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Simulation of High Efficiency CIGS solar cells with SCAPS-1D software

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Abstract

In this paper, the high efficiency Cu(In,Ga)Se₂ (CIGS)-based solar cells was analyzed and designed by SCAPS-1D software. This paper deals with the influence of a buffer layer on the performance of the CIGS-based solar cells. The photovoltaic parameters have been calculated in different buffer layer materials (CdS, ZnS, ZnSe), we give great alternative for Cadmium sulphide (CdS). Starting with a good structure, we simulated the J-V characteristics and showed how the absorber and buffer layers thickness, defect density influence the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and efficiency (η) of solar cell. The optimized solar cell shows an efficiency of > 22% under the AM1.5G spectrum and one sun.

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Keywords: Solar cells; Cu(In,Ga)Se₂; Photovoltaic parameters; buffer layer ;defect density; SCAPS-1D

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1. Introduction

Copper indium gallium (di) selenide Cu(In,Ga)Se_2 (CIGS) is a I-III-VI₂ semiconductor material composed of copper, indium, gallium, and selenium. The material is important for terrestrial applications because of their high efficiency, long-term stable performance and potential for low-cost production. Thin film solar-cells with polycrystalline Cu(In,Ga)Se_2 (CIGS) absorber layers provide a good alternative to wafer based crystalline silicon solar cells, which currently constitute the major share of photovoltaics installed and used worldwide. The CIGS based solar cells exhibit excellent outdoor stability, radiation hardness and highest efficiencies (19.2%) [1-4].

These compounds are direct bandgap semiconductors which minimize the requirement for long minority carrier diffusion lengths. Such p-type semiconductors with high absorption coefficient are the promising absorbing materials for thin film photovoltaic technology [5]. Buffer layer is an intermediate layer film between the absorber and window layers with two main objectives, to provide structural stability to the device and to fix the electrostatic conditions inside the absorber layer [6]. Cadmium sulphide (CdS) is a prominent candidate to be used a buffer layer in Cu(In,Ga)Se_2 based solar cell. Note that Cadmium (Cd) is a metal that can cause severe toxicity in humans and the environment.

In this work, we present a numerical study of the thin film CIGS-based solar cells with SCAPS, is used to calculate the photovoltaic parameters (J_{sc} , η , V_{oc} and FF) under standard illumination (AM1.5G, 100 mW/cm², 300K). We study the influence of a buffer layer on the performance of the CIGS solar cells. The J-V characteristic has been calculated in different buffer layer materials (CdS, ZnS, ZnSe). The purpose is to replace the CdS by Other materials like Zinc Sulphide (ZnS) and Zinc Selenide (ZnSe). At last, we examine the effects of defect density on the photovoltaic parameters (J_{sc} , η , V_{oc} and FF).

2. Numerical Modeling and Material Parameters

A typical CIGS-based solar cell structure consists of a p-type wide-band gap absorber layer (CIGS) which is deposited on the Molybdenum (Mo) coated back glass substrate. An n-type buffer layer made of n-CdS(CdS, ZnS, ZnSe) and window layer made of n-ZnO:Al. The cell is illustrated schematically in Fig. 1.

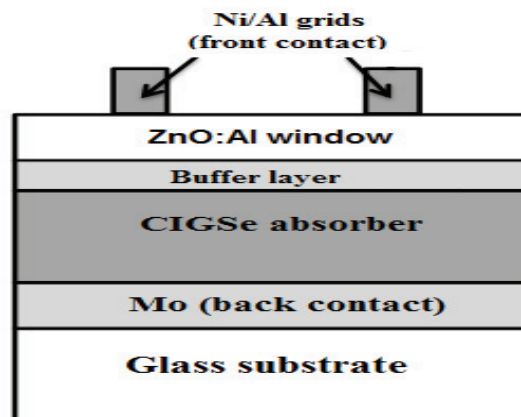


Fig. 1. Schematic structure of a CIGS solar cell.

In this paper, we use the Solar Cell Capacitance Simulator structures (SCAPS-1D) to analyse the CIGS-based solar cells. SCAPS is a one-dimensional solar cell device simulator, developed at ELIS, University of Gent, which is freely available to the PV research community [7-9].

