Research Article

Numerical Analysis of Copper-Indium-Gallium-Diselenide-Based Solar Cells by SCAPS-1D

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We used a one-dimensional simulation program Solar Cell Capacitance Simulator in 1 Dimension (SCAPS-1D) to investigate Copper-Indium-Gallium-Diselenide- (CIGS-) based solar cells properties. Starting with a conventional ZnO-B/i-ZnO/CdS/CIGS structure, we simulated the parameters of current-voltage characteristics and showed how the absorber layer thickness, hole density, and band gap influence the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and efficiency of solar cell. Our simulation results showed that all electrical parameters are greatly affected by the absorber thickness (w) below 1000 nm, due to the increase of back-contact recombination and very poor absorption. Increasing hole density (p) or absorber band gap (E_g) improves V_{oc} and leads to high efficiency, which equals value of 16.1% when $p = 10^{16} \text{ cm}^{-3}$ and $E_g = 1.2 \text{ eV}$. In order to reduce back-contact recombination, the effect of a very thin layer with high band gap inserted near the back contact and acting as electrons reflector, the so-called back-electron reflector (EBR), has been investigated. The performances of the solar cells are significantly improved, when ultrathin absorbers ($w < 500 \text{ nm}$) are used; the corresponding gain of J_{sc} due to the EBR is 3 mA/cm^2 . Our results are in good agreement with those reported in the literature from experiments.

1. Introduction

Continuously increasing demand for photovoltaic (PV) modules and the need for low-cost PV options have stretched these advantages to the limit and have exposed some inherent disadvantages of c-Si technology, such as the scarcity of feedstock material, costly processing of materials, and device fabrication steps, as well as the inability for monolithic interconnections [1].

Thin films solar cells, mainly CIGS in this context, are enrolled as an alternative to the silicon technology. One of the advantages of thin films solar cells based on CIGS is the reduction of production cost compared to crystalline silicon sector, related to the power used during the deposition process. The recent performance in the laboratory for CIGS solar cell is 20.3% [2]; close to crystalline silicon whose performance is around 25%. Increasing this performance focused researchers, and it is becoming a central topic in the field of thin films solar cells. Despite the fact that there exists an extensive literature on CIGS solar cells, which has

best performances compared to other thin film photovoltaic sector, scientific knowledge of this family of solar cells are not yet exhaustive. This concerns mainly the loss mechanisms in the cell, the substitution of the toxic CdS layer by other alternative layers, and the reduction of the absorber thickness beyond 1000 nm [3, 4]. In order to improve CIGS solar cell performances, it is necessary to increase the understanding of the basic factors limiting the electrical parameters of the cell.

The purpose of this work is to study, using SCAPS-1D [6] simulation package, factors limiting the performance of CIGS solar cells. We examine the influence of the absorber layer thickness, band gap, and hole density, as well as the effect of the back-electron reflector (EBR), on the electrical parameters of CIGS solar cell.

2. Materials and Methods

2.1. Cell Structure. The structure of the solar cell is (Ni/Al)/MgF₂/ZnO:B/i-ZnO/CdS/OVC/CIGS/Mo/substrate

FIGURE 1: Structure of CIGS-based solar cells.

(Figure 1). The key parts of the cell are the CIGS absorber and the CdS buffer layer. The layer between the CdS and CIGS absorber is a thin layer named ordered vacancy compound (OVC). This layer, is formed by the interface states between the buffer layer and the absorber [7]. The OVC layer is considered to be beneficial to the performance of CIGS cells because the electrical junction is shifted away from the high-recombination interface between the CdS and CIGS layer, and hence, the recombination rate is reduced [8]. A ZnO intrinsic layer (i-ZnO) and boron-doped ZnO (ZnO:B) layer are deposited on the top of the buffer layer. These two layers are commonly referred to as transparent conductive oxide (TCO), because of their wide band gap which makes them transparent to most of the solar spectrum. Most solar cells based on CIGS use ZnO:Al as TCO. But in this paper, we use the boron-doped ZnO as TCO. Indeed, the ZnO:Al has absorption losses, leading to a decrease of the quantum efficiency of the solar cells in the near infrared regions. A boron doping would be more beneficial for the solar cells [9]. The TCO is covered with an antireflection layer MgF_2 , which increases the absorption of photons in the absorber.

