (cm/s)	1.00×10^{17}	1.00×10^{17}
SP_0 (cm/s)	1.00×10^{17}	1.00×10^{17}
ϕ_m (eV)	4.95	4.40
Reflectivity/Transmittivity	0.80 (Reflectivity)	0.90 (Transmittivity)

TABLE III
Interface properties

Parameter	CIGS/CdS	CdS/i-ZnO
Defect type	Acceptor	Acceptor
σ_n	1.00×10^{-14}	1.00×10^{-15}
σ_p	1.00×10^{-14}	1.00×10^{-15}

III. RESULTS AND DISCUSSIONS

A. CIGS Absorber Layer Thickness Optimization

The performances of solar cell depend on the thickness of the cell. In this study, CIGS absorber layer has varied between 500 nm and 2000 nm where CdS is 50 nm and i-ZnO is 50 nm. In Fig. 2 the performances of simulated cells are shown in respect to V_{oc} , J_{sc} , FF and efficiency. All those solar cell output parameters in Fig. 2 have shown an upward trend with the absorber layer is increment. This is because with rise in CIGS absorber layer thickness, to be absorbed wavelengths of illumination are also increased. The long wavelength photons will go deep within the CIGS layer and which will result rise in electron hole formation, so that the V_{oc} , J_{sc} , FF and efficiency has elevated with rise in CIGS layer thickness and the best value of the efficiency found at the thickness 2000 nm

with highest efficiency 22.67%. On the other hand for a very thin absorber layer, back contact is very close to it, so that capturing electrons by back contact will grow up. Thus reduces the V_{oc} and J_{sc} . However, further increase in CIGS layer can increase the efficiency but it will ultimately increase the material cost.

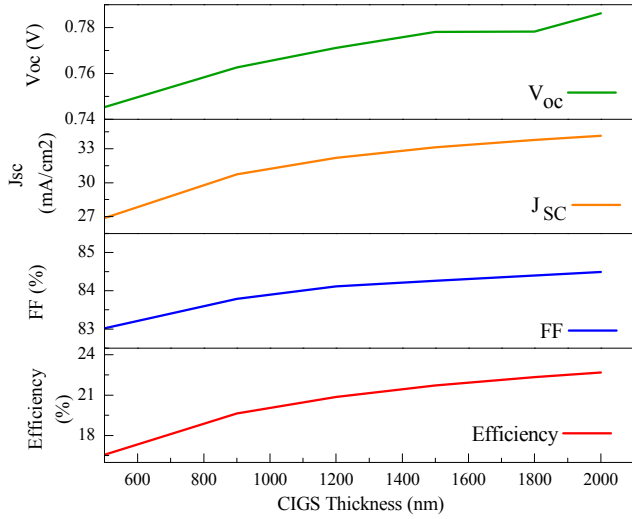


Fig. 2. CIGS absorber layer thickness variations on solar cell performance.

Fig. 3 illustrates the quantum efficiency (QE) of variable CIGS absorber layer thickness. Thicker CIGS layer will lead to rise in number of longer wavelength photons and it will contribute to more electron hole formation and collection. The effect can clearly be seen in the QE of the solar cell.

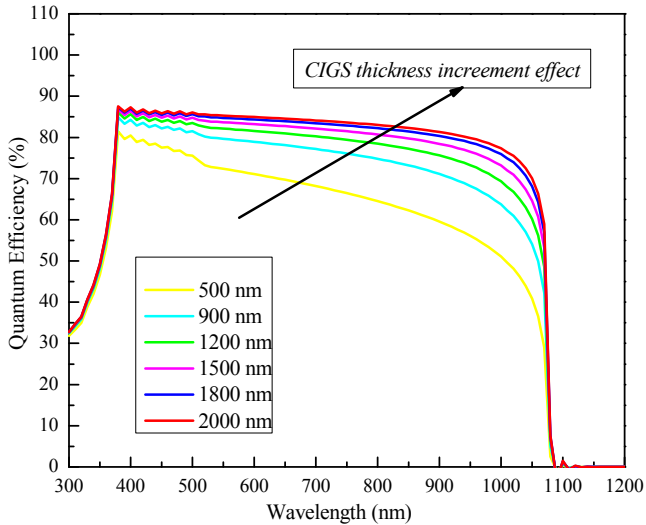


Fig. 3. CIGS absorber layer thickness variations on Quantum Efficiency.

QE in thicker absorber layer is much higher than the thinner absorber layer as illustrated in Fig.3. In case of thick absorber layer generation process has occurred far from the back contact region in the long wavelength portion.

B. CdS Buffer Layer Thickness Optimization

The optimum thickness of CdS layer found is (50-60) nm. Here CdS layer is changed from 50 nm to 200 nm with CIGS 2000 nm and i-ZnO 50 nm to observe the optimum

performance. Fig. 4 illustrates the effects in details of with increase in thickness of CdS layer.

