Two-dimensional Modelling and Simulation of CIGS thin-film solar cell

S. Tobbeche[1,*] and H. Amar[1]

[1]*Laboratoire des matériaux semi-conducteurs et métalliques, Faculté des Sciences et de la Technologie,
Département de Génie-Electrique, Université de Biskra,B.P 145, Biskra 07000, Algérie.*

Abstract: *2 D Silvaco Atlas software is used for the study of a CIGS thin film solar cell in the configuration: ZnO(200 nm)/n-type CdS(50 nm)/ p-type CIGS(350 nm)/Mo. The cell performance is evaluated by implementing the defects created at the grain boundaries of the polycrystalline CdS and CIGS material and at the interface CdS/CIGS.The J-V characteristics and the external quantum efficiency EQE are simulated under AM 1.5 illumination. The conversion efficiency η of 20.35% is reached and the other characteristic parameters are simulated: the short circuit current density J_{sc} equals 35.62 mA/cm^2, the open circuit voltage V_{oc} is of 0.69 Vand the fill factor FF is of 82.7 %. The calculated external parameters of the solar cell are in good agreement with the measured characteristics. The simulation results also showed that the rise of the CdS thickness decreases all output parameters and the external quantum efficiencywhile the rise of the CIGS thickness improves all photovoltaic parameters and the external quantum efficiency. The highest efficiency of 21.08 % is reached for the CIGS thickness of 5 μm.*

1. Introduction

Thin film solar cells have the potential for low-cost and large-scale terrestrial photovoltaic applications. A number of semiconductor materials including polycrystalline CdTe, CIGS and amorphous silicon (a-Si) materials have been developed for thin-film photovoltaic solar cells. The CIGS based solar cells exhibit an excellent outdoor stability and aradiation hardness [1, 2]. They are attracting considerable interest for space applications, because proton and electron irradiation tests of CIGS and CdTe solar cells have proven that their stability against particle irradiation is superior to Si or III–V solar cells [3]. CIGS is an excellent material for highefficiency thin-film solar cells because it is a suitable energy band gap semiconductor with a high opticalabsorption coefficient in the visible spectrum of incident sunlight. The absorption coefficient of CIGS films in the visible spectrum is 100 times larger than silicon material. The best performance of CIGS is due to its tunable bandgap to match well the solar spectrum. When alloying the CuInSe$_2$ (CIS) with Ga to form CIGS thin films, the wider band-gap energy of the CIGS absorber layer can potentially better match the solar spectrum, as well as increase the open circuit voltage of the fabricated cells.The maximum efficiency for the best CIGS cell grown on stainless steel substrates is 17.5 % under AM1.5G illumination [4]. The device structure consists ofMgF$_2$/ITO/ZnO/CdS/CIGS/Mo/stainlesssteel substrates.The CIGS cell with a Ga composition x=0.3 which corresponds to a bandgap energy range of 1.1-1.2 eV fabricated on sodalime glass substrates has an efficiency of 20% [5]AM1.5G, as reported by the NREL (National Renewable Energy Laboratory) research team. In recent years, progress hasshowed that the best thin-filmCIGS solar cells by using thin film CIGS of thickness between 2.5 and 3 μm, and a band gap in the range 1.2 to 1.3 eV

have surpassed the 20% efficiency barrier for CIGS solar cells and have reached a new world record efficiency of 20.3% [6]. It was established numerically [7], by using AMPS-lD simulation tool that the maximum efficiency obtained numerically for a simple CdS/CIGS solar cell was 19 %. An increase in efficiency is expected mainly using denominated tandem, triple, and multi-junction solar cells, consisting of layers with different band gaps in order to exploit different energy regions of the solar spectrum.

The numerical simulation is a powerful tool and many parameters can be varied to model the observed phenomenon. It can also offer a physical explanation of the observed phenomenon since internal parameters such as the recombination rate and the free carrier densities can be calculated. In this work we have used Silvaco Atlas software on the design and the study of a CIGS solar cell. It makes it possible to design and predict the performance of semiconductor-based devices and solar cells. This work contributes to obtain a better understanding and insight in CIGS solar cells.In this study, we have investigated the thickness effect of the absorber layer CIGS and the buffer layer CdSon the photovoltaic parameters of the solar cell.