2.2. Numerical Modeling and Material Parameters. CIGS polycrystalline solar cells are complicated structures, due to the large number of layers and the fact that the effects of some particular phenomena, mechanisms or material parameters often result from intuition. Numerical simulations can be used to provide insight to interpret measurements and to assess the potential merits of a cell structure. Indeed, once multiple measurements are (more or less) quantitatively described, the simulations can be used to analyse the effect of the variation of material parameters, that is, the presence or absence of particular properties, or variation of all properties in the range of values, to obtain the optimal values for optimizing the solar cells efficiencies, and should give the manufacturers additional ideas of how to vary their production methods to improve the product performance. Several software, among which SCAPS-1D [6], ASA [10], PC-1D [11], AFORS-HET [12], and AMPS-1D [13], have been developed in order to simulate the functioning of thin film

FIGURE 2: Comparison between the photocurrent density-voltage (J - V) curves for the simulated (red line) and the reported experimental data (blue line) [5].

solar cells. SCAPS is widely used for the simulation of CIGS- and CdTe- based solar cells. The good agreements between SCAPS-1D simulation results and the existing experimental ones [14] motivated us to use this tool in our work. SCAPS calculates the steady-state band diagram, recombination profile, and carrier transport in one dimension, based on Poisson equation together with hole and electron continuity equations. Recombination currents are calculated with the Shockley-Read-Hall (SRH) model for bulk defects and an extension of the SRH model for interface defects. To keep the model as simple as possible, one type of single level defects is introduced in each layer. These are all compensating defects positioned at the intrinsic level that is close to midgap. To pin the Fermi level at the absorber (CIGS)/OVC and OVC/(CdS) layer interface, neutral defects were placed 0.2 eV below the conduction band. These have a small capture cross-section to separate between pinning and recombination parameters of the OVC. The optical and electrical parameters used in this paper are derived from numerical models [5, 15, 16]. The influence of the series resistance and shunt resistance are not taken into consideration. Band discontinuity at the interface of the different materials is assumed small and neglected. The solar spectrum AM.1.5 is used for this numerical simulation, and the temperature is set at 300 K. Table 1 summarizes the parameters of the different layers used in this paper.

Figure 2 shows a superposition of J - V curve of experimental data [5] and a simulated CIGS solar cell for our baseline, where the absorber thickness taken as the default thickness is 1800 nm. The resulting performance parameters of the open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and efficiency are determined using J - V characteristics and are shown in Table 2.

Although the experimental values are slightly higher than the simulated ones, excellent agreement was observed in the J - V curve. The agreement between experiment and simulation is good for the J - V characteristic and validates our set of parameters as a baseline for simulating the influence of the variation of absorber parameters on the solar cell performances.

TABLE 1: Baseline parameters for modelling CIGS solar cells.