SCAPS is capable of solving the basic semiconductor equations, the Poisson equation and the continuity equations for electrons and holes (Eqs. (1)- (3)) [10, 11]:

$$\frac{d^2}{dx^2} \psi(x) = \frac{e}{\epsilon_0 \epsilon_r} (p(x) - n(x) + N_D - N_A + \rho_p - \rho_n) \quad (1)$$

Where ψ is electrostatic potential, e is electrical charge, ϵ_r is relative and ϵ_0 is the vacuum permittivity, p and n are hole and electron concentrations, N_D is charged impurities of donor and N_A is acceptor type, ρ_p and ρ_n are holes and electrons distribution, respectively. The continuity equations for electrons and holes are :

$$\frac{dJ_n}{dx} = G - R \quad (2) \quad \frac{dJ_p}{dx} = G - R \quad (3)$$

Where J_n and J_p are electron and hole current densities, R is the recombination rate, and G is the generation rate. Carrier transport in semiconductors occurs by drift and diffusion and can be expressed by the equations:

$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx} \quad (4) \quad J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\phi}{dx} \quad (5)$$

SCAPS calculates solution of the basic semiconductor equations in 1 dimensional and in steady state conditions.

The parameters used for simulations of a standard CIGS-based solar cell are summarized in the following table1.

Table 1. The parameters for the CIGS-based solar cell at 300K.

Parameters	CIGS	ZnO :Al	CdS	ZnS	ZnSe
Eg(eV)	1.5	3.5	2.4	0.06	0.08
ϵ_r	13.6	9	10	10	10
χ (eV)	4.5	4.65	4.2	3.5	2.9
μ_n (cm ² V ⁻¹ s ⁻¹)	100	100	100	50	50
μ_p (cm ² V ⁻¹ s ⁻¹)	25	25	25	20	20
Nc (cm ⁻³)	2.2.10 ¹⁸	2.2.10 ¹⁸	1.5.10 ¹⁸	1.5.10 ¹⁸	1.5.10 ¹⁸
Nv (cm ⁻³)	1.8 .10 ¹⁹	1.8 .10 ¹⁹	1.8.10 ¹⁹	1.8.10 ¹⁸	1.8.10 ¹⁸
Vt(cm/s)	1.10 ⁷	1.10 ⁷	1.10 ⁷	1.10 ⁷	1.10 ⁷
Vt (cm/s)	1.10 ⁷	1.10 ⁷	1.10 ⁷	1.10 ⁷	1.10 ⁷

3. Results and discussion

3.1. Effect of buffer layer on the J-V characteristics

Fig.2 shows the simulated characteristics J-V, with the AM1.5 illumination conditions (100mW/cm²), for different buffer layer. The table 2 includes all the photovoltaic parameters (I_{SC} , η , V_{OC} and FF) of the CIGS-based solar cell with different buffer layer. From these figure, one can notice that solar cells with CdS and ZnS as buffer

layer gives high conversion efficiency. As for the solar cell buffer With ZnSe layer had the least conversion efficiency.

Table 2. The photovoltaic parameters for the CIGS-based solar cell for different buffer layer.

	CdS	ZnS	ZnSe
V _{oc} (V)	0.668	0.668	0.669
J _{sc} (mA /Cm ²)	35.76	36.42	36.02
FF %	80.48	81.30	50.33
η %	19.23	19.80	12.13

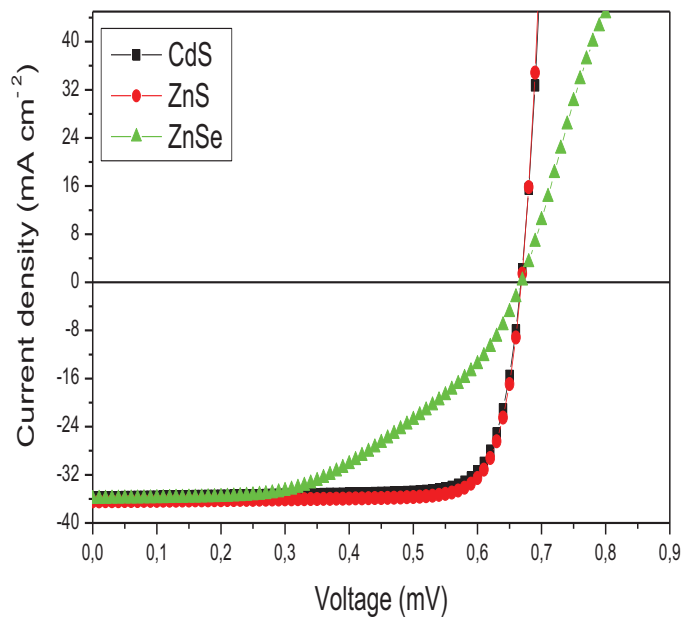


Fig. 2. J-V characteristics of cells with different buffer layer.