2. CIGS solar cell structure

A solar cell structure used in an experimental work [6] was simulated. The cell setup was described as follows:soda-lime glass (3 mm), sputtered molybdenum (500–900 nm), CIGS (2.5–3.0 μm), chemical bath deposited CdS buffer layer (40–50 nm), sputtered undoped ZnO (50–100 nm), sputtered aluminium doped ZnO (150–200 nm) and nickel/aluminium-grid.CIGS solar cells with an efficiency of 20.3 % were produced with varying composition (Ga/(Ga+In) from 0.30 to 0.35. Oursimulated solar cell structure is formed by a p-typedoped CIGS absorber and an n-type doped CdS buffer. A transparent contact of ZnO layer is deposited on the top of the structure to achieve a low series resistance. The solar cell structure is completed

by molybdenium rear metallization contact. The Ga composition is about 0.30, corresponding to a band gap energy of 1.15 eV [7, 8].Baseline case parameters are shown in Table 1.

3. Physical models and imput parameters

Most numerical simulators use the Shockley-Read-Hall (SRH) model to describe carrier recombination currents. We considered two Gaussian deep acceptor (donor) defect distributions for the CdS(CIGS) layer. The position of the recombinative defect states is in a narrow distribution close to themiddle of the band gap. A surface recombination at the CdS-CIGS interface which effectively recombines minority carriers that reaches the interface. Absorption coefficients of ZnO, polycristalline CdS and CIGS are defined in Silvaco database.

We modeled CIGS solar cell with the parameters defined in Table 1. The purpose was to see if it is possible to obtain a reasonable simulation which could be compared with experimental results and other simulation calculations.

Table 1. The solar cell parameters used in the simulation

Parameter and units e, h for electronsand holes, respectively	CdS	CIGS
Thickness (nm)	50	350
Permitivity	10	13.6
Electron affinity (eV)	4.5	4.8
Band gap (eV)	2.4	1.15
Effective conduction banddensity (cm^{-3})	10^{19}	10^{19}
Effective valence band density(cm^{-3})	10^{19}	10^{19}
Electron mobility (cm^{2}V^{-1} s^{-1})	140	140
Hole mobility (cm^{2}V^{-1} s^{-1})	25	25
Acceptor concentration (cm^{-3})	0	10^{16}
Donor concentration (cm^{-3})	10^{17}	0
Gaussian density of states (cm^{-3})	10^{15}	10^{15}
Distribution width (eV)	0.1	0.1
Capture cross-section for e (cm^2)	10^{-17}	5×10^{-13}
Capture cross-section for h (cm^2)	10^{-13}	10^{-15}
Recombination velocity at CdS/CIGS interface for e (cm/s)	10^5	10^5
Recombination velocity at CdS/CIGS interface for h (cm/s)	10^5	10^5

4. Simulation results and discussion

Fig. 1 shows the variation curve of the current density J with the applied voltage V, the solar cell's top surface is subjected to AM 1.5 with a power density of 100 mW/cm^2.
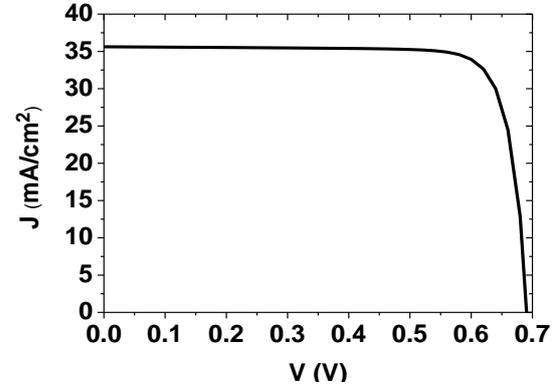

Fig. 1 Current density vs. voltage of the CIGS solar cell.

The photovoltaic parameters of the solar cell obtained by simulation and experiment [6] such as, J$_{sc}$, V$_{oc}$, FF and η are illustrated in Table 2. These simulation results are in good agreement with those measured. The efficiency is equal to the high record efficiency 20.3% observed experimentally.

Table 2. Simulation and experiment parameters of CIGS solar cell

	J$_{sc}$ (mA/cm^2)	V$_{oc}$ (V)	FF (%)	η(%)
Simulation	35.62	0.69	82.7	20.35
Experiment	35.4	0.74	77.5	20.3

The external quantum efficiency spectrum is illustrated in Fig. 2. This shows a peak response of nearly 86 % and falls off in the range below 0.6 μm due to the absorption and recombination in the CdS layer.
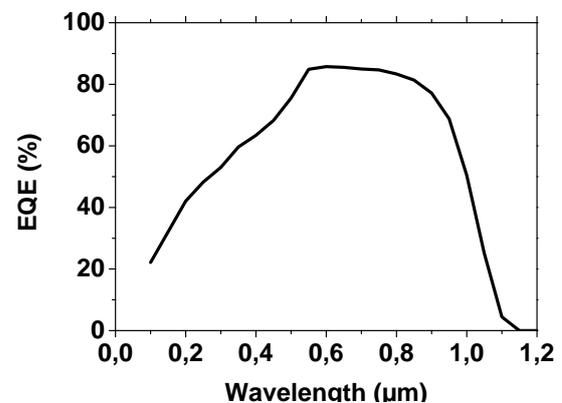

Fig. 2. The external quantum efficiency of the CIGS cell.

