

OPTIMIZATION OF COPPER INDIUM GALLIUM Di-SELENIDE (CIGS) BASED SOLAR CELLS BY BACK GRADING

S. OUEDRAOGO^{a,b}, R. SAM^a, F. OUEDRAOGO^a, M. B. KEBRE^a,
J.M. NDJAKA^b, F. ZOUGMORE^a

^a*UFR-SEA, Laboratoire de Matériaux et Environnement (LA.ME), Université de Ouagadougou, BURKINA FASO*

^b*Université de Yaoundé I, Faculté des Sciences, Département de Physique, B.P. 812 Yaoundé, CAMEROUN*

We performed modeling and simulation of Cu(In,Ga)Se₂ (CIGS) thin film solar cell, using SCAPS-1D device simulator, and we especially investigated the influence of absorber back surface region grading. The band-gap in the back surface region, as well as the thickness of the back surface grading layer, were varied to achieve the optimal performances. Based on these results, an optimal back-grading structure for Cu(In,Ga)Se₂ solar cell is proposed. It is shown that, the short-circuit current density (J_{sc}) improves with increasing the absorber band-gap in the back surface region. Very high J_{sc} of 32.72 mA/cm² was obtained, when the band-gap of the absorber near the back contact is 0.2 to 0.5 higher than the absorber bulk band-gap. The Open-circuit Voltage (V_{oc}), the fill factor (FF) and the efficiency (η) of the solar cell decrease for high band-gap near the back contact. The efficiency and the fill factor obtained for our model are respectively 16% and 75%. A comparison with published data for the Cu(In,Ga)Se₂ cells shows an excellent agreement.

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Keywords: Cu(In,Ga)Se₂; simulation ; back-grading

1. Introduction

CuInSe₂ based solar cells has shown good performance in photoconversion and long-term stability against exterior aggression [1,2]. The low consumption of materials, the energy used in the manufacturing process and the low cost of substrates or superstrates make CuInSe₂ based solar cells attractive in industrial and research fields [3]. This material has a direct band-gap and high absorption coefficient (10⁵cm⁻¹) [4], requiring only a few micrometers to absorb the maximum of incident photons. One of the most interesting qualities of this material is its band-gap, depending on its composition. The partial substitution of indium (In) in CuInSe₂ by gallium (Ga), commonly refer to as Ga-grading, to form CuIn_{1-x}Ga_xSe₂, affects the band-gap of the material according to the following equation [5] :

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

Where x represents the proportion of Ga i.e. the ratio Ga/(Ga+In), and b is the optical bowing parameter, for which values ranging between 0.11 and 0.24 have been reported [5]. By adjusting x , the band-gap can increase from 1.02 eV (CuInSe₂) to 1.68 eV (CuGaSe₂), which affects principally the conduction band level of the absorber Cu(In,Ga)Se₂ (CIGS) [5]. The probability of carrier recombination can be reduced by an additional electric field, which improves the separation of the free carriers [7,8].

* Corresponding author: ouedraogo@univ-ouaga.bf; ouedraogosoumaila81@yahoo.fr

The record performance of 20.3% [9] obtained for CIGS based solar cells are related to the intentional or unintentional graduation of the absorber. Usually three profiles of graduation are performed on CIGS based solar cells:

- i. Back grading, which consists to increase the conduction band level towards the back surface region of the absorber [11].
- ii. Front grading, the conduction band level of the absorber is increased near the junction [12]
- iii. Double grading, which combines (i) and (ii), has an increased band-gap both towards the back and the front contact [13].

Many works are unanimous on the beneficial effect of the absorber graduation on the solar cell performances [11,14]. However, the effect of Ga-grading on the electrical parameters of the solar cell is poorly understood. Some contradictions appear on the electrical parameters affected by the back-grading. Indeed, starting with several profiles of back-grading, the authors [12] show that the back-grading improves both the short-circuit current density (J_{sc}) and the open-circuit voltage (V_{oc}), while those of [5,14] show that no significant gain of the V_{oc} is obtained for devices with a standard thick CIGS layer (1.5-2 μm). The purpose of this work is to highlight by numerical simulations, the electrical parameters affected by the back-grading. SCAPS 3.0 software is used [15].

