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Research Article

Simulation of the Effects of the Thickness and the Bandgap of the Absorber on the Performance of the Quaternary Thin Film Solar Cell Based on $Cu(In,Ga)Se_2$

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Abstract

In the field of energy transformation, the share of renewable energies continues to grow and gives hope to fight against global warming. In the global electricity mix we have: 15% for hydropower, and 14.5% for other renewables, according to 2022 figures. Among renewable energies, photovoltaic (PV) solar energy is the most promising with very high record yields of around 29% theoretically, 27.3% experimentally for record-breaking PV solar cells in the laboratory and 22% in industrial production for a solar panel. The selenide, gallium, indium and copper (CIGS) sector is very promising, one of its major advantages coming that the fact the quaternary alloy $Cu(In,Ga)Se_2$ is a material with an adjustable bandgap (Eg). The freely available and highly stable one-dimensional solar cell capacities simulation software, is the tool used for the simulation. Digital simulation is an essential tool because it makes it possible to predict the behavior of the solar device and to be able to estimate its performances. The study of effects of the thickness (W_{CIGS}) and the gap of the CIGS absorber with a cadmium sulfide buffer layer of 30 nm shows that current-voltage density characteristic is enormously affected for $W_{CIGS} \leq 1000$ nm. We therefore note a significant decrease in the values of the short-circuit current density (J_{SC}) and the open-circuit voltage (V_{OC}) when W_{CIGS} decreases. These results are explained by a significant reduction in the quantity of incident photons absorbed and an increase in the recombination rate of the charge carriers photogenerated in the absorber. V_{OC} increases and J_{SC} decreases with the increasing of the absorber gap, the increase in V_{OC} is therefore linked to a significant reduction in the recombination rate at the CIGS/Mo interface and inside the space charge region. The maximum efficiency is 26.33% for Eg = 1.45 eV and W_{CIGS} = 3000 nm.

Keywords

Numerical Simulation, Quaternary Thin Film Solar, $Cu(In, Ga)Se_2$ Absorber, Thickness, Bandgap, Electricals Parameters

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1. Introduction

In the field of energy transformation, the share of renewable energies continues to grow and gives hope to the important decisions taken by international policies in the fight against global warming [1, 2]. Global warming, which is caused largely by the consumption of fossil fuels through industrial processing. The share of renewable energies continues to grow in the global electricity mix: 15% for hydropower, and 14.5% for other renewables, according to 2022 figures [3].

Renewable energies are positioned in the short and long term as a solution to the various problems encountered in the use of fossil energies. Among the different type of renewable energies, photovoltaic (PV) solar energy is becoming more and more promising with very high record yields of around 29% theoretically, 27.3% experimentally for record-breaking PV solar cells in the laboratory and 22% in industrial production for a solar panel [4]. For a tandem Perovskite-Silicon solar cell and multi-junction solar cell in GaAs, the record yield is respectively 34, 85% and 44, 7% [5, 6].

In the solar photovoltaic field, we note several sectors among which we can cite the first-generation PV sector, made up of mono-crystalline and polycrystalline silicon technologies. The second-generation PV sector or thin film sector is made up of silicon technologies in its amorphous and polymorphic forms, indium copper selenide (CIS) and its variant selenide, gallium, indium and copper (CIGS), gallium arsenide (GaAs), cadmium telluride CdTe and copper, zinc, tin and sulfur technology (CZTS) [7]. The third-generation PV sector is made up of technologies based on organic solar cells and dye or Gra ëtzel solar cells, all of these PV sectors are promising.

In the rest of this paper, we will focus on copper, indium, gallium, and diselenide ($Cu(In,Ga)Se_2$) PV technology. This PV technology shows great promise in terms of stability and conversion efficiency.

Our objective is to study the performance of the quaternary CIGS-based solar cell as a function as certain variable parameters of the CIGS absorber in order to make the PV conversion optimal.

Firstly, we will study the effect of the thickness of the absorber layer (CIGS) on the opto-electrical characteristics, then we will address the effect of the graduation of the CIGS gap on the electrical characteristics and efficiency quantum. Secondly, we investigate the bandgap effects on the quaternary CIGS solar device. Finally, we study the electrical parameters as a function of the simultaneously variation of the bandgap and the thickness of the CIGS.