4.1. Impact of thickness of the CdS layer

In the simulation, the CdS layer thickness was ___ from 10 nm to 100 nm while the CIGS laye___ ness remained constant (350nm). Fig.3.(a) shows the effect on
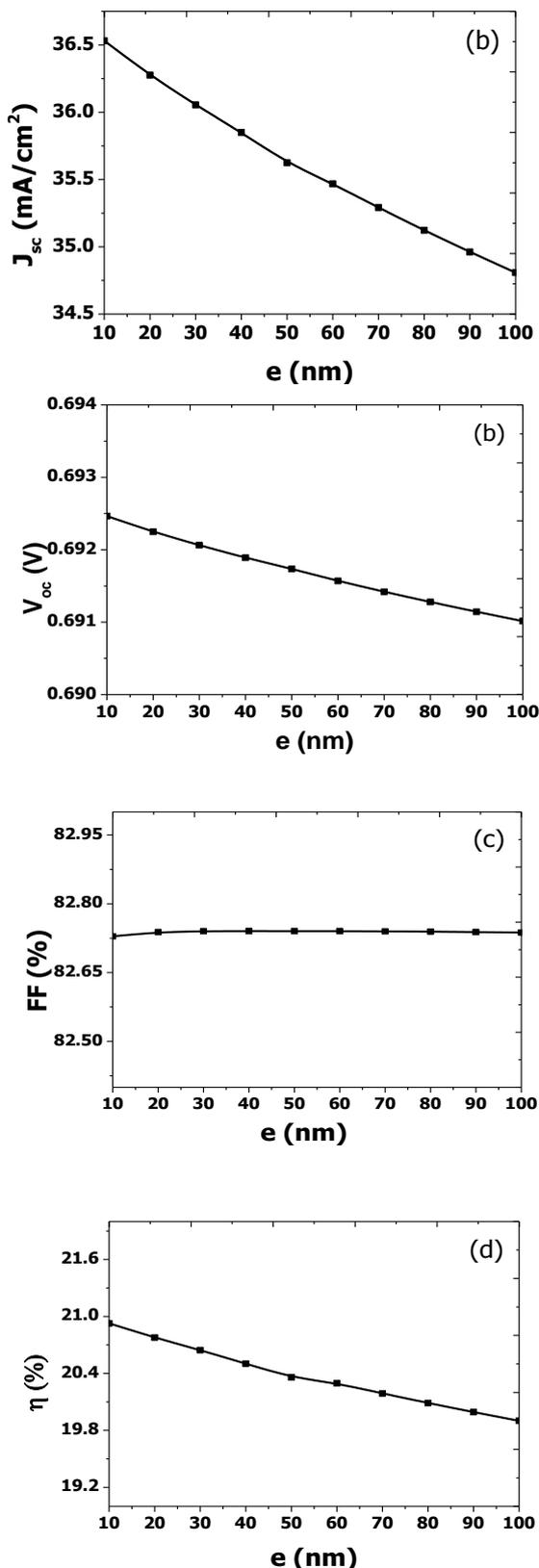

the short circuit current, this latter decreases with the increase of the thickness. In fig.3.(b) we displayed the influence on the open circuit voltage, it is clear that the thickness does not have much effect on V_{oc}. In fig.3. (c), the fill factor is nearly constant with the increase of the CdS thickness. It can be seen in fig.3.(d) that the efficiency decreases with the increase the CdS thickness. This is obviously due to the fact that with a thinner CdS layer, most of the photogenerated carriers are collected.When the thickness increases, the photons of short wavelengths are absorbed at a further distance of the CdS/CIGS junction. Though the CdS layer is characterized by defect states which act as recombination centres reduce the lifetime of the minority carriers(holes)and consequently the photogenerated carriers recombinebefore reachingthe junction. Therefore, there's a drop of the short circuit current, the open circuit voltage and the efficiency with the increase of the CdS thickness. These observations are fairly in agreement with simulation in [9]. Generally the thickness of the optimum CdS buffer layer should be within 50 nm and 60 nm [10].

