Optimization of Baseline Parameters and Numerical Simulation for Cu(In,Ga)Se_2 Solar Cell

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***Abstract*—For the purpose of designing a highly efficient Cu(In,Ga)Se_2 (CIGS) solar cell, an understanding of the structural, optical and electronic properties of each constituent layers in the heterojunction cell is very crucial. Important parameters such as thickness, doping concentration, electron affinity and band gap energy are identified to govern the electrical characterization of the cell. In this paper, an extensive study on the effects of these parameters on the short circuit current density (J_{SC}) and open circuit voltage (V_{OC}) known as *J-V* characteristics is performed. Optimized values of each parameter obtained from different numerical simulations are summarized and presented. An optimal CIGS solar cell model is later identified and simulated using Silvaco ATLAS software. Performance analysis is carried out on the completed cell under standard irradiance with air mass 1.5 (AM1.5) spectrums. This proposed model provides simulated conversion efficiency of 23.58% and fill factor (FF) of 77.89% which is in agreement with experimental efficiencies found in literature.**

Keywords—CIGS solar cell, numerical simulation, parameters optimization, proposed baseline data, Silvaco ATLAS software, conversion efficiency

I. Introduction

CIGS solar cell has emerged as a promising alternative to conventional silicon solar cells, leading other thin-film technologies with an efficiency reaching 22.6%, as certified in 2016 [1], [2]. Despite this high efficiency level, CIGS has not yet attained its full potential. The efficiency of current solar devices is limited by optical, collection, and recombination losses. According to Shockley-Queisser limit, maximum theoretical conversion efficiency of *p-n* junction-based solar cell is 32.8% at a band gap of 1.15 eV [3]. If all loss mechanisms were addressed at the same time, an efficiency approaching this level would be technically feasible.

Improvement of CIGS solar cell efficiency requires device optimization. Numerical simulations are advantageous for optimization because all the input parameters of the model in terms of device and material properties are well controlled. Parameters such as layer thickness, doping concentration, band gap, electron affinity, and many more can affect solar cell's characteristics and its electrical performance. Currently, a number of simulation packages such as AMPS-1D, SCAPS-1D, and Silvaco ATLAS are commonly used to perform an in-depth simulation study of CIGS solar cell for the purpose of optimization

This paper starts with an introduction to the structure of a typical CIGS solar cell and the importance of each layers' material properties. Afterwards, the results from different simulation studies on CIGS cell are discussed and optimized baseline parameters which can be used to develop a theoretical model of the cell are presented. Subsequently, numerical simulation was conducted using the obtained layer data. Starting with a conventional n-ZnO/n-CdS/p-CIGS structure, we simulated the parameters of current density-voltage (*J-V)* characteristics. The purpose of the study was to set optimum baseline parameters for CIGS solar cell and evaluate its characteristics with valid experimental results.

II. CIGS Solar Cell Structure and Selection of Material Parameters

Generally, a typical CIGS solar cell structure consists of a top contact, followed by three layers of semiconductor material: doped zinc oxide (n-ZnO) which serves as the window layer, cadmium sulfide (CdS) as the n-type buffer layer, and CIGS as a p-type absorber layer. Molybdenum (Mo) is commonly used as a back contact in the stack, with soda-lime glass as the substrate. The standard structural layout of a CIGS cell is illustrated in Fig. 1.

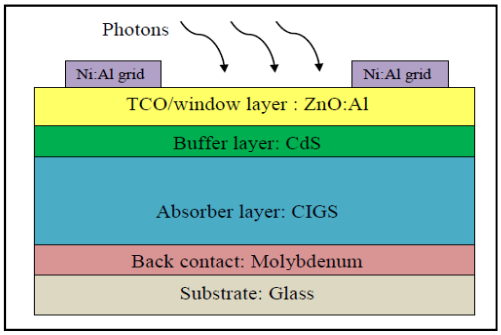

Fig. 1. Schematic representation of a typical thin-film CIGS solar cell

This basic structure could be modified in terms of layer thickness, cell surface area, and material properties. Our focus lies in particular on the influence of thickness and carrier concentration of the absorber-buffer-window region, as well as band gap energy of the absorber layer on the electrical parameters. Properties of these layers are evident to directly contribute in the performance of the cell [4]–[14].