2. Materials and Methods

The diagram of the typical model of a CIGS solar cell presents a structure where we have an absorber layer which occupies most of the solar device. The absorber is indeed the centerpiece of the $Cu(In,Ga)Se_2$-based solar cell, its physico-chemical and opto-electric properties are of capital importance for the proper functioning of the CIGS solar cell [8-11]. More particularly the bandgap and the thickness of the absorber are very sensitive parameters for optimizing performances.

Figure 1 shows the structure of the CIGS-based solar cell with cadmium sulfide buffer layer.

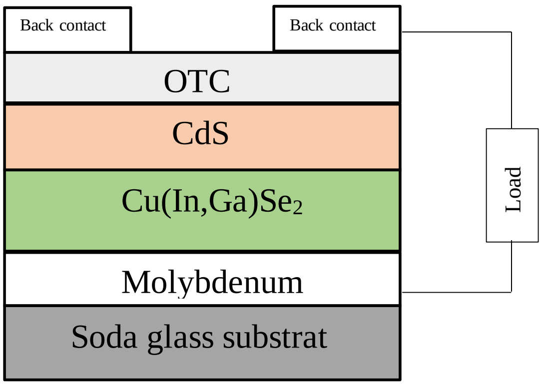


Figure 1. *Structure of CIGS-based solar cell.*

We distinguish from bottom to top the soda glass substrate layer (Na_2O_2) (W_{Na2O2}=1000 nm), the rear contact layer consisting of molybdenum (Mo) (W_{Mo}=500 nm), the absorber layer (CIGS) (W_{CIGS}=100-3000 nm), the buffer layer (CdS) (W_{CdS}=30 nm), the oxide layer transparent conductive (OTC) (W_{ZnO}=100 nm) and the front contact layer (Ni/Al/Ni) ($W_{Ni/Al}$ =500 nm).

In many studies, the standard absorber thickness is 3000 nm. Reducing the thickness of the absorber is currently the subject of several studies [12-15]. It must make it possible to miniaturize the size of the cells, reduce the deposition time of the absorber and also minimize the production and transport costs of solar PV modules.

The absorber layer, the most important of the device, is made up of copper indium gallium diselenide ($Cu(In, Ga)Se_2$). In high-efficiency CIGS devices, CIGS has a direct bandgap of 1.2 eV [16, 17]. One of the major advantages of the CIGS solar cell is the fact that the quaternary alloy $Cu(In,Ga)Se_2$ is an absorber material with an adjustable bandgap, its bandgap can vary from 1.02 to 1.68 eV depending on of the ration x = [Ga]/([Ga] + [In]) [10, 18, 17] according to equation (1):

$$E_g\left(eV\right)=1.02+0.67x+0.11x\left(x-1\right) \qquad (1)$$

A combination consisting to graduate the absorber bandgap and the using alternative buffer layers are now part of the innovative prospects of CIGS-based technology. With p-type conductivity and a large absorption coefficient of around 10^5 cm^{-1} [16], the absorber layer is where the conversion of incident photons into electron-hole pairs is optimal. The working principle of this solar cell structure is described in [19-22].

The freely available and highly stable one-dimensional solar cell capacities simulation software SCAPS-1D for the simulation of thin-film solar cells is the tool used for the simulation. More details regarding this very attractive numerical simulation software can be obtained in this works [10, 19-21, 23-27]. In the field of photovoltaic solar energy, digital simulation is an essential tool because it makes it possible to predict the behavior of the solar device and to be able to estimate its performance.

Table 1. Base parameters of CIGS cell properties. Φ_b —barrier height ($\Phi_{bn} = E_c - E_F$, $\Phi_{bn} = E_F - E_v$), Se and S_h—surface recombination velocity electron and hole, W —layer width, ε —dielectric constant, μ —mobility, Doping (electron/hole density), Eg—band gap energy, N_C and N_V —effective density of states, ΔE_C —conduction band offset, N_{AG} —acceptor-like defect density, N_{DG} —donor-like defect density, E_A and E_D —peak energy in, σ_e and, σ_h —capture cross section electrons and holes, χ_e —electron affinity, υ —thermal velocity, W_G —characteristic energy, Na, Nd —shallow uniform acceptor and donor [13-15, 17, 19, 21, 28, 29].