2. Material and methods

2.1 Structure of CIGS based solar cells

The structure of the studied solar cell is (Ni/Al) / MgF_2 / ZnO:B / i-ZnO / CdS / OVC / CIGS / Mo / substrate (fig.1). The fundamental parts of the cell are the absorber (CIGS) and the buffer layer (CdS). The layer between the absorber and CdS is a thin layer called OVC (ordered vacancy compound). This indefinite layer, difficult to define is formed by the interface states between the buffer layer and the absorber [16]. An intrinsic (i-ZnO) and Boron-doped ZnO (ZnO:B) layers are deposited at the top of the buffer layer. These two layers are commonly known as transparent conductive oxide (TCO) because of their wide band-gap which makes them transparent to most part of the solar spectrum. The surface of the TCO layer is covered with an antireflection layer MgF_2 , thus increasing the absorption of the photons in the absorber

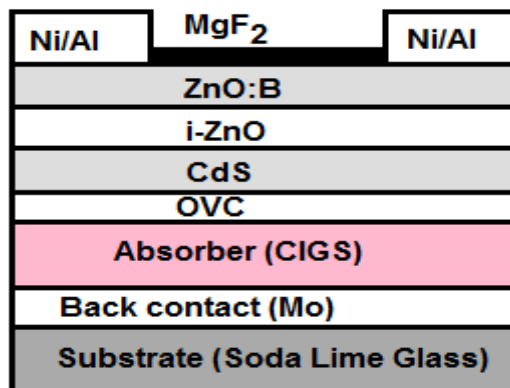


Fig. 1 : Structure of the solar cells used in the simulation

2.2 Phenomenological parameters of CIGS based solar cells and numerical simulation

CIGS polycrystalline based solar cell is a complex structure given the number of layers (higher than six), and the effects of some particular phenomena, mechanisms or materials parameters are often beyond intuition. Numerical simulation 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 numerical simulation can be used to analyze the effect of the variation of material parameters i.e. the presence or absence of particular properties, or variations of all properties in the range of values, to obtain the optimal values for optimizing the solar cells efficiencies.

Several softwares have been developed to simulate the functioning of thin film solar cells. Among these include SCAP-1D [15], which is widely used in the simulation of CIGS and CdTe based solar cells. The good agreement between the simulation results and those of experiments [17] motivates 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 the Poisson equation, the 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)/buffer layer (CdS) interface, donor defects were placed 0.2 eV below the conduction band. These have 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 experimental work [6] and numerical models [18,19]. The influence of the series resistance and shunt resistance are not taken into account. The 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. The OVC layer differ to the bulk CIGS by the following values of parameters:

- Thickness: 30 nm,
- Band-gap (E_g): 1.3 eV,
- Electron mobility (μ_e): 10 cm/V.S,
- Carrier density (N): 10^{12} cm⁻³

Table 1: CIGS baseline input parameters used for this simulation.