The effect of the CdS layer thickness on the external quantum efficiency spectrum is illustrated in fig. 4. As mentioned earlier, when the thickness increases, more photons with shorter wavelength can be lost in the CdS layer. As expected, the higher the CdS thickness, the lower the external quantum efficiency. The external quantum efficiency for a thicker CdS layer is much lower for wavelengths below 0.6 μm.
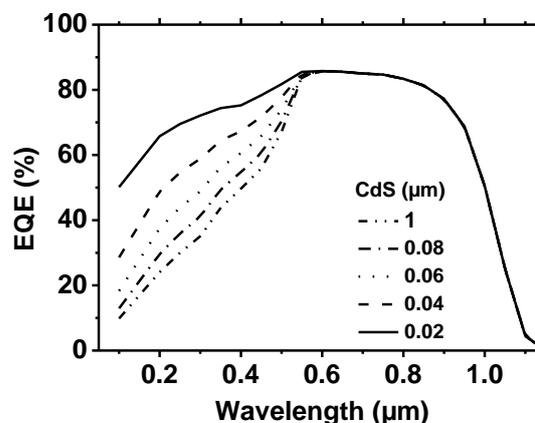

Fig.4. The external quantum efficiency for different thicknesses of CdS layer.

4.2. Impact of thickness of the CIGS layer

The photovoltaic parameters in terms of J_{sc}, V_{oc}, FF and η were simulated for the CIGS thicknesses varying from0.5 μm to 5μm and the CdS thickness isconstant (50 nm) (fig.5). We observe an increase of these parameters with the CIGS layer thickness. For the thickness equal to 0.5 μm, the efficiency is 13.64%. The highest efficiency of 21.08 % is reached for the thickness of 5 μm. The increase in the conversion efficiency is mainly due to the increase of the CIGS thickness. A possible explanation is that more the thickness increases, more photons with longer wavelengths can be collected in the CIGS layer. Therefore,

Fig.3. Relationship between CIGS solar cell parameters and CdS layer thickness

this will contribute to more generation of electron-hole pairs which
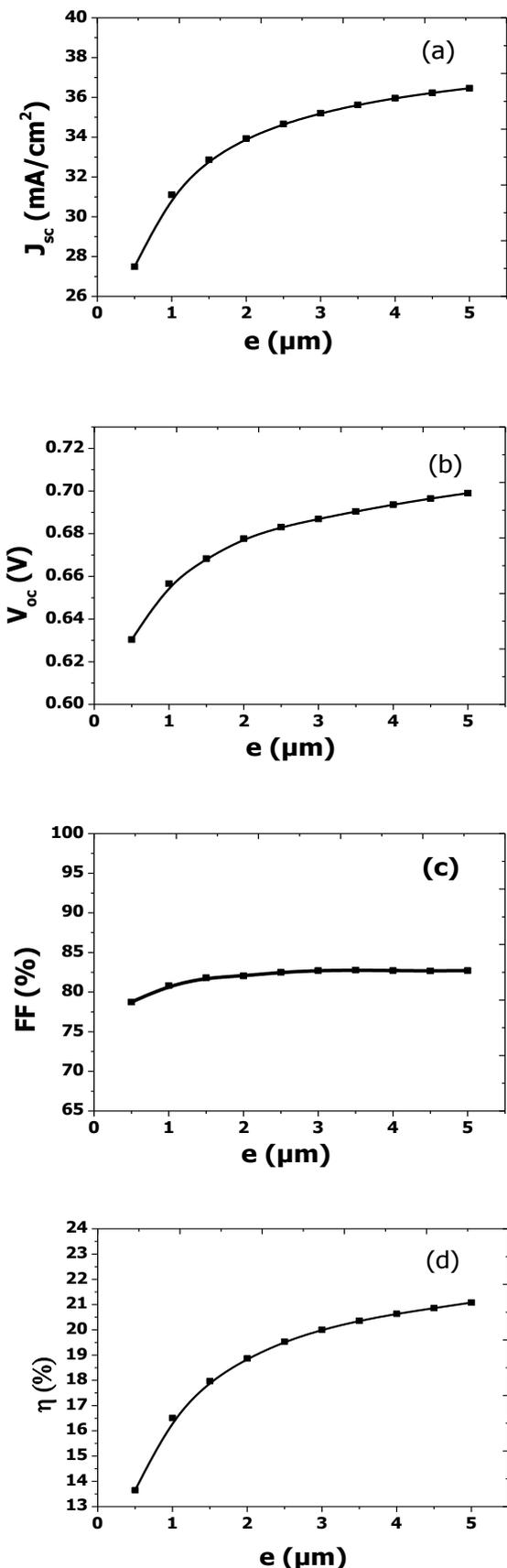
will increase the short circuit current, the open circuit voltage and the efficiency. A very thin CIGS layermeans physically that the backcontactand thedepletion region are very close. This effect more promotes the electron recombination at the back contact. This type of recombination is detrimental to the cell performance because it affects J_{sc}, V_{oc} and η. These observations are in good agreement with simulation in [9, 11].The external quantum efficiency also increases as the thickness of the CIGS layer increases (fig. 6). As mentioned previously when the thickness increases, more photons are absorbed, especially the long wavelengths of the illumination. Thus a greater number of electron–hole pairs would be produced from the absorbed photons. Therefore and as illustrated, the higher the CIGS thickness, the higher the external quantum efficiency for wavelengths above 0.55μm.
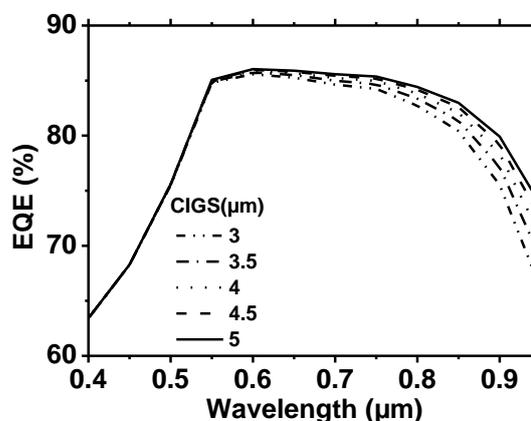