Contacts properties		
Parameters	**Right**	**left**
$\Phi_b(eV)$	$\Phi_{bn} = 0.0$	$\Phi_{bp} = 0.15$
$S_e(cm/s)$	10^7	10^7
$S_h(cm/s)$	10^7	10^7
Reflectivity	0.05	0.8

	p-CIGS	**n-CdS**	**n-OVC**	**i-ZnO**	**n-ZnO**
Layers properties					
W (nm)	1000	30	1	80	100
Eg (eV)	1.2	2.4	1.45	3.4	3.3
χ_e (eV)	4.5	4.45	4.5	4.55	4.45
$\varepsilon/\varepsilon_0$	13.6	10	13	9	9
Nc (cm^{-3})	$2.2*10^{18}$	$2.2*10^{18}$	$2*10^{18}$	$4*10^{18}$	$2.2*10^{18}$
Nv (cm^{-3})	$1.8*10^{19}$	$1.8*10^{19}$	$2*10^{19}$	$3*10^{19}$	$1.8*10^{19}$
v_e (cm/s)	$5*10^6$	10^7	$5*10^5$	10^7	10^7
v_h (cm/s)	$5*10^6$	10^7	$5*10^5$	10^7	10^7
μ_e (cm^2/Vs)	10^2	10^2	1	50	10^2
μ_h (cm^2/Vs)	25	25	1	20	25
Na (cm^{-3})	$2.5*10^{16}$ (a)	-	10^{13} (a)	-	-
Nd (cm^{-3})	-	$2.5*10^{16}$ (d)	-	$5*10^{17}$ (d)	10^{18} (d)
ΔE_C (eV)	0.35	-0.3	-	-	-
Bulk defect properties					
σ_e (cm^2)	$6.1*10^{-14}$	10^{-17}	-	-	10^{-14}
σ_h (cm^2)	10^{-14}	10^{-13}	-	-	10^{-15}
N_{AG}, N_{AG} (cm^{-3})	$3*10^{14}$ (d)	10^{17} (a)	-	-	10^{13} (a)
E_A, E_D (eV)	0.6	1.2	-	-	1.65
W_G (eV)	0.1	0.1	-	-	0.1

3. Results and Discussions

3.1. Effect of the Thickness of the Absorber Layer (CIGS) on the Opto-electric Characteristics

In this part of our work, we study the effects of the thickness and the gap of the CIGS absorber which are two parameters sensitive to the optimization of the performance of the solar cell. We keep the properties of the different layers [14] constant and we vary the thickness and the bandgap of the absorber. We also set the thickness of the CdS buffer layer to 30 nm in order to minimize the recombination rate inside this layer [14].

Figure 2 shows that the variation in the thickness (W_{CIGS}) of the absorber enormously affects the J-V characteristic for $W_{CIGS} \leq 1000$ nm. We therefore note a significant decrease in the values of the short-circuit current density (J_{SC}) and the open-circuit voltage (V_{OC}) (Figure 2) when the W_{CIGS} of the absorber layer decreases.