Parameters	CIGS	CdS	i-ZnO
Layers thickness (nm)	3000	50	200
Dielectric constant	13.6	10	9
Electron affinity (eV)	4.5	4.2	4.45
Band-gap (eV)	Varied	2.4	3.3
Effective conduction band density (cm ⁻³)	$2.2 \cdot 10^{18}$	$2.2 \cdot 10^{18}$	$2.2 \cdot 10^{18}$
Effective valence band density (cm ⁻³)	$1.8 \cdot 10^{19}$	$1.8 \cdot 10^{19}$	$1.8 \cdot 10^{19}$
Electron thermal velocity (cm/s)	$1.0 \cdot 10^7$	$1.0 \cdot 10^7$	$1.0 \cdot 10^7$
Electron thermal velocity (cm/s)	$1.0 \cdot 10^7$	$1.0 \cdot 10^7$	$1.0 \cdot 10^7$
Electron mobility (cm ² v ⁻¹ s ⁻¹)	100	100	100
Hole mobility (cm ² v ⁻¹ s ⁻¹)	25	25	25
Doping concentration of acceptors (cm ⁻³)	$2.0 \cdot 10^{16}$	0	0
Doping concentration of donators (cm ⁻³)	0	10^{17}	10^{18}
Defects			
Type of defects	neutral	neutral	neutral
Total density of defect (cm ⁻³)	$1.0 \cdot 10^{14}$	$1.0 \cdot 10^{18}$	$1.0 \cdot 10^{17}$
Electrons capture cross section (cm ²)	$5.0 \cdot 10^{-13}$	$1.0 \cdot 10^{-17}$	$1.0 \cdot 10^{-12}$
Electrons capture cross section (cm ²)	$1.0 \cdot 10^{-15}$	$1.0 \cdot 10^{-12}$	$1.0 \cdot 10^{-15}$
Energetic distribution	Gaussian	Gaussian	Gaussian
Defect energy level	Mid-gap	Mid-gap	Mid-gap

To better understand the effect of the back-grading, the absorber is divided in two parts as shown in fig.2. The first part, the bulk of the absorber, has a thickness d and constant band-gap of 1.15 eV, which correspond to a $Ga/(Ga+In) = 0.3$. The second part, near back contact has a band-

gap linearly increasing from 1.02 eV (pure CuInSe₂) to 1.68eV (pure CuGaSe₂) and represents the back surface grading layer. Its thickness is denoted by d_{grad} . CB and VB in Fig.2. denote respectively the conduction band and the valence band of the absorber. The back-grading shifts the minimum of the conduction band value. The schematic energy band diagram of CIGS solar cells with back-grading is shown in fig.3. The conduction band minimum E_c is changed for a CIGS layer with an increase Ga concentration towards the back contact.

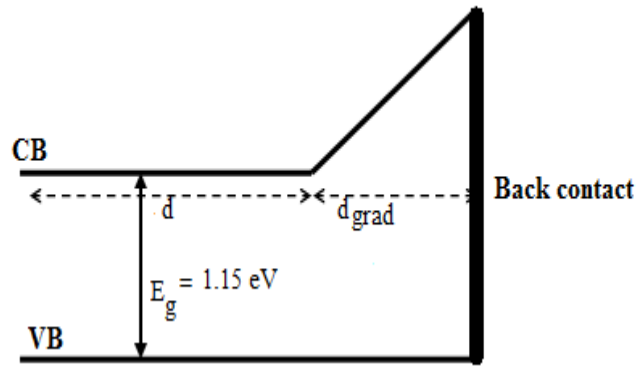


Fig.2: Simulated absorber layer band-gap profile. The band-gap variation at the back surface region shifts the minimum of the conduction band value

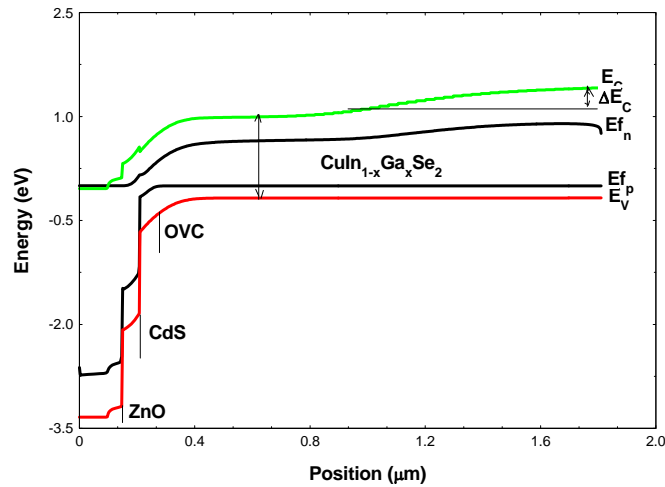


Fig.3: Band edge diagram of CIGS based solar cells, where the conduction band minimum E_c is changed for a CIGS layer with an increase Ga concentration towards the back contact.