A. Layers Thickness

ZnO is used both as a window or a transparent conducting oxide (TCO) layer and also as n-type junction. TCO serves as the first contact between photons and the cell thus this layer should allow the largest possible percentage of photons to reach the absorber layer while simultaneously allowing for good conduction of current generated by the cell [15]. ZnO is commonly doped with Aluminum to enhance the electrical conductivity [16]. Similarly, the role of CdS buffer layer other than optimizing the band alignment of the CIGS solar device [17] is to be as much transparent as possible, allowing a maximum sunlight absorption in the absorber layer [13]. Therefore, in the CIGS structure, ZnO and CdS layers are very thin. Contrary to ZnO and CdS, the CIGS layer acts as the absorber and is very important in determining the cell efficiency. It is reported that the performance of a CIGS cell increases with the increased thickness of the CIGS absorber layer.

B. Doping Concentration

Theoretically, donor (N_D) or acceptor (N_A) concentration of the component layers of CIGS solar cell can be determined from the capacitance voltage measurement [18], [19]. The effect induced by N_A and N_D on the V_{OC} and J_{SC} can be observed from the diode equations presented in [20].

C. Conduction band and valence band effective density of states

For direct band gap material such as ZnO, CdS, and CIGS, the recommended relations of effective masses for electrons and holes are discussed in [19]. Based on this, the effective densities of states in the conduction band N_C and the valence band N_V can be obtained via an equation presented in [20]. According to the equation, the N_C and N_V are temperature dependent. For CIGS solar cell, N_C and N_V at 25°C (300K) are determined to be $2.2\text{x}10^{18}$ cm^{-3} and $1.8\text{x}10^{19}$ cm^{-3} respectively. The same values are used as simulation parameters in [4], [6], [7], [9], [12], [18], [21]–[24].

D. Band gap energy

The band gaps of ZnO and CdS semiconductors are constant [20]. Conversely, in the chalcopyrite $Cu(In_{1-x},Ga_x)Se_2$ alloy system, the band gap can be tuned by varying the relative amount of Gallium (Ga) in the composition denoted by compositional ratio $x = (Ga)/(Ga+In)$. According to [19], the band gap can range from 1.04 eV for pure $CuInSe_2$ to 1.67 eV for pure $CuGaSe_2$. The band gap of CIGS layer is dependent on "x" following (1) as in below:

$$E_g(x) = 1.02 + 0.67x + 0.11x\,(x-1) \quad (1)$$

From a number of simulation studies [8], [11], [19], [24]–[27], it is shown that V_{OC} increases linearly with an increase in band gap energy as expected, while J_{SC} decreases. The trade-off between V_{OC} and J_{SC} leads to an optimal value of absorber layer band gap energy. Currently, CIGS solar cell with $x = 0.3$ which corresponds to a band gap energy between 1.1 to 1.2 eV yields optimum efficiency both in simulation and laboratory results [1], [28]. Electron affinity of the CIGS material is also dependent on the Ga composition of the material and the relation can be deducted from curve fitting as shown in [8]. The difference between electron affinity of CIGS absorber layer and CdS buffer layer plays an important role in the band alignment at the buffer/absorber interface [29].

III. Discussion on the Optimization Studies of ZnO, CdS, and CIGS Material Properties

For the purpose of cell performance optimization, the variation of photovoltaic-parameters as a function of thickness and doping concentration were simulated in a number of investigations. Optimum values for the two properties determined through simulations discussed in recent publications are presented in Table 1.