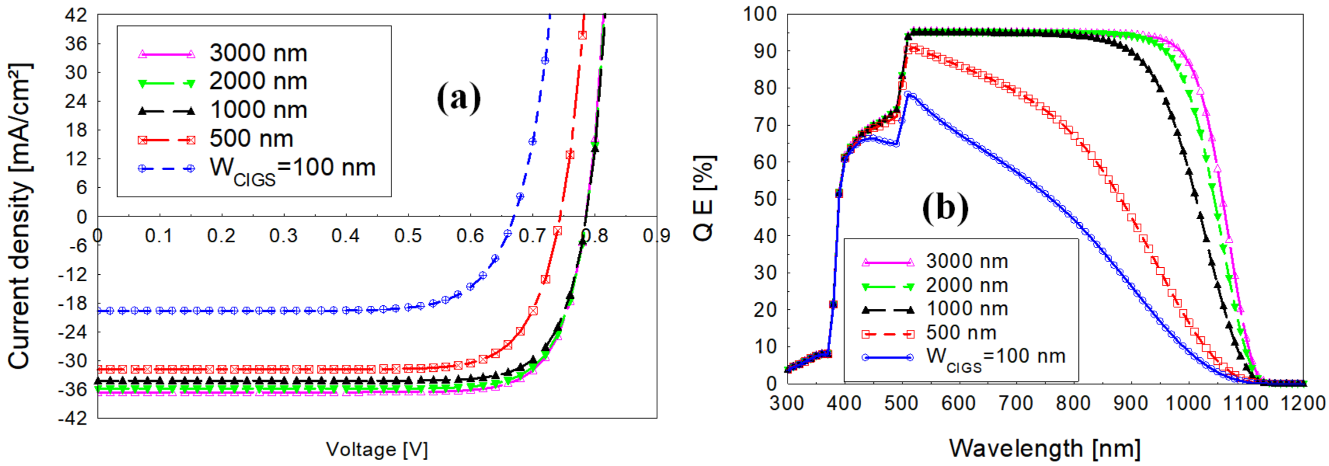
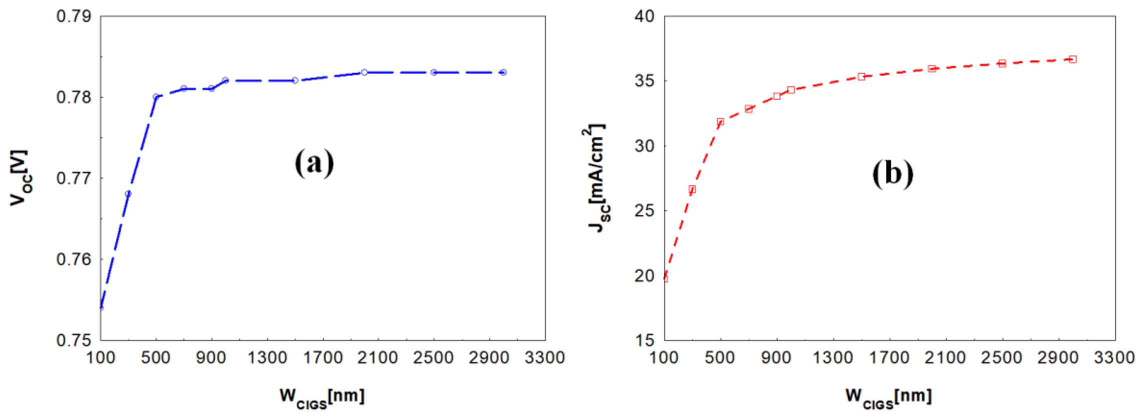


Figure 2. *(a) J-V characteristics, (b) quantum efficiency as a function of CIGS thickness.*

From the analysis of the curve of Figure 3, we note that the values of the different electrical parameters decrease with the decrease in the thickness of the CIGS layer. This reduction becomes very significant when the thickness is less than 500 nm ($W_{CIGS} < 500$ nm). We notice that J_{SC} and η are the most affected parameters. Their values go from 36.66 to 19.73 mA/cm^2 and from 22.99 to 11.58% respectively for W_{CIGS} equal to 3000 nm and 500 nm. These results are explained by:

1) a significant reduction in the quantity of incident photons absorbed in the layer CIGS (Figure 2b).
2) an increase in the recombination rate of the charge carriers photogenerated in the absorber.