Fig.6. The external quantum efficiency for different thicknesses of CIGS layer.

5. Conclusion

Silvaco Atlas software was used in the simulation of the CIGS solar cell operating under AM1.5. It was shown that the numerical simulation is an important tool for understanding and achieving high efficiency CIGS solar cells. The numerical calculations provide not only a good understanding but they also allow us to predict ways to improve the efficiency. The simulation of the CIGS solar cell gives an efficiency of 20.35 % in good agreement with the experimentalhigh record efficiency of 20.3 % in the CIGS solar cell [6]. The effect of the CdS and CIGS thicknesses on the photovoltaic parameters and the external quantum efficiency were studied. It was found that the rise of the CdS thickness decreases all output parameters and the external quantum efficiency while the rise of the CIGS thickness improves all photovoltaic parameters and the external quantum efficiency. The highest efficiency of 21.08 % is reached for the CIGS thickness of 5 μm.

References

[1] Ullal HS, Zweibel K, Von Roedern B, Proc. 26th IEEE Photovoltaic Specialists Conf., Anaheim, CA, USA; 1997, p. 301.

Fig.5. Relationship between CIGS solar cell parameters and CIGS layer thickness.

[2] Yamaguchi M., J. Appl. Phys. **78 (**1995)1476.

[3] Bätzner DL, Romeo A, Terheggen M, Döbeli M, Zogg H, Tiwari AN,Thin Solid Films 451-452 (2004) 536-543.

[4]Tuttle JR, Szalaj A, Keane J, Proceedings of the 28th IEEE Photovoltaic Specialists Conference, Anchorage, 2000; 1042–1045.

[5] I.Repins, S. Glynn, J. Duenow, T.J. Coutts, W. Metzger, and M.A. Contreras, Conference Paper NREL/CP-520-46235, juin 2009.

[6] P. Jackson, D. Hariskos, E. Lotter, S. Paetel, R. Wuerz, R. Menner, W. Wischmann and M. Powalla, Prog. Photovolt. Res.Appl.19(2011)894-897.

[7] K. Ramanathan, M.A. Contreras, C.L. Perkins, S. Asher, S.F. Hasoon, J. Keane, D. Young, M. Romero, W. Metzger, R. Noufi, J. Ward, A. Duda, Prog. Photovolt: Res. Appl 11 (2003) 225.

[8] M.A. Contreras, B. Egaas, K. Ramanathan, J. Hiltner, A. Swartzlander, F. Hasoon, R. Noufi, Prog.Photovolt: Res. Appl 7 (1999) 311.

[9]Puvaneswaran Chelvanathan, Mohammad Istiaque Hossain, Nowshad Amin, Current Applied Physics 10 (2010) S387–S391.

[10] Yamamoto, Y. Saito, K. Takahashi, M. Konagai, Sol. Energy Mater. Sol. Cells 65 (2001)125–132.

[11] Nowshad Amin, Puvaneswaran Chelvanathan, M. Istiaque Hossain and Kamaruzzaman Sopian, Energy Procedia 15 (2012) 291 – 298.