TABLE 1. PHYSICAL PARAMETERS PROPERTIES USED IN SIMULATIONS AND EXPERIMENTS FOR OPTIMAL CELL

Sim.[a] /Exp.[b]	Thickness (nm)			Doping Concentration (cm^{-3})			η %
	ZnO	*CdS*	*CIGS*	*ZnO*	*CdS*	*CIGS*	
[4][a]	20	50	4000	$1x10^{16}$	$1x10^{16}$	$1x10^{16}$	25.90
[9][a]	150	40	3000	$1x10^{17}$	$2x10^{19}$	$1x10^{18}$	23.20
[11][a]	200	50	3000	$1x10^{18}$	$5x10^{18}$	$1x10^{19}$	20.34
[14][a]	NA[c]	60	4000	NA[c]	$1x10^{17}$	$1x10^{17}$	21.4
[30][a]	800	50	3000	$1x10^{18}$	$1x10^{17}$	$8x10^{16}$	19.75
[15][a]	400	50	2000	NA[c]	NA[c]	NA[c]	17.2
[1][b]	150 - 200	30-50	2500 - 3000	NA[c]	NA[c]	NA[c]	22.6

[a] Simulation [b] Experiment [c] Information not available in publication

A. Effect of ZnO, CdS, and CIGS thickness on V_{OC}, J_{SC}, and conversion efficiency

Simulation studies performed by [4], [5], [9], [12], [31] show that both the cell efficiency and J_{SC} are significantly influenced by the variation of the ZnO window layer thickness. As the ZnO film thickness increases, the optical transmission and the electrical resistivity of this layer decrease. Reduction in J_{SC} in case of increased thickness is attributed to the low optical transmission of light that allows less amount of light to be absorbed to the CIGS layer thus affecting the creation of electron-hole pairs [4], [5], [9], [12]. Conversely, if the thickness of this layer is to be too thin, the cell performance degrades due to the increase of loss because of reflection [4], [12]. It is suggested that the best efficiency should be achieved using ZnO window layer with an optimum thickness that is from 100 to 200 nm.

Analysis of the results from simulation [4], [9], [12], [22] show that except for V_{OC} which remains constant, all remaining photovoltaic parameters (J_{SC}, η, and FF) are decreasing with the increase of CdS buffer layer thickness. When CdS thickness increases, a large number of short wavelength photons are absorbed in this layer before reaching the absorber layer, leading consequently to degraded cell performance [24]. This is because the absorbed photons in CdS do not contribute significantly in the collected photo-current. Hence, it is preferable to minimize its thickness in

order to reduce optical absorption loses. Though CIGS cell with thinner buffer layer shows higher performance, thicknesses less than 40nm currently is not reachable due to limitation in fabrication techniques and instruments. Based on these considerations, the range of 40 nm to 60 nm is determined to be the optimized thickness of buffer layer in CIGS solar cell [7], [24], [32], which is in agreement with CdS thickness (50 nm) commonly adopted in the lab [1], [28].

The general performance of a CIGS cell increases with the increased thickness of the CIGS absorber layer but with a much slower rate over 3000 nm [6], [8], [14]. By increasing the absorber layer thickness, more photons with longer wavelengths can be collected in this layer which will contribute to more generation of electron-hole pairs (EHP). This will results in higher J_{SC} and V_{OC} which will collectively increase the conversion efficiency of the cell [4]–[6], [9], [10], [25]. Though a thicker absorber layer benefits for complete photons absorption, too thick of the layer will lead to material waste and will eventually promote recombination. Moreover, simulations in [8], [18], [24], [31] show that for film thickness exceeding 3000 nm, the values of J_{SC} and V_{OC} are almost unchanged which will not result in major efficiency gains. On the contrary, if the absorber layer thickness is reduced, the back contact will be very close to the depletion region, thus promoting more recombination events at the back contact. Due to the recombination, less amount of electrons will contribute to the quantum efficiency, affecting both V_{OC} and J_{SC} [4], [6], [10], [24], [25].