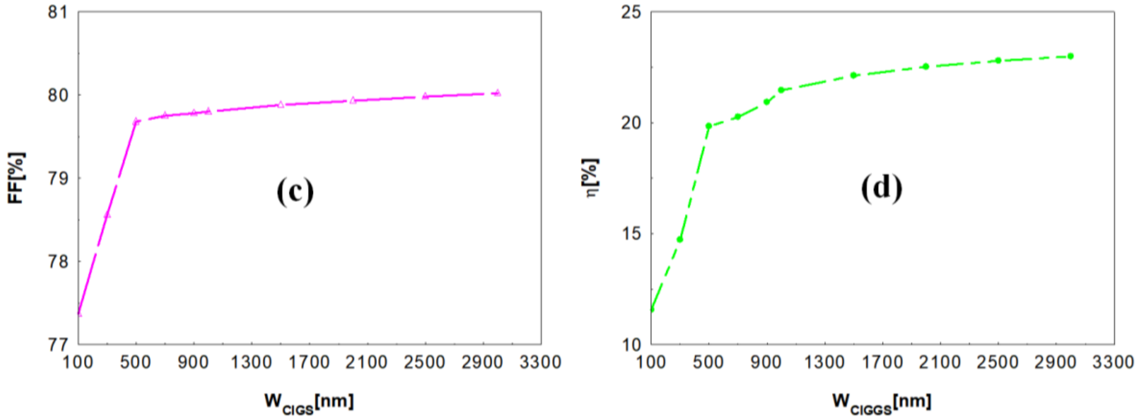


Figure 3. Electrical parameters as function on the thickness of the CIGS.

Indeed, when $W_{CIGS} \leq 500$ nm (Figure 2b), the absorption of incident photons with wavelengths between 500 and 1100 nm decreases considerably. This is the origin of the decrease in J_{SC} observed (Figure 2a) and Figure 3b. In addition, if the thickness of the CIGS is greatly reduced ($W_{CIGS} < 500$ nm), the short wavelength photons penetrate deep into the absorber and generate electron-hole pairs near the back contact (Mo). Some photons dissipate as heat radiation through the Mo and Na_2O_2 layers. Thus, recombinations become important at these levels. This large quantity of electron-hole pairs which recombine results in a significant reduction in V_{OC} (Figure 2a) and (Figure 3a).

The results for ultra-thin absorbers are extremely sensitive to interface recombination, and in our previous paper we have aborded it [29]. We also aborded the dominate recombination mechanism in the chalcopyrite $Cu(In,Ga)Se_2$ thin film solar cell by highlighting the dominant type of recombination and its area of predominance [8].

Experimentally, the reduction of thickness of the absorber to 500 nm leads to a significant reduction in the performance of the CIGS cell to around 6% [12]. Our model shows a loss in conversion efficiency of 3% if W_{CIGS}= 500 nm (Figure 3d). The recombination rate at the CIGS/Mo interface becomes increasingly important with the decrease in the thickness of the CIGS, this can explain the loss of the stability and the performances of the CIGS PV solar device (Figure 3c and d). However, in order to reduce the thickness of the CIGS layer, for a thickness of the CdS layer of 30 nm, the range from 1000 to 1500 nm presents acceptable performances and good stability.

3.2. Effect of the Graduation of the Bandgap of CIGS on the J-V Characteristic and Quantum Efficiency

From Figure 4a, we note that the V_{OC} increases and the J_{SC} decreases when the absorber bandgap increases. On the other hand, with regard to quantum efficiency (Figure 4b), we see a significant decrease in the quantity of photons absorbed in the CIGS and which explains the decrease in J_{SC} (Figure 4a). The increase in V_{OC} (Figure 4a) is therefore linked to a significant reduction in the recombination rate at the CIGS/Mo interface and inside the SCR.