	Layer Properties				
	CIGS	OVC	CdS	i-ZnO	ZnO : B
W (nm)	Variable	30	50	200	400
E_g (eV)	Graded	1.3	2.4	3.3	3.3
X (eV)	4.5	4.5	4.45	4.55	4.55
ϵ/ϵ_0	13.6	13.6	10	9	9
N_c (cm ⁻³)	$2.2 * 10^{18}$	$2.2 * 10^{18}$	$1.3 * 10^{18}$	$3.1 * 10^{18}$	$3 * 10^{18}$
N_v (cm ⁻³)	$1.5 * 10^{19}$	$1.5 * 10^{18}$	$9.1 * 10^{18}$	$1.8 * 10^{19}$	$1.8 * 10^{19}$
v_e (cm/s)	$3.9 * 10^7$	$3.9 * 10^7$	$3.1 * 10^7$	$2.4 * 10^7$	$2.4 * 10^7$
v_h (cm/s)	$1.4 * 10^7$	$1.4 * 10^7$	$1.6 * 10^7$	$1.3 * 10^7$	$1.3 * 10^7$
μ_e (cm ² /Vs)	100	10	72	100	100
μ_h (cm ² /Vs)	12.5	1.25	20	31	31
Doping (cm ⁻³)	Variable (a)	10^{13} (a)	$5 * 10^{17}$ (d)	10^{17} (d)	10^{20} (d)
Bulk defect properties					
N (cm ⁻³)	10^{14} (D)	10^{14}	$5 * 10^{16}$ (A)	10^{16} (A)	10^{16} (A)
σ_e (cm ²)	10^{-15}	10^{-15}	10^{-15}	10^{-15}	10^{-15}
σ_h (cm ²)	10^{-11}	10^{-11}	$5 * 10^{-13}$	$5 * 10^{-13}$	$5 * 10^{-13}$
Interface	Interface properties				
	CIGS/OVC		OVC/CdS		
ΔE_c (eV)	0.0		0.0		
N (cm ²)	10^{11} (N)		$3 * 10^{13}$ (N)		
σ_e (cm ²)	10^{-15}		10^{-15}		
σ_h (cm ²)	10^{-15}		10^{-15}		

(a) and (d) denote shallow acceptor and donor defect while (A), (D), and (N) denote deep acceptor, donor, and neutral defects.

TABLE 2: Results from simulation compared with experimental data [5].

	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	Efficiency (%)
Experimental	0.646	33.6	76.1	—
Simulation	0.635	32.2	77.8	15.7

3. Results and Discussion

3.1. Effect of Absorber Layer Thickness on the Solar Cell Characteristics. The standard thickness of the Cu(In,Ga) Se₂ layer in CIGS solar cells is about 3000 nm. If this thickness could be reduced, with no or only minor loss in the performance, the deposition time of CIGS layer would be reduced for thinner CIGS layers. A thinner CIGS layer would reduce the direct materials usage and thereby the materials costs. A reduction of materials usage is important for indium (In) and gallium (Ga) since the supply of these metals might become an issue if CIGS thin-film solar cells are produced in large volumes [17]. However, the reduction of the absorber thickness is associated with a number of problems [3, 4]. With SCAPS-1D, the properties of the different layers are kept constant while varying the absorber thickness, in order to obtain qualitative information of the absorber layer thickness on the solar cell electrical parameters. The band gap of the absorber is also kept constant to 1.15 eV. Figure 3 shows the absorber layer thickness (w) effect on the electrical parameters of the solar cells. For all electrical parameters (J_{sc} , V_{oc} , FF, and efficiency), we can distinguish two zones of the absorber thickness (w)

which influence strongly the electrical parameters. The first zone is $w < 1000$ nm, and the second one corresponds to $1000 < w < 2500$ nm.

All electrical parameters decrease significantly in the first zone. The short-circuit current density (J_{sc}) is the parameter which is most affected by the decrease of the absorber thickness. This is mainly due to the recombination of photogenerated electrons at the back contact (Mo) [3, 4]. For a thinner absorber, photons of short wavelength (higher energy) penetrate deeply into the absorber and generate electron holes near the back contact, which is a zone of high recombination, thereby resulting in the decrease of the current density. The J_{sc} passes from 29.4 mA/cm² for $w = 1000$ nm to 5.3 mA/cm² for $w = 100$ nm, that is, a loss of 24.1 mA/cm² corresponding to the recombination current at the back contact. The quantum efficiency curve (Figure 4) shows that the absorption of the incident light greatly reduces in the first zone of thickness ($w < 1000$ nm); mainly the wavelength is greater than 500 nm, related to the combined effect of light transmission and high recombination of electrons at the CIGS/Mo interface. The decrease of the open-circuit voltage is related to degradation of the junction in the case of ultrathin thickness. The decrease of J_{sc} and V_{oc} leads to the decrease of the efficiency of the solar cells according to (1), where FF is the fill factor.

