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Investigation of the effect of thickness, band gap and temperature on the efficiency of CIGS solar cells through SCAPS-1D

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Abstract— **In this paper, we present numerical simulations results of a Copper Indium Gallium diselenide thin-film solar cell (or CIGS cell) using the SCAPS-1D simulations code. We investigate the effect of absorber thickness, band gap and temperature on cell performances parameters. We have shown that the electric property of solar cell such as : the fill factor, the tension in open circuit, the short circuit current density and the power conversion efficiency are affected by variations of cell thickness, band gap and temperature. The best efficiency performance of 23.26% is obtained with a 1.4 □m thickness of the absorber layer and at temperature 260K.**

Index Terms— **Solar cells, CIGS, Numerical simulation, SCAPS-1D.**

I. INTRODUCTION

The photovoltaic market knew a strong grow in the last few years. Although various sectors and technologies splits the market, the cells containing Silicon dominates it with more than 85%, this is due primarily to the maturity of the nanoelectronic industry which uses massively the Silicon and good performance of the cells. However, the many steps of production make this material technology expensive and greedy, which justifies the interest to develop the cells in less expensive thin layers. In addition CIGS cells offer many advantages: Cells CIGS are fabricated sonochemically [1], offer a significant absorption capacity which requires 100 times less material (~1μm) than the Silicon cells (~100μm), and they can be deposited on various types of substrates (flexible or rigid) of large [2].

Furthermore, different conversion efficiencies of CIGS cells are mentioned in the literature [3-10]. By changing the material of the buffer layer, the most efficient CIGS/CdS thin film solar cell with a flexible polymer has achieved 20.4% efficiency [11]. The efficiency improvement from 20.4% to over 22% [12] or even 25% with adding an extra layer of SnS [13] are found by different research groups. All these efficiency records were obtained from CIGS solar cells with the CdS buffer layer. Despite the high efficiency level of the CIGS/CdS buffer layers the development of Cd-free buffer layers is one of the main objectives in the field of CIGS thin film solar cells. This is mainly because of CdS toxicity [14] and its incompatibility with in-line vacuum-based production methods [6].

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In this work, we used the code of simulation SCAPS-1D to examine the performances of the solar cells containing Copper indium gallium (di)selinide (CIGS). We carried out a series of studies of the parameters of the cells according to the thickness of the absorbing layer, energy of the band gap and the temperature in order to improve them.

The solar spectrum AM 1.5G with an intensity of 1 kw/m2 and temperature between 260 K and 360 K are used in our simulations

II. MODELING OF THE DEVICE

A. Method of simulation

SCAPS-1D stands for "Solar Cell Capacitance Simulator one-dimensional" is a one-dimensional solar cell device simulator, developed at ELIS, University of Gent, which is freely available to the PV research community [15-17]. This program is designed for simulation of photonic devices such as CdTe and CIGS cells. An unlimited number of layers can be modelled with SCAPS-1D, which makes it sufficiently flexible to optimize the performance of conversion of the solar cells. This code is based on the two equations of continuity of the holes and the electrons and the resolution of the Poisson's equation which are used to describe the phenomena of transport in a device-based semiconductor.

In absence of a magnetic field and in the one-dimensional case, the Poisson's equation connecting the potential to the densities of the charge carriers is given by:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{q}{\varepsilon}\left[-n(x) + p(x) - N_A^- + N_D^+ + \rho(n,p)\right] = 0 \qquad \text{(Eq.1)}$$

Where is the electrostatic potential at the point x, ε is the permittivity ; N, p, ρ are the concentration of the free electrons, that of the free holes and the density of the charge carriers respectively; N_D^+ and N_A^- are the densities of the ionized donors and acceptors ; q is the electron charge.

At steady state and under illumination, the continuity equations are given by:

$$\frac{1}{q}\frac{dJ_n}{dx} = -G_{op}(x) + R(x) \qquad \text{(Eq. 2)}$$

$$\frac{1}{q}\frac{dJ_p}{dx} = G_{op}(x) - R(x) \qquad \text{(Eq. 3)}$$

J_n and J_p are the current densities of the electrons and holes, G_{op} is the rate of generation electron hole and R is the rate of direct and indirect recombination.

Simulation is done in three stages which represent the ambient conditions, the electric parameters of defects of each layer and the model of tunnelling (will intra band or traps assisted) and finally the execution of the programs to extract the results.