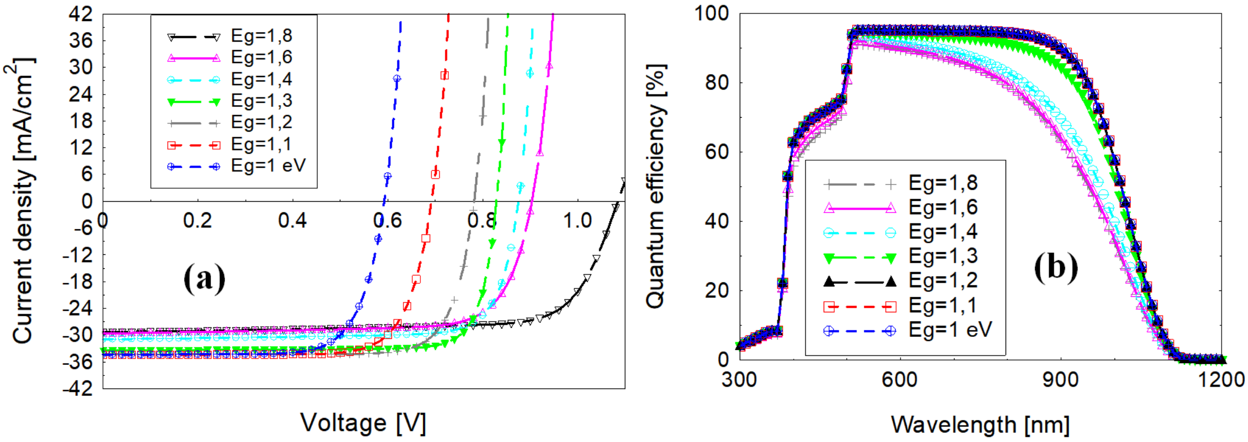


Figure 4. (a) J-V characteristic, (b) quantum efficiency as a function of the bandgap of the CIGS absorber.

3.3. Electrical Parameters as a Function of the Thickness and Bandgap of the CIGS Absorber

In this section, we study the performance of the CIGS-based solar cell through the graduation of the bandgap of the absorber for different thicknesses, in order to make the photovoltaic conversion optimal.