Consider

$$\eta = \frac{V_{oc} \cdot J_{sc} \cdot FF}{1000}. \quad (1)$$

FIGURE 3: Absorber thickness effects on the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and the efficiency. The solid red circles denote the experimental data extracted from [17].

The cell efficiency decreases from 14.13% for $w = 1000$ nm to 1.35% for $w = 100$ nm. The decrease of the efficiency is even more abrupt when the thickness of the absorber exceeds 500 nm, due to the simultaneous action of degradation of the absorption and electrons capture by the back contact. When the thickness of the absorber decreases, fewer photons are absorbed in the absorber. The quantity of electron hole is reduced, which reduces the efficiency of the solar cell.

In the second zone ($w > 1000$ nm), all electrical parameters are almost constant. However, the short-circuit current density passes from 29.3 mA/cm² for $w = 1000$ nm to 31.53 mA/cm² for $w = 2500$ nm, that is, a gain of 2.23 mA/cm², leading the cell efficiency to 16.10%. This is related to the increase in the collection of photogenerated carriers and complete absorption of the photons, as shown in Figure 4 (second zone). The quantum efficiency of the cells is high in this zone of thickness and reaches 90%. More photons are absorbed for $w > 1000$ nm, which increased the solar cell performances. Attempts are made to compare the simulation results with reported experimental data for the CIGS cells. The results are shown in Figure 3, where the solid red circles denote the experimental values extracted from [17]. Excellent

agreement was obtained between the simulated solar cell electrical parameters (V_{oc} , J_{sc} , FF and efficiency) trends and experimental values. Although the experimental values are slightly higher than the simulated ones because an intentional high defect density is introduced into the layers, we find that the main tendencies of the experimental data are reproduced by the simulation.

In sum, J_{sc} and V_{oc} decrease very significantly for thicknesses $w < 1000$ nm. These observations are also similar to those of references [18].

3.2. Effect of Absorber Hole Density. Figure 5 shows the influence of hole density on V_{oc} , J_{sc} , FF, and efficiency, for different thicknesses of the absorber. The open-circuit voltage (V_{oc}) increases significantly with increasing absorber doping. This increase is particularly important when the thickness of the absorber is larger. The V_{oc} reaches a peak at $p = 10^{16}$ cm⁻³, beyond this value, there is a saturation of the open-circuit voltage independently of the absorber thickness.

This saturation is related to the dependence of the space charge region width (SCRW) and the hole density in the absorber. If we assume that no voltage is applied to the diode

FIGURE 4: Quantum efficiency of the cell as a function of incident light wavelength for the two zones of the absorber thickness. 1 and 2 denote, respectively, the first zone and second zone.

and the build-in potential is equal to unity, the SCRW is given by approximation as the following equation:

$$\text{SCRW} = \sqrt{\frac{2\epsilon_r\epsilon_0}{qp}}, \quad (2)$$

where ϵ_r is the relative permittivity of the absorber, ϵ_0 the absolute vacuum permittivity, and q the elementary charge. Increasing hole density (p) reduces the space charge region width, and thus, causes the saturation of the V_{oc} for large values of p . For $w < 1000$ nm, the thickness of the absorber may become order of magnitude or smaller than the space charge region width and tends to be fully depleted [3]. In this case, the effect of doping on the open-circuit voltage remains insignificant. The short-circuit current density follows the same trend for all thicknesses of the absorber. It decreases significantly with increasing hole density. However, the decrease of J_{sc} is more brutal for $w < 1000$ nm. For this range of thickness, increasing the doping may lead to a reduction of the space charge width below the thickness of the absorber, thereby reducing the collection of the carriers by the junction.

The fill factor is affected by the increase of the hole density. For all thicknesses, the voltage gain is higher than the loss of the J_{sc} ; thus, the overall efficiency of the device increases with doping and reaches a peak of 16.10% for $p = 10^{16} \text{ cm}^{-3}$. Beyond $p = 10^{16} \text{ cm}^{-3}$, the combined effect of the saturation of V_{oc} and the brutal drop of J_{sc} for all thicknesses makes the performance of the device almost constant independently of doping.