3. Results and discussion

3.1 Influence of band-gap variation ΔE_g

The difference between the minimum band-gap E_g in the bulk absorber CIGS and the maximum $E_{g\text{back}}$ close to the back contact defines the quantity ΔE_g . The resulting performance parameters of open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF) and conversion efficiency are determined using current density-voltage (J-V) characteristics. Fig. 4 shows the influence of band-gap variation and the surface recombination velocity (V_R) on these parameters. The short-circuit density (J_{sc}) of the device seem to be more affected by back-grading.

Initially, J_{sc} is enhanced with the increase of the band-gap of the absorber near the back contact from $\Delta E_g = 0$ to 0.5 eV and is dramatically decreased for $\Delta E_g > 0.5$ eV. The gain of the J_{sc} is about 3% due to the back grading. The interface CIGS/Mo is expected to have a relatively high recombination; it would be desirable to keep the photoelectrons away from this interface. A quasi-electrical field can be established in the back region of the CIGS layer due to back-grading. This quasi-electrical field can keep a high conductivity for the majority holes and at the same time reject the minority electrons, which allows to increase the short-circuit current density for $0 < \Delta E_g < 0.5$ eV. For high Ga content, $\Delta E_g > 0.5$ eV, the decrease of the J_{sc} should be due to the increase of defect near the Mo.

The open-circuit voltage (V_{oc}), the fill factor (FF) and the efficiency of the device have the same trend with increasing the barrier high ΔE_g . For $\Delta E_g < 0.3$ eV, these electrical parameters are substantially constant, and systematically decreases when $\Delta E_g > 0.3$ eV, due to the high defect near back contact.

Fig.4 also shows that back surface recombination velocity (V_R), which increases the recombination mechanisms near the back contact, can be reduced by the back grading. No evident aspect of increasing back recombination velocity is observed on the electrical parameters. The V_{oc} , FF and the efficiency of the device follow the same trend with increasing the back contact surface recombination velocity. For $\Delta E_g < 0.5$, only the short-circuit current density increases when $V_R < 10^5$ cm/s eV, since the reduction of the surface recombination velocity reduces the surface recombination rate and therefore leads to an improve of J_{sc} .

Attempts are made to compare the simulation results with the reported experimental data [6] for CIGS solar cells with back grading. Fig.4 shows good correlation between simulated electrical parameters (V_{oc} , J_{sc} , FF, efficiency) and the experimental values, especially for conversion efficiency and the short-circuit density (J_{sc}). Discrepancies observed should be related to the use of boron doped ZnO (ZnO:B) layer as transparent conductive oxide (TCO) in place of the conventional ZnO:Al. Hagiwara et al. [20] have demonstrated that, the ZnO:Al has absorption losses, leading to a decrease of the quantum efficiency of the solar cells in the near infrared regions. Even though the values of the simulation are slightly different to the experimental ones, we find that the main tendencies of the experimental data are reproduced by the simulation.