3.2. The thickness effects on the photovoltaic parameters

The analysis of all the results shows that the best photovoltaic parameters (J_{sc} , η , V_{oc} and FF) are obtained with ZnS buffer material. For achieving the best the photovoltaic parameters (J_{sc} , η , V_{oc} and FF) of a solar cell, the thickness of the p-CIGS, n-ZnS region then should be optimized, without defects.

We begin the simulation by changing the thickness of the absorber layer from 1 to 2, 5 μm and the thickness buffer layer was changed from 10nm to 90nm (see Table 2). We observed also from Table 3 that the best photovoltaic parameters obtained for 2, 5 μm for the thickness of absorber layer and 10nm for the thickness buffer layer.

Table 3. The thickness effects on the photovoltaic parameters for the cigs solar cell.

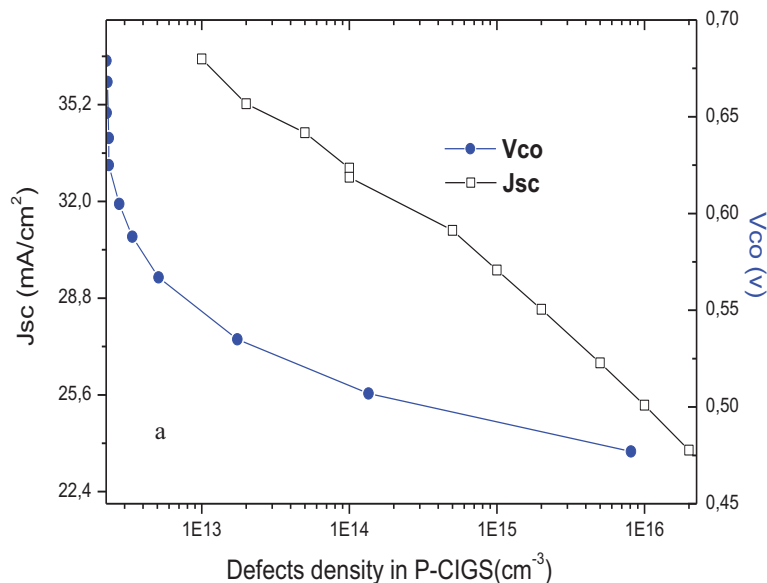
Absorber layer p-CIGS				
Thickness(μm)	V _{co} (V)	J _{sc} (mA /cm ²)	η %	FF %
1	0,683	36,45	20,75	83,27
1,5	0,687	37,23	21,36	83,46
2	0,690	37,71	21,78	83,60
2,5	0,693	38,06	22,11	83,71
Buffer layer n-ZnS				
Thickness(nm)	V _{co} (V)	J _{sc} (mA /cm ²)	η %	FF %
10	0,693	38,13	22,16	83,73
30	0,693	38,08	22,12	83,71
50	0,693	38,06	22,11	83,71
90	0,693	38,04	22,10	83,70

The cell with thinner buffer layer shows higher performance, thicknesses less than 40nm currently is not reachable because of fabrication techniques and instruments limitation. Thus, the range of 40nm to 50nm is the preferred and the optimized thickness of the buffer layer in CIGS-based solar cell [12].

3.3. Effects of defect density in CIGS thin film solar cell

After the optimization of cell thickness without defects state, the photovoltaic parameters by assuming the defects in the region p-CIGS and n-ZnS have been calculated.

Effects of defect state in p-CIGS and n-ZnS are shown in figs.3 (a,b) and Figs.4 (a,b). The location of the defect density is theoretically changed from the bottom of the conductivity band to the top of the valance band.