B. Structure of the solar cell and parameter setting

CIGS is a I-III-VI2 semiconductor material composed of copper, indium, gallium, and selenium. The material is a solid solution of copper indium selenide (often abbreviated "CIS") and copper gallium selenide (CGS). It has a chemical formula of $CuIn_xGa_{(1-x)}Se2$ where the value of x =%Ga /(%Ga+%In) determine the rate of Gallium atoms that replace Indium atoms in the structure. CIGS is a tetrahedrally bonded semiconductor, with the chalcopyrite [2] crystal structure, and a band gap varying continuously with x from about 1.0 eV (for CIS) to about 1.7 eV (for CGS) [18]. The simulated cell containing CIGS consists of several layers: Mo/p-CIGS/n-CdS/i-ZnO/ZnO: B, and illustrated in figure 1.

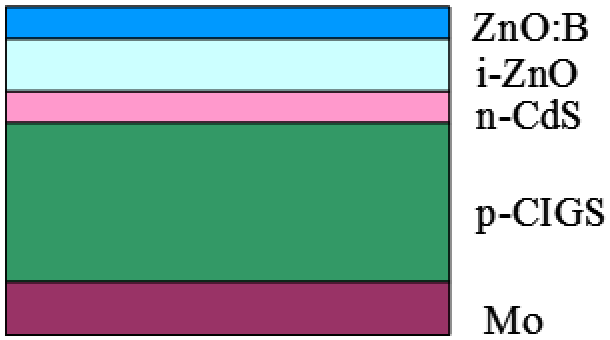

Fig. 1: Structure of a CIGS device

The characteristics of the various layers are gathered in table 1 [10]. Several authors [19] demonstrate that the work function for back surface of Ag can be tuned from 3.8 to 5.5 eV. In our work, we used the latter value which allows the best performances of CIGS solar cell.

	Surface avant	Surface arrière
Sn (cm/s)	107	107
Sp (cm/s)	107	107
Metal work Function (eV)	4.45	5.5
Majority carrier Barrier height relative to Ef (eV)	0	0.8
Majority carrier barrier height relative to Ev or Ec (eV)	0.0908	0.553
Optical filter	From file	Reflection From file (MoSe2)
Réflectivité Rf	0.95	0.8

Table 1: General Property of front and back surface metal contacts.

All required parameters for the simulation are given in table 2 [10]. The most common substrate is glass of silicate. This last is covered on a side with molybdenum (Mo) being used as metal back contact. The heterojunction is formed between the semiconductors CIGS and ZnO with a fine layer of interface made up of CdS and ZnO. The CIGS has a doping of the type *p* coming from intrinsic defects, an energy of variable band gap between 1 and 1.7 eV and a thickness varying from 100 to 3000 nm. In this layer the majority of the photons are absorbed to form the pairs electron hole. A plug layer of CdS, type n and thickness fixes of 50 nm, trains the second part of heterojunction *p-n*. The windows layer of intrinsic ZnO (i-ZnO) thickness 200 nm is of type *n* thanks to the incorporation of boron (B).

	n-ZnO	i-ZnO	n-CdS	p-CIGS
d (μm)	0.02	0.2	0.03	Variable
Eg (eV)	3.3	3.3	2.4	Variable
x (eV)	4.45	4.45	4.2	4.5
εr (1)	9	9	10	13.6
Nc (cm-3)	3×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
Nv (cm-3)	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
VthN	2.4×10^{7}	107	107	107
VthP	1.3×10^{7}	107	107	107
μn (cm2/Vs)	100	100	100	100
μp (cm2/Vs)	31	25	25	25
Nd (cm-3)	1020	1017	5×10^{17}	10
Na (cm-3)	1	1	1	1.3×10^{15}

Table 2: Properties of each layer.

The performances of a solar cell can be examined starting from important parameters that are the density of current of short-circuit J_{sc}, the tension of open circuit V_{oc}, the fill factor *FF* as well as the conversion efficiency η.

III. RESULTS AND DISCUSSION

Several research groups have an attempt to improve the efficiency of CIGS based solar cell. We will analyze and interpret the impact of physical and optical parameters of the CIGS absorber layer on the performance of the device as the thickness and gap as well as the effect of temperature on the conditions of illumination of AM1.5G (1KW / m2) and a zero voltage. Reflectance occurred at back contact was considered to be 90% while the front reflectance was neglected. The back surface recombination velocity was supposed to be 107cm/s.

Before investigating the effects of the thicknesses of absorber, at first, optimum band gap value of the CIGS absorber layer was determined. Minimum and maximum band gap values for the simulation were selected as 1.1eV and 1.7eV (pure CGS) according to the reference [10].