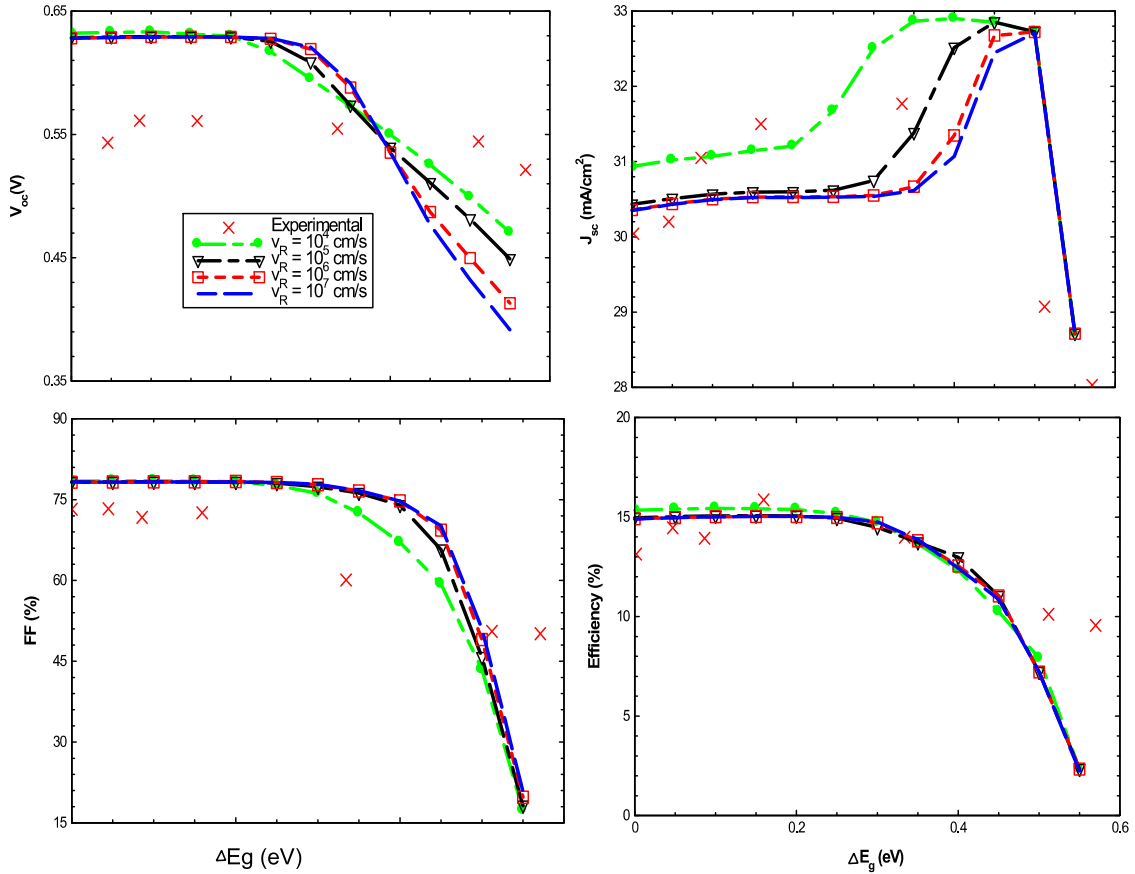


Fig.4. The solar cell output parameters depend on barrier height ΔE_g

3.2 Influence of the absorber back surface region band-gap and its thickness

A proper optimization of the back surface grading layer can significantly improve the performances the solar cell. In this section, the band-gap variation ΔE_g in the back surface region and the thickness of the back surface grading layer d_{grad} have been varied to achieve the optimal performance. Current-voltage parameters for $E_g = 1.15$ eV, $\Delta E_g = 0-0.5$ eV, and $d_{grad} = 0-0.6$ μm are shown in Fig. 5. The performances of the devices are shown in term of V_{oc} , J_{sc} , FF and efficiency. It is quite obvious from the figure that, the short-circuit current density increases with increasing d_{grad} . The increase of the J_{sc} is mainly due to the increase in the p-type CIGS absorber layer. As the p-type layer is increased, more photons with longer wavelengths can be collected in the absorber. The open-circuit current density (V_{oc}), fill factor (FF) and efficiency decrease steadily with increasing d_{grad} . The optimal values for d_{grad} and ΔE_g are in the range 0.1– 0.3 μm and 0.2–0.4 eV respectively, which lead to high performances of the solar cells. The efficiency and fill factor (FF) obtained under these conditions for our model are respectively about 16% and 75%.