3.3. Effect of Ga-Grading on the Cell Performance. The band-gap of CIGS can be tuned from 1.04 eV (pure CIS) to 1.65 (pure CGSe) depending on the Ga content. The Ga dependence of the band gap follows the equation [19]

$$E_g [\text{eV}] = 1.02 + 0.67x + bx(x - 1), \quad (3)$$

where x denotes the proportion of gallium in the absorber, that is, the ratio $\text{Ga}/(\text{Ga} + \text{In})$, b is the optical bowing coefficient for which values between 0.11 and 0.24 have been reported [19].

Thereafter, we assume that the band gap of the absorber [19], bulk defect densities [20], absorption coefficients, and electron affinities [21] is varied according with the Ga contents in the absorber. The other parameters of the absorber as well as the properties of the other layers of the cells are assumed constant in this simulation. With a uniform band gap profile, we analyze the effect of increasing absorber band gap on the electrical parameters.

As shown in Figure 6, the open-circuit voltage (V_{oc}) increases with the increase of the band gap, almost independently of the absorber thickness. However, this increase is not proportional to the band gap. The dependence of V_{oc} with the band gap is linear for $E_g < 1.15$ eV, corresponding to $x < 0.3$, and less linear $x > 0.3$. The short-circuit current density decreases dramatically with increasing gallium concentration but strongly depends on the thickness of the absorber. For $w < 1000$ nm, the decrease of J_{sc} is brutal, due to the combined effect of the decrease of absorption coefficient with increasing the band gap [22] and the reduction of absorption in the long wavelength region of the solar spectrum in the thin absorber. These results are also confirmed in [22, 23]. The efficiency of the solar cell as well as the fill factor (FF) increases with the band gap for $E_g < 1.25$ eV; beyond this value, the increase of the band gap by introducing the gallium has no effect and becomes detrimental to the performance of the device. These results are in good agreement with the experimental results from the literature. The best solar cell was obtained with a ratio $x = \text{Ga}/(\text{In} + \text{Ga}) = 0.3$ [24], which corresponds to a band gap of 1.15 eV. Despite attempts to increase the band gap and therefore increase the V_{oc} , CIGS solar cell shows poor electrical characteristics when the rate of gallium exceeds 0.3%, that is, $E_g = 1.15$ eV. Rau et al. [25] and Hanna et al. [20] have shown experimentally that the increase of the band gap by introducing gallium creates defects in the volume of the absorber. These defects become detrimental to the performance of the device when the gap exceeds 1.15 eV ($x = 30\%$) corresponding to the minimum defect density [20].

3.4. Potential Improvement by Using Back-Electron Reflector. The short-circuit current density (J_{sc}) is the most affected parameter by the variation of the thickness, especially for ultrathin absorber ($w < 1000$ nm), where the capture of electrons by the back contact is established as the main source of reduction of the J_{sc} [3, 4, 26].

At the CIGS/Mo interface, it would be desirable to keep the photoelectron away from this interface, which is expected to have a relatively high recombination velocity. By using a very thin layer rich in gallium (Ga) at the CIGS/Mo interface, commonly called back-electron reflector (EBR), we can keep the high conductivity for the majority holes and at the same time reflect the minority electrons.

To better understand the beneficial effect of the EBR on the electrical parameters, all the parameters of layers are kept constant, except the band gap and the thickness of

FIGURE 5: The simulated performance of hole density on V_{oc} , J_{sc} , FF, and the efficiency as a function of the CIGS absorber thickness.

the absorber. The properties of EBR layer are summarized in Table 3. In order to obtain qualitative information on the beneficial effect of the EBR, we show in Figure 7, the quantities ΔV_{oc} , ΔJ_{sc} , ΔFF , and $\Delta \text{efficiency}$, which represent the electrical parameters gained with the EBR, as a function of absorber thickness and absorber band gap.

Except the fill factor (FF), which shows a loss for $E_g < 1.1$ eV, the other electrical parameters have a gain due to the EBR.