A. Thickness effect

One of the main challenges in CIGS based solar cell is the cost of materials which it is limited the mass production of these devices that of module price in comparison with conventional single or polycrystalline silicon solar cell is too high. CIGS layer is so important in cell efficiency. CIGS absorbers today have a typical thickness of about 1-3 µm. In part to reduce the consumption of the raw material and the cost of these cells, we consider the effects of the thickness *d* on the electric parameters of the solar cell. Figure 2 presents the variations of these parameters according to *d*. Figure 2(a) shows that the values of open circuit voltage V_{oc} increases with the thickness mainly to $E_g > 1.2$, and from the value of *d* = 1.4 µm, the increase in the thickness has no effect on this parameter. The maximum value $V_{oc} = 0.76$ V is obtained for d = 2 µm and E_g =1.5 eV. The results in figures 2(b) and 2(d) shows that there is an increase of the parameters: efficiency η and current density in short circuit (J_{sc}) with increasing the thickness of the CIGS layer and from a certain value (1µm for J_{sc} and 1.4 µm for η) there is a decrease in these parameters. We were able to get a maximum performance of 22.02% with a thickness of *d* = 1.4 µm. On the other hand, the fill factor decreased to a value minimum at *d* = 1.4 µm for all values of E_g and it remains almost constant as shown in figure 2(c).

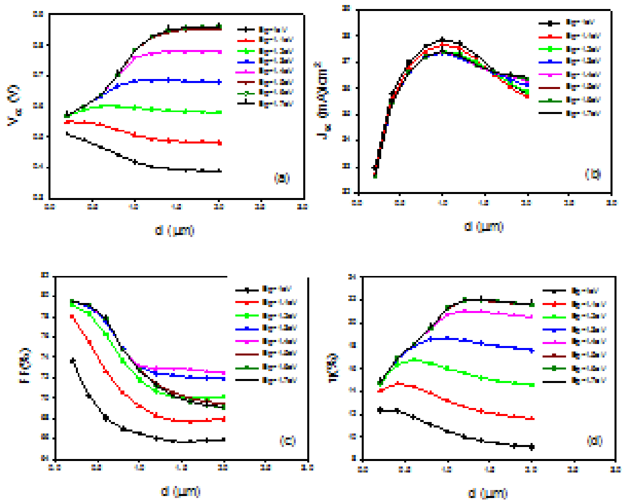

Fig. 2: (a) Variation of V_{oc} (a), J_{sc} (b), *FF* (c) and η (d) as a function of CIGS layer thickness.

B. Band gap effect

There are many parameters that influencing the efficiency and performance in PV cell structure. The reason is due because of a complicated physical mechanism taken place inside. In order to get confidence into a solar cell model, we have to take different characteristics as well as different possible conditions to be simulated and compared. Taking this into account we have considered the variation of band gap of CIGS absorber layer. This last have a very important influence on the parameters of the working structure n-ZnO / i-ZnO / CdS / CIGS.

The calculated V_{oc}, J_{sc}, *FF* and efficiency η values for the studied band gap range are shown in table 3 and the band gap dependence of calculated efficiencies is given in figure 3. As can be seen from figure 3, the efficiency increases significantly up to 1.5 eV then saturates.

CIGS Eg values (eV)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)
1	0.3955	37.2602	65.75	9.69
1.1	0.4878	37.0853	67.77	12.26
1.2	0.586	36.9914	70.12	15.2
1.3	0.6845	36.8546	72.2	18.21
1.4	0.7805	36.8483	72.95	20.98
1.5	0.8452	36.876	70.5	21.97
1.6	0.8504	36.8772	70.2	22.02
1.7	0.8505	36.8772	70.2	22.02

Table 3: The calculated cell output values in the studied band gap range.

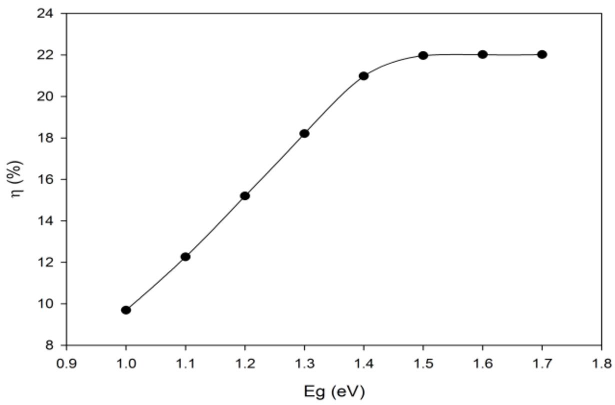

Fig. 3: The efficiency vs. band gap dependence of the simulated cells

C. Temperature effect

Operating temperature plays a vital role in the performance of the solar cells. The optimum operating temperature that has been used for most of the simulation in this study is 300 K. The temperature dependence of photovoltaic parameters of cell CIGS is studied for a solar cell in the range (260-360K) under a constant illumination (1000W/m²). From Fig. 4, it has been found that the overall efficiency in case of CdS buffered cells is severely affected by the operating temperature. At higher temperature, parameters such as the electron and hole mobility, carrier concentrations and band gaps of the materials would be affected that result in lower efficiency of the cells [20].