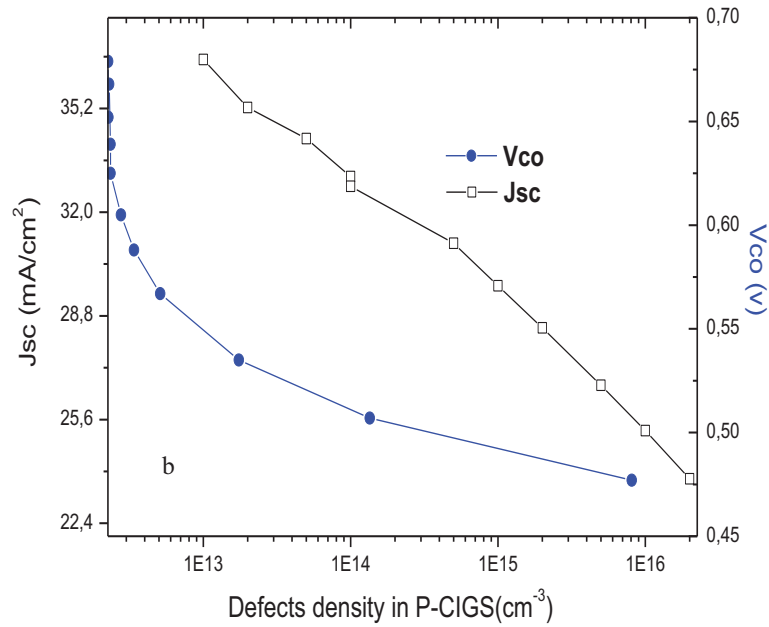
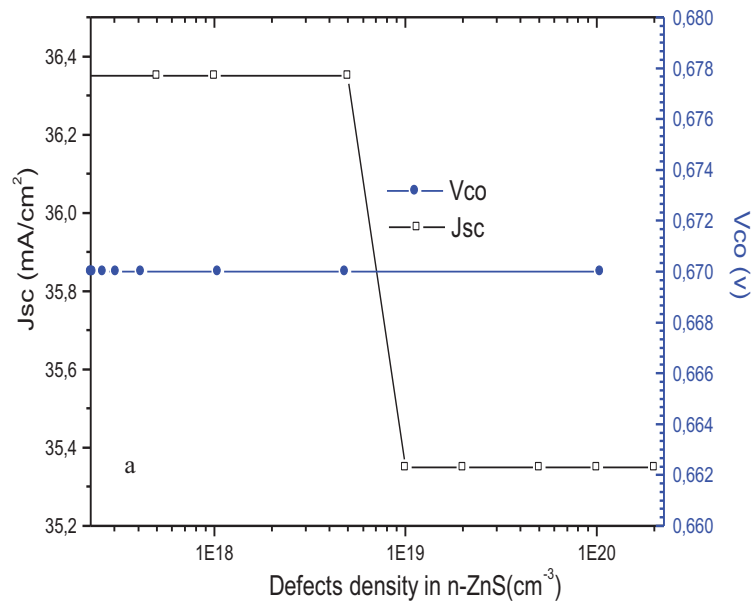


Fig. 3 (a,b). Variation of J_{sc} and V_{oc} and (b) Efficiency and FF in CIGS-based solar cell as a function of natural defects density in p-CIGS layer.



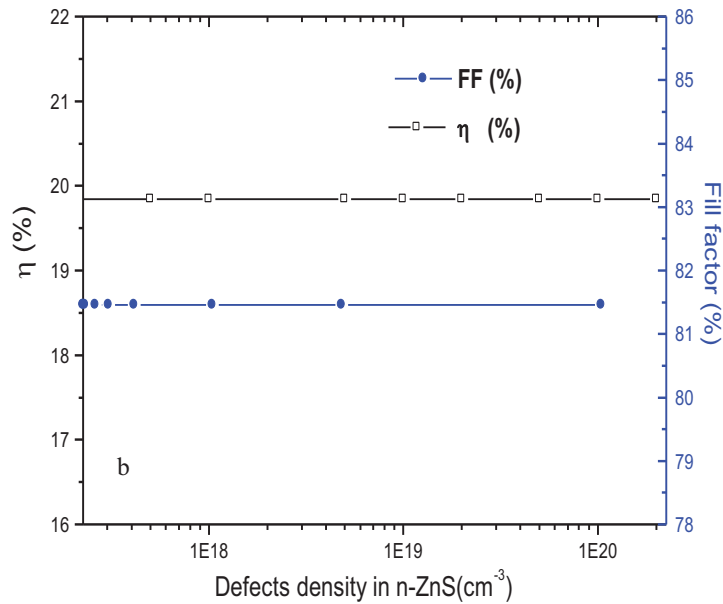


Fig.4 (a,b). Variation of J_{sc} and V_{oc} and (b) Efficiency and FF in CIGS-based solar cell as a function of natural defects density in n-ZnS layer.