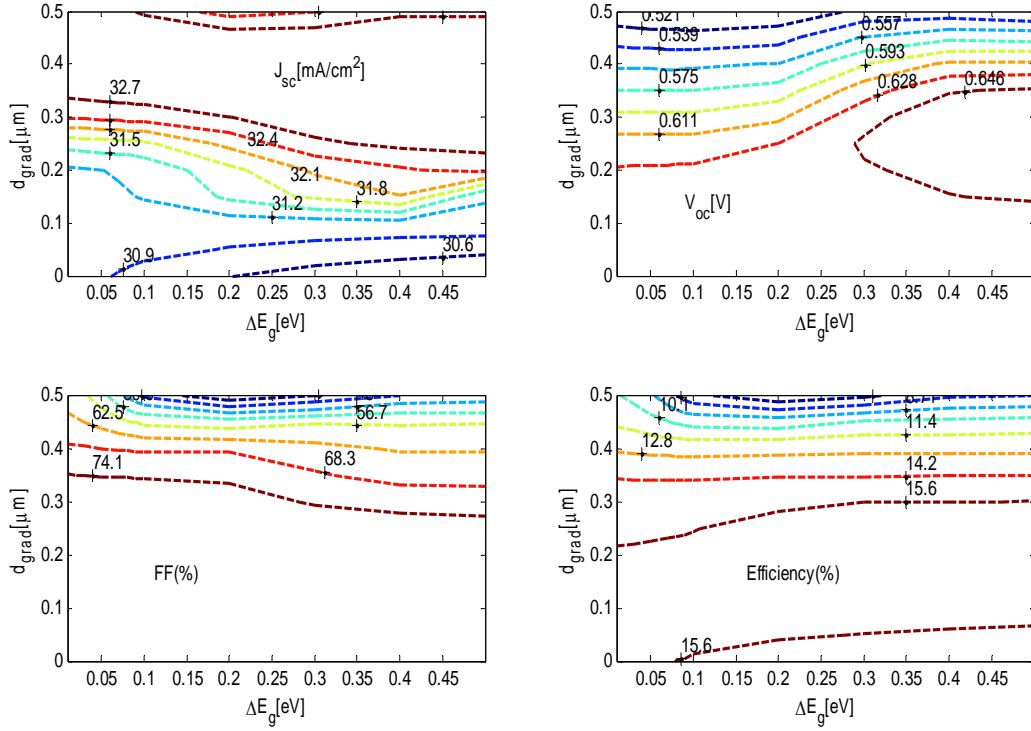


Fig.5: The short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF) and conversion efficiency of the solar cells as function of the back surface region band-gap variation ΔE_g and the thickness of the back surface grading layer d_{grad}

3.3 Influence of the Cu(In,Ga)Se₂ bulk thickness and the absorber back surface grading layer thickness variation

The standard thickness of the Cu(In,Ga)Se₂ (CIGS) layer is about 1.5–2 μm [21]. If this thickness could be reduced, with no, or only minor, loss in performance, production cost could be lowered and the materials usage would reduce. The reduction of the absorber thickness is, however, associated with a number of problems such as the reduction of the light absorbed in the CIGS layer. Another potential problem for thinner CIGS layer is that, electrons will be generated closer to the back contact (Mo) with higher probability for back contact recombination. By using graded compositional profiles towards the back contact, an additional drift field is obtained due to the band gap variation that assists carrier collection and reduces back contact recombination. This motivated us to study in this section the effect of the absorber thickness d and d_{grad} on the solar cell performance. The absorber bulk band gap is fixed to $E_g = 1.15$ eV and its thickness d , is varied in the range from 0.5 μm to 2 μm . The absorber back surface band gap is taken as 0.3 eV larger than the absorber bulk band gap, i.e. $\Delta E_g = 0.3$ eV and its thickness is varied from 0 μm to 0.5 μm . Fig.6 shows the simulated CIGS solar cell performances with d and d_{grad} . The efficiency of the device increases with increasing the absorber bulk thickness d . This gain is mainly due to an increased J_{sc} , which varies from 29 mA/cm² for $d = 0.5$ μm to 32.2 mA/cm² for $d = 2$ μm , i.e. a gain of 3.2 mA/cm². The FF and V_{oc} increase with increasing d due to an increased light absorption and the reduction of the back contact recombination. Fig. 6 also shows that the performances of the devices are strongly depend on d_{grad} . FF, V_{oc} show a negligible decrease with large d_{grad} . A small increase is observed for $d_{grad} < 0.2$ μm . For thicknesses of the absorber d exceeding 1 μm , the effect of d_{grad} on the solar cells performances is more pronounced, since the thickness of the absorber is thick enough that the absorption takes place in the bulk of the absorber, far from CIGS/Mo interface. The thickness of the absorber near the back contact d_{grad} becomes more important when d is more than 0.5 μm . The net gain of the efficiency is 7%. This is a serious track to reduce the absorber thickness without affecting the performance of the device.