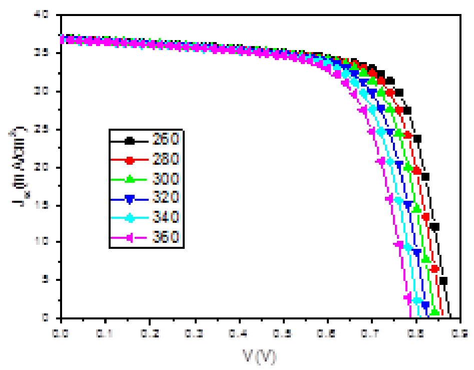

Fig. 4: Influence of temperature on the J-V characteristics

Figure 4 shows the effect of temperature on the characteristic $J(V)$. It is clear that increasing the temperature leads to an inevitable decrease of the voltage. Furthermore, for low voltages, the temperature variation has weak effect on the current density which remains nearly constant.

We then examined the effect of temperature on the characteristic parameters of the solar cell, namely the density of short-circuit current (J_{sc}), the open circuit voltage (V_{oc}), the fill factor (*FF*) and the PV conversion efficiency (η) are influenced by temperature. These parameters are presented in table 4, for various temperatures between 260 K and 360 K for the cell with 1.4 μm thickness and 1.7 eV band gap of the absorber.

Temperature (K)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)
260	0.9306	36.9261	67.7	23.26
280	0.882	36.9026	69.6	22.66
300	0.8505	36.8772	70.2	22.02
320	0.8272	36.8506	70.07	21.36
340	0.8071	36.8237	69.59	20.68
360	0.7878	36.7978	68.93	19.98

Table 4: Output parameters of simulated cells various temperatures.

Figure 5 shows a general decrease in these parameters with the increase in temperature. Their maximum values, in particular that of the efficiency, are all achieved at ambient temperature. The decrease of J_{sc} and η is almost linear in the range studied temperatures (260-360K). The thermal behaviour of V_{oc} under constant illumination is shown in figure 5(a), we also observed a linear decrease of J_{sc} in function of temperature in a narrow thermal range and may be insignificant. The *FF* decreases with increasing temperature, then it increases slightly from 300K.

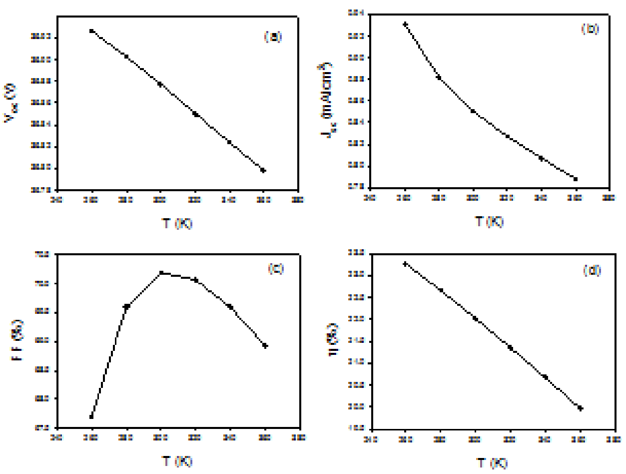

Fig. 5: influence of temperature on photovoltaic parameters of cell CIGS: (a) V_{oc}, (b) J_{sc}, (c) *FF* and (d) η.

We find that the maximum value of η is obtained by below ambient temperature. Specifically, at T=260K, the best performance of 23.26% is obtained with a 1.4 μm thickness and E_g=1.7 eV of the absorber layer.

IV. CONCLUSION

The objective of our work was to study the integration of thin-film chalcopyrite Cu(In,Ga)Se2 in photovoltaic technology and its influence on the electrical performance while identifying some locks that limit this technology. In order to optimize the time and cost of manufacture of such photovoltaic thin film (CIGS), numerical simulations have been done by adjusting parameters such as the absorber thickness and gap as well as the temperature, using the code SCAPS-1D. Photovoltaic parameters of cell CIGS : V_{oc}, J_{sc}, FF and η has been calculated which simulation results shows that optimized of CIGS thickness is 1.4μm and an improvement of conversion efficiency of 22.02% (at ambient temperature) and 23.26% (at temperature 260K) has been observed in comparison to the other conventional CIGS.

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