The gain is very important when the thickness of the absorber is very small ($w < 1000$ nm). For thickness greater than 1000 nm, the effect of EBR on the electrical parameters is insignificant, given the fact that the thickness of the absorber is thick enough that the absorption takes place in the bulk of the absorber, away from the interface CIGS/Mo. However, when the absorber is thin ($w < 1000$ nm), photons of long wavelengths pass through the absorber and generate carriers at the CIGS/Mo interface, which is a zone of high recombination. The presence of the EBR can repel the electrons away from this interface, avoiding their capture by the Mo, and the short-circuit current density (J_{sc}) increases. For thin thicknesses, the gain of J_{sc} due to the EBR is $3 \text{ mA}/\text{cm}^2$ on average, and it is less than $0.5 \text{ mA}/\text{cm}^2$ for thickness greater

TABLE 3: Properties of the EBR layer used in our simulations.

W_{EBR} (nm)	10
E_g (eV)	1.4
ϵ/ϵ_0	13.6
N_c (cm^{-3})	2.2×10^{18}
N_v (cm^{-3})	1.8×10^{19}
v_e (cm/s)	10^7
v_h (cm/s)	10^7
μ_e (cm^2/Vs)	100
μ_p (cm^2/Vs)	25
Do paging (cm^{-3})	2.10^{19}

W_{EBR} denotes the thickness of EBR.

than 1000 nm. These results agree very well with those of Kanevce [27], who also showed that the gain of J_{sc} due to the EBR for ultrathin absorber is about $3 \text{ mA}/\text{cm}^2$.

4. Conclusion

Using SCAPS-1D package, we analyzed the variation of the absorber layer thickness, absorber holes density, the band

FIGURE 6: Effect of increasing absorber band gap on the electrical parameters (V_{oc} , J_{sc} , FF, and efficiency) as a function of the CIGS absorber thickness.

gap, and the effect of the introduction of the EBR on the electrical parameters of a CIGS solar cells. We have shown the following.

- Electrical parameters of CIGS solar cell are affected by reducing absorber thickness, but the most significant loss is the short-circuit current density that shows a loss of $24.1 \text{ mA}/\text{cm}^2$ when the thickness decreases from 1000 to 100 nm, due to the increasing of recombination at the CIGS/Mo interface.
- Increasing hole density in the absorber can significantly increase the performance of the device. This increase is mainly due to the gain of the open-circuit voltage (V_{oc}) when the hole density is lower than 10^{16} cm^{-3} .
- Ga grading can increase the performance of the solar cells. However, the short-circuit current density decreases considerably with increasing Ga in the absorber but strongly depends on the absorber layer thickness. The dependence of the V_{oc} with the band gap is linear for $E_g < 1.15 \text{ eV}$.
- The use of the EBR at CIGS/Mo interface can increase the short-circuit current density, especially, when the absorber thickness is less than 1000 nm. The gain due to the EBR is estimated at $3 \text{ mA}/\text{cm}^2$.

Nomenclature

Abbreviation

AM.1.5:	Standard terrestrial solar spectrum "Air Mass 1.5"
SCAPS-1D:	Solar Cell Capacitance Simulator in 1 Dimension
CIGS:	Copper Indium Gallium Diselenide
SCRW:	Space Charge Region Width
EBR:	Back-electron reflector.

Symbols

ΔE_c :	Conduction-band offset
ϵ/ϵ_0 :	Dielectric constant
E_g :	Band-gap energy of the semiconductor
FF:	Fill factor
J_{sc} :	Short-circuit current density
μ_e, μ_h :	Electron and hole mobility
N_c, N_v :	Effective density of states in the conduction and valence band
V_{oc} :	Open-circuit voltage
σ_e, σ_h :	Electron and hole capture cross section

FIGURE 7: Gain of electrical parameters due to presence of the EBR.

v_e, v_h : Electron and hole thermal velocity

X : Electron affinity

w : Absorber layer width

W : Layers width.

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