B. *Effect of ZnO, CdS, and CIGS doping on V_{OC}, J_{SC}, and conversion efficiency*

Based on the diode equations [20] discussed earlier, it can be observed that as the values of N_A and N_D increases, the saturation current I_S decreases which leads to a logarithmic increase in the open-circuit voltage, V_{OC}. On the other hand, with increasing doping level, the output current I of the cell is controlled by two limiting factors: higher drift velocity of the majority carriers which increases the output current and increased minority carrier recombination rate that will reduce the output current. Therefore, the output current depends on which of the two factors dominates the other at a particular doping concentration [11], [30].

According to [4], [9], [30], as N_D of ZnO window layer increases, the cell efficiency increases as well and becomes almost constant when N_D reaches a value of $1x10^{18}$ cm^{-3}. The increase in output conversion efficiency is attributed to the improve collection of photo-generated carriers as the doping concentration increases. The same trend can be observed in the efficiency variation versus CdS buffer layer carrier concentration (N_D) [4], [9], [13], [18]. Above 10^{17} cm^{-3}, the efficiency increases only slightly then starts to decrease as N_D becomes higher. Therefore, the optimized doping level of the CdS buffer layer is restricted to $1x10^{17}$ cm^{-3} [18], [30]. For CIGS layer, as N_A increases further than 10^{16} cm^{-3}, the efficiency of the solar cell reduces due to the recombination process at the back contact, suggesting 10^{16} cm^{-3} to be in optimum range [4], [18], [30], [33], [34]. These results are in good agreement with default values presented in [19].

IV. Proposed Baseline Data for Numerical Simulation

Based on recent publications and trends, the recommended values for different parameters required for numerical simulation of CIGS solar cell is presented in this section. The values are displayed in Table 2.

TABLE 2. BASELINE PARAMETERS FOR OPTIMAL CELL

Parameters	Layers		
	ZnO	***CdS***	***CIGS***
Thickness (nm)	150	50	3000
Band gap, E_g (eV)	3.3	2.4	1.27
Donor concentration, N_D(cm^{-3})	$1x10^{18}$	$1x10^{17}$	0
Acceptor concentration, N_A(cm^{-3})	0	0	$2x10^{16}$
Conduction band effective density of states, N_C (cm^{-3})	$2.2x10^{18}$	$2.2x10^{18}$	$2.2x10^{18}$
Valence band effective density of states, N_V (cm^{-3})	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$

V. Simulation Approach Using Silvaco Atlas Software

Properties of the device layers defined in Table 2 were used as input parameters to design a theoretical model of CIGS solar cell. Then, the output characteristics of the optimized cell were numerically simulated.

The schematic device structure of CIGS solar cell developed using Silvaco simulation tool is shown in Fig. 2. The stack is composed of Molybdenum (Mo) back contact, a p-type wide-band gap absorber layer (CIGS), followed by n-type buffer layer made of CdS and a window/TCO layer made of doped ZnO of thickness as per Table 2 respectively.

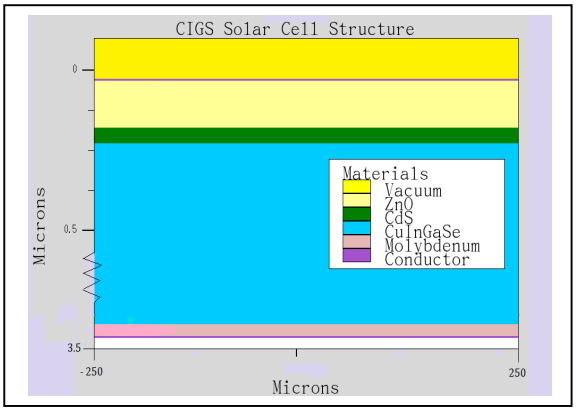

Fig. 2. Schematic CIGS solar cell structure used for simulation.