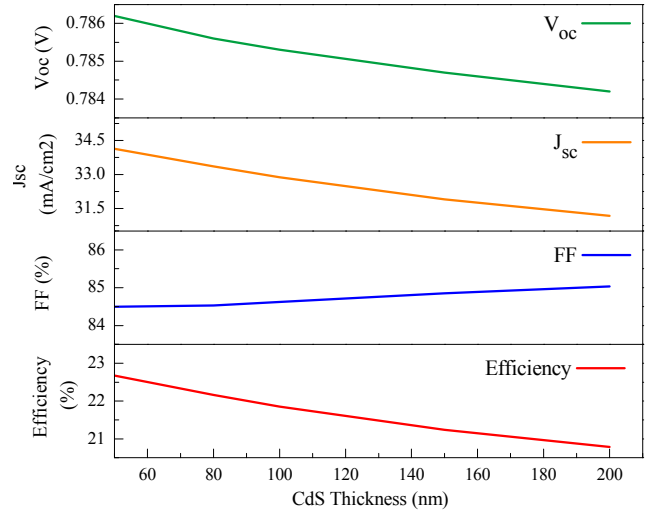


Fig. 4. CdS buffer layer thickness variations on solar cell performance.

It depicts that J_{sc} reduces greatly with increased CdS layer and V_{oc} affected a little. Meanwhile FF has increased slightly as it is inversely proportional to V_{oc} and J_{sc} . Thus, from the overall effect finally the efficiency has decreased with the rise in CdS layer thickness. This is because with increment in buffer layer, more energy carrying photons will be absorbed here. Therefore it lessens the number of photons which could have the possibility to go near the absorber layer and hence the efficiency has been decreased from 22.67% to 20.78%.

C. i-ZnO Layer Thickness Optimization

The effect of i-ZnO thickness on the output parameter is similar to the effect of CdS buffer layer but is varied in magnitude.

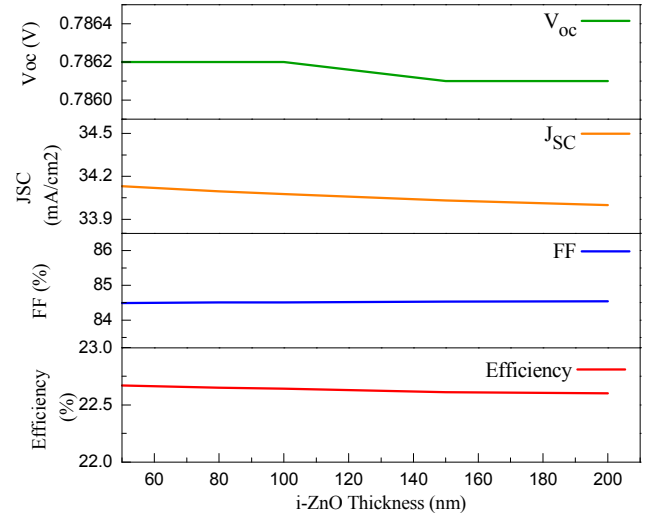


Fig. 5. i-ZnO window layer thickness variations on solar cell performance.

An increase in the thickness of i-ZnO layer from 50 nm to 200 nm Fig. 5 shows that efficiency reduced from 22.67% to 22.60% where other layer is as follows CIGS 2000 nm and CdS 50 nm. Besides, V_{oc} is also dropped by a little margin and

J_{sc} decreased from 34.130 mA/cm² to 33.999 mA/cm² whereas FF is almost remained same.

These effects have also reduced QE as it depends on the thickness of window layer. Light crossed through window layer first to arrive near the p-n junction. QE will be reduced when light is absorbed by the layer most as because carriers number is decreased. The maximum QE is found with 50 nm i-ZnO as shown in Fig. 5.

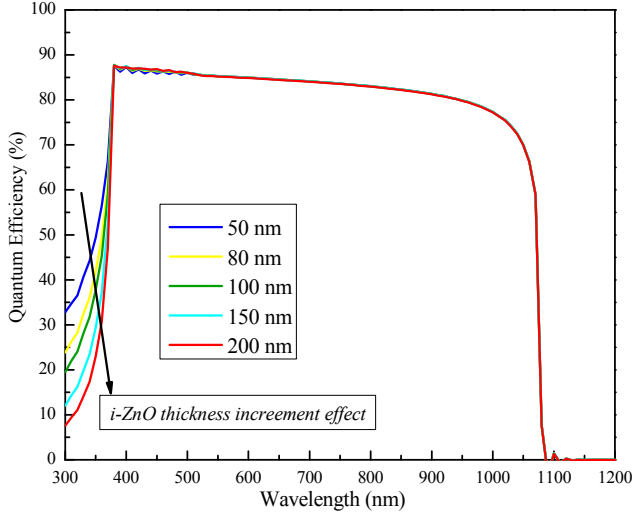


Fig. 6. i-ZnO window layer thickness variations on Quantum Efficiency.