From figs.3 (a,b) , we note that the best photovoltaic parameters is obtained for a Effects of defect density in from 1.0×10^{13} to $1.0 \times 10^{14} \text{ cm}^{-3}$. It is shown that V_{oc} and J_{sc} are degraded by increasing the defect density because of the recombination with the localized energy levels which is created by defects and it reduces the conversion efficiency of the solar cell. We observed that the conversion efficiency η decrease with increasing the defects density in p-CIGS layer.

Figs.4 (a,b) shown the effects of defect density in n-ZnS . We observed that the defect density is idealized from 1.0×10^{17} to $1.0 \times 10^{19} \text{ cm}^{-3}$. We also note that defect density in n-CdS layer always have little effect on J_{sc} , As for V_{oc} , η and FF no change was observed.

3.4. Current–voltage simulation

Fig.5 shows the simulated characteristics J-V with and without defects state, with the AM1.5 illumination conditions (100 mW/cm^2).

The fig.5 represents the current voltage characteristics with and without defects density for the CIGS thin film solar cell. We observe that the photovoltaic parameters (J_{sc} , η , V_{oc} and FF) decrease when we added the defects density.

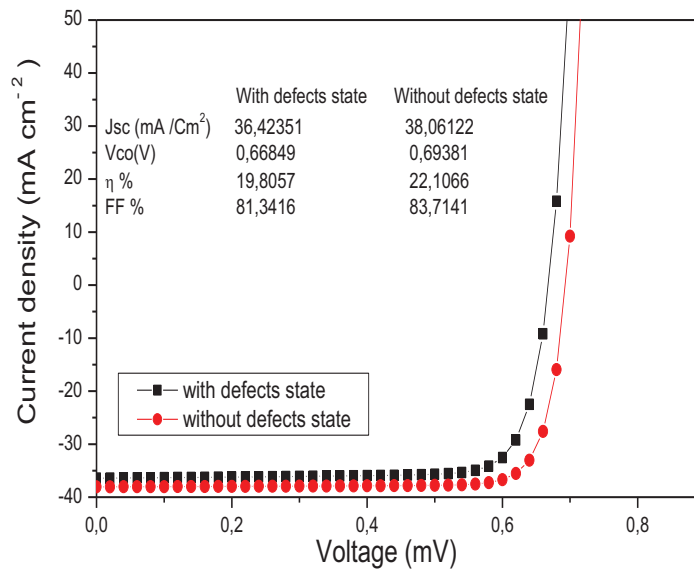


Fig.5.The J–V characteristic of the CIGS-based solar cell with and without defects.

4. Conclusion

In this investigation, we study the performance of the CIGS-based solar cells. The CdS buffer layer is replaced by other materials like Zinc Sulphide (ZnS) and Zinc Selenide (ZnSe). We concluded that ZnS can be used as alternative material to CdS. We have also demonstrated in this study, that the variation in the thickness of the absorber layer (and buffer layer) and of defect density in p-CIGS layer and n-ZnS layer affect the conversion efficiency.

The photovoltaic parameters (J_{sc} , η , V_{oc} and FF) have been calculated and it was found that optimized value of the cell thickness is 2.5 μm for p-CIGS layer and 50nm for n-ZnS layer. For the defect density, we can also say that have a significant impact on the performance of CIGS-based solar cells. High defect density in p-CIGS layer lead to pronounced decrease in the photovoltaic parameters (J_{sc} , η , V_{oc} and FF). In n-ZnS layer we note no effect of this defect density on the photovoltaic performance in particular (η , V , and FF), as for short circuit current J_{sc} is degraded by increasing the defect density. We have used a simulation of CIGS thin film solar cell via SCAPS-1D.

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