Fig 3. shows current density-voltage *(J-V)* characteristics curve for CIGS solar cell simulated under standard test condition of AM 1.5 illumination spectra, 1000 W/m^2 irradiance, and 25℃ (300K) temperature.

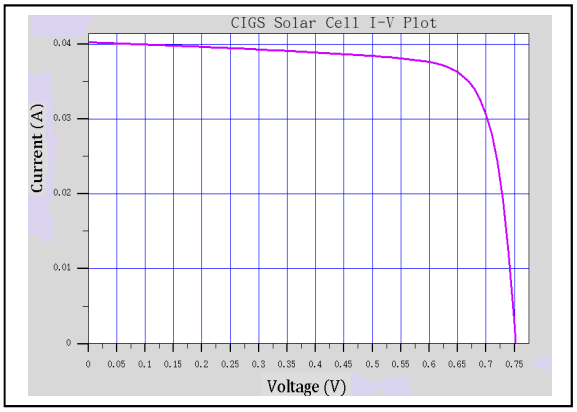

Fig. 3. J-V characteristic curve for optimized CIGS solar cell

The resulting performance parameters of the V_{OC}, J_{SC}, FF, and η determined using *J-V* characteristics are displayed in Table 3, and compared with gathered experimental values [1],

[35]. It can be observed that the efficiency is slightly higher than the highest recorded efficiency of 22.6% [1], [2] observed experimentally. Based on the simulation's results and analysis given in previous sections, the simulated cell's V_{OC} is improved by setting the absorber layer band gap at optimum value which is around 1.2 eV. The cell's J_{SC} on the other hand is enhanced by setting the absorber, buffer and window layers thickness at optimum value which leads to the increase in absorber layer's absorption rate. However, the simulated cell is not an exact comparison to the experimental cell reported in [1], [35]. This is because the information on some of the parameters used such as doping concentration, band gap, and exact thickness of each layer are not reported for the experimental cell in the reference. In addition, the simulation of CIGS cell in this work is performed in an ideal environmental condition hence moderate resistive loss is expected out of the cell. The changes in CIGS solar cell efficiency introduced by the presence of grain boundary (GB) are also not considered in our baseline case. According to [36] GBs that are presence within the space-charge region (SCR) will lower the V_{OC}, whereas GBs in the bulk material are observed to reduce the J_{SC} of the cell. Nonetheless, the close agreement between experimental and simulation values from this work validates our set of parameters as a baseline data for numerical simulation and modelling of CIGS solar cell.

TABLE 3. PERFORMANCE PARAMETERS - SIMULATION (FROM THIS WORK) VS EXPERIMENT

Performance Parameter	This work	Experiment [1][a]	Experiment [35][b]
Open Circuit Voltage, Voc (V)	0.75	0.74	0.72
Short Circuit Current Density, Jsc (mA/cm^2)	40.27	37.80	39.40
Fill Factor, FF (%)	77.89	80.60	78.20
Efficiency, η (%)	23.58	22.60	22.30

[a] P. Jackson et al. 2016 [b] R. Kamada et al. 2016

CONCLUSION

In this paper, based on gathered simulation and experimental studies, we provide a guideline that should be considered when assigning input parameters for numerical simulation of CIGS thin film solar cell. Numerical simulation is proven to play a vital role to understand the basic factors influencing and limiting the electrical parameters of the cell and to optimize the performance before experimental procedure can be conducted. The combination of optimum parameters gathered from recent simulation studies are subsequently used in our simulation. In optimum condition, we achieved conversion efficiency of 23. 58% and fill factor of around 78%. The simulated results are in close agreement with experimental values though the efficiency is 0.98% higher than the champion laboratory CIGS cell efficiency. The analysis and examination of the simulation results suggest that the optimization of material properties has an advantage in improving the cell efficiency.

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