D. Optimization of Operating Temperature

Operating temperature plays a critical role in solar cell electrical parameters. The operating temperature is optimal at 300 K or 27 °C. In a solar cell, V_{oc} and efficiency is mostly affected by an increase in temperature.

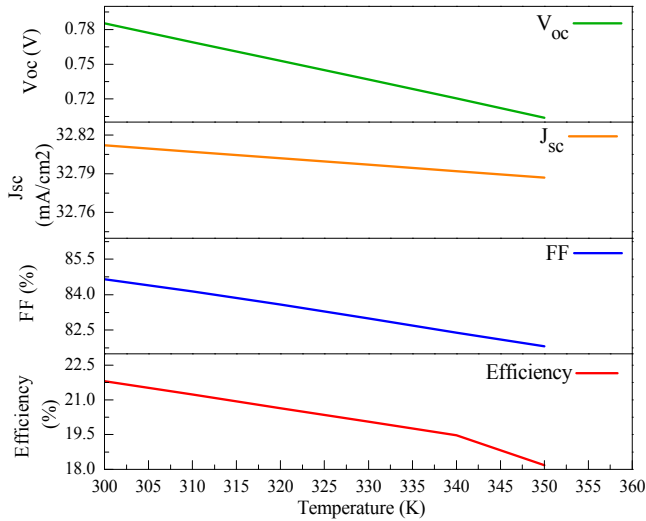


Fig. 7. Temperature variations on solar cell performance.

Fig. 7 represents that solar cell performances have degraded with increase in temperature. With temperature increment band gap energy becomes unstable [9] resulting electrons and holes recombination in the regions. This causes reduction in J_{sc} , V_{oc} and FF. Hence, efficiency has also reduced.

E. J-V Characteristic Curve of High Efficiency CIGS Cell

Fig. 10 shows the J-V curve of high efficient CIGS solar cell under light and dark condition on AM 1.5G where $V_{oc} = 0.7862$ V, $J_{sc} = 34.130$ mA/cm², FF = 84.49% with the layers as follows 2000 nm CIGS, 50 nm CdS, 50 nm i-ZnO and 100 nm ZnO:Al

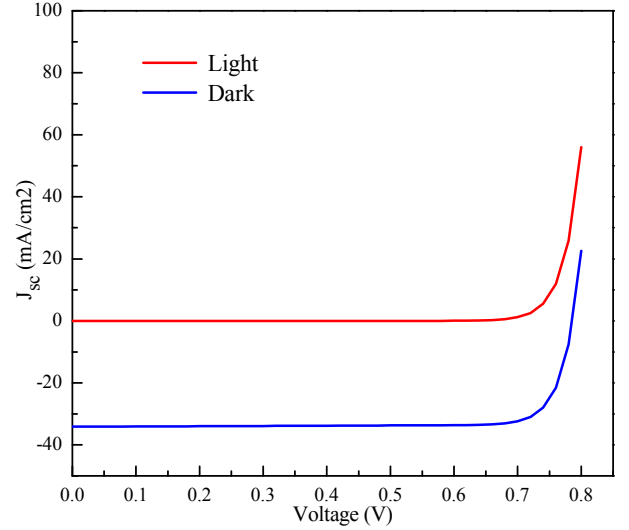


Fig. 8. Light-Dark J-V Curve of high efficiency CIGS cell.

In proposed model simulation, CIGS solar cell has crossed over the highest efficiency of the laboratory based cell as shown in TABLE IV. Though current density of simulated CIGS cell is less compared to laboratory produced CIGS cell, open circuit voltage and fill factor is much higher than that cell.

	Efficiency (%)	V_{oc} (V)	FF (%)	J_{sc} (mA/cm ²)
Simulated CIGS	22.67	0.7862	84.49	34.13
Solar frontier [4]	22.30	0.4219	78.2	39.38
ZSW [5]	21.70	0.746	79.3	36.6
Solibro [4]	21.0	0.757	77.6	35.70

IV. CONCLUSION

In this work, numerical modeling and analysis of CIGS solar cell has carried out using SCAPS-1D simulator by varying the layer thickness of the CIGS solar cell. The output parameters depicts that optimum efficiency is obtained with increment in the thickness of CIGS absorber layer from 500 nm to 2000 nm. Besides V_{oc} , J_{sc} and FF are also enhanced with increased absorber layer. As well as QE also improved with widen CIGS absorber. Meanwhile, a rise in buffer layer and window layer reduces the performances of CIGS solar cell. The highest efficiency of CIGS cell obtained is 22.67% whereas at present best efficiency is 22.3%. These results can be useful for a desired CIGS solar cell fabrication. But some other parameters need be investigated in further studies.

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