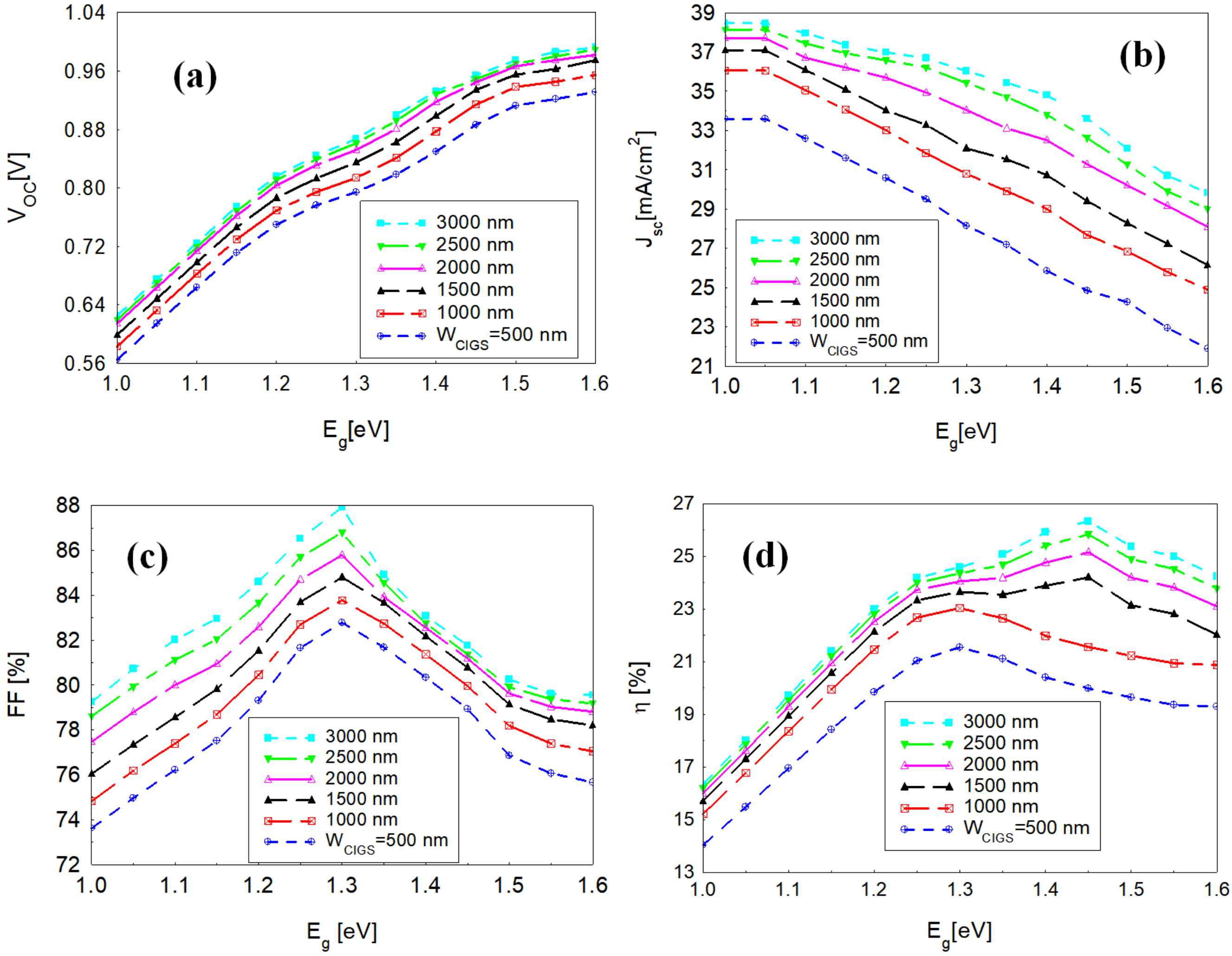


Figure 5. Electrical parameters as a function of the bandgap and for different thicknesses of the absorber.

Figure 5 shows that the curves of all the electrical parameters increase when W_{CIGS} increases. Regarding the increase in the bandgap, the curves relating to V_{OC} increase (Figure 5a), those of J_{SC} (Figure 5b) decrease. It should be noted that the FF and η curves reach their maximum for the absorber bandgap value of 1.3 eV (Figure 5c and d) if W_{CIGS} ≤1000 nm. For W_{CIGS} >1000 nm, η is maximum for Eg = 1.45 eV. The decrease in the J_{SC} values can be explained this time by a decrease in the optical absorption coefficient of the absorber conforming to equation (2) [30, 31]:

$$\alpha = \frac{B}{h\nu}\left(h\nu - E_g\right)^{1/2} \qquad (2)$$

This leads to a reduction in the absorption of photons arriving in the absorber. The increase in the bandgap of the absorber which leads to an increase in the V_{OC} and FF values and a decrease in the J_{SC} values, makes it possible to obtain a maximum efficiency of 22.95% for Eg = 1.3 eV and W_{CIGS} = 1000 nm (Figure 5d) and 26.33% for Eg = 1.45 eV and W_{CIGS} = 3000 nm (Figure 5d). Likewise, we note that the fill factor (Figure 5c) is optimal for a bandgap of 1.3 eV.

It emerges from our various analyzes that the widening of the bandgap of the absorber has the effect of reducing the recombination of the charge carriers inside the SCR and at the interface CIGS/Mo.

4. Conclusion

In the field of photovoltaic solar energy, digital simulation is an essential tool because it makes it possible to predict the behavior of the solar device and to be able to estimate its performance.

In the present study, the investigations that we carried out on the thickness and the bandgap of the CIGS absorber using a thickness of 30 nm of the CdS buffer layer, present results which show on the one hand a significant reduction in the values of J_{SC}, V_{OC}, FF and η when W_{CIGS} decreases. This drop in performance, which is explained by a reduction in the quantity of incident photons and an increase in the recombination rate of the charge carriers photogenerated in the CIGS absorber, results in a reduction in J_{SC} from 36.66 to 19.73 mA/cm^2 and η from 22.99 to 11.58% respectively for W_{CIGS} equal to 3000 nm and 500 nm. On the other hand, the results obtained show that the increase in the bandgap leads to an increase in V_{OC} and a decrease in J_{SC}. The maximum value of FF is obtained for a bandgap of 1.3 eV when $W_{CIGS} \leq 1000$ nm, the maximum values of conversion efficiency are obtained respectively for a bandgap of 1.3 eV (22.95%) when $W_{CIGS} \leq 1000$ nm and for Eg = 1.45 eV (26.33%) for $W_{CIGS} \leq 3000$ nm.

Abbreviations

CdS	Cadmium Sulfide
CdTe	Cadmium Telluride
CIGS	Copper Indium Gallium Selenide
CIS	Copper Indium Selenide
CZTS	Copper Zinc Tin Sulfur
Eg	Bandgap Energy
GaAs	Gallium Arsenide
Na_2O_2	Soda Glass
OTC	Oxide Transparent Conductive
PV	Photovoltaic
SCAPS-1D	One-dimensional Solar Cell Capacities Simulation
ZnO	Zinc Oxide

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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