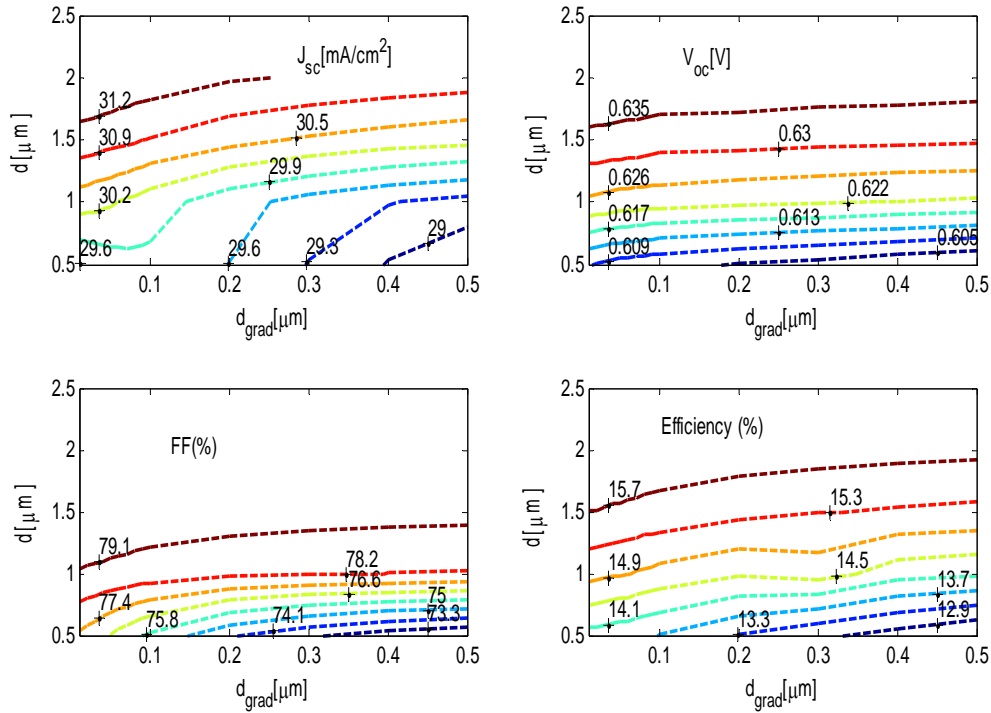


Fig. 6: The short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF) and conversion efficiency of the solar cell as function of the absorber bulk thickness d and the thickness of the back surface grading layers d_{grad}

4. Conclusion

In the present study, the role of the absorber back surface grading is investigated numerically by one dimensional SCAPS-1D computer software. In the simulation studies, the band-gaps in the back surface region, the thickness of the back surface grading layer and the absorber bulk thickness are varied to achieve optimal performances. We showed that back surface grading greatly improves the performances of CIGS, especially, the short-circuit current density which shows an effective gain of 3% due to the reduction of back contact recombination. High performances of $\text{Cu}(\text{In,Ga})\text{Se}_2$ solar cell are obtained, when the variation of band-gap ΔE_g of the back surface region is in the range 0.2–0.4eV higher than the absorber bulk band-gap and its thickness is in the range 0.1–0.3 μm . The efficiency and the fill factor obtained for our model are respectively 16% and 75%. Comparison with published experimental data shows good correlation with simulated values. Discrepancies should be related to some solar cell characteristics, such as serie and shunt resistances neglected in this study, and the use of (ZnO:B) layer as transparent conductive oxide (TCO) in place of the conventional ZnO:Al. Further studies should be focused on numerically and experimentally double and front grading case.

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