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Numerical Simulation Study of CIGS-based Thin Film and Heterojunction Solar Cells: Doping and Buffer/Absorber Layer Optimization for Maximum Efficiency

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Abstract

In this work we present the results of the numerical simulation study of the electrical characteristics of a CIGS-based thin film and heterojunction solar cell and their interpretations. First, we will simulate two solar cells of structures: ZnO/CdS(n)/CIGS(p)/Mo and ZnO/ZnS(n)/CIGS(p)/Mo using the SCAPS-1D software.
We will compare the results of the electrical simulation of the CdS cell with those found experimentally. Next, we will compare the electrical simulation results of the CdS cell with the ZnS cell. After that, we will choose the best cell to study the effect of doping and buffer/absorber layer thickness on the photovoltaic parameters (Jsc, Voc, FF, η) of the solar cell with the aim of achieving maximum efficiency of the CIGS-based solar cell.

Keywords: Thin films, Absorber Layer, Buffer layer**,** SCAPS-1D, photovoltaic parameters.

1. Introduction

Many scientists use optical and electrical calculations to simulate the solar cells they study. CIGS solar cells are a popular subject thanks to their recent popularity. One of the major disadvantages of CIGS and CdTe thin-film solar cells is loss of their buffer layers due to the high absorption rate of the material [1]. Alternative materials for thinning the CdS layer include replacing it with a material with a higher bandgap or adding a different one.

New materials are needed for several reasons: (a) Minimize power loss through windowing and buffer absorption (instead of CdS). (b) Establishment of favourable band offsets for wider bandgap CIGS. (c) Use as transparent front and rear contacts in tandem devices. Several alternative buffer layers have been explored, including Zn(OH,S), ZnSe, Zn(Se, OH) [2,3], zinc sulfide (ZnS) [4], possible replacements for II-VI semiconductor materials and Directly wider compound bandgap, with a bandgap energy of about 3.8 eV, implies that further improvement in short-circuit current (Jsc) can be achieved in CIGS solar cells by replacing the CdS buffer layer with a ZnS buffer layer. Taking these factors into account, there is compatibility of the CIGS absorption layer with other wide band gap buffer layers. Zinc sulphide (ZnS) prepared by chemical bath deposition (CBD) is proving to be an attractive alternative to CdS in combination with CIGS absorbers [5, 6] because of its wide bandgap of the order of 3.68 eV and its non-toxicity to the environment.

The main purpose of this paper is to investigate the performance of thin-film Cu (In, Ga)Se_2 (CIGS) based solar cells using the SCAPS-1D software. The performance of solar cells has been achieved. First, we evaluated quiescent current density J_{SC}, quiescent current voltage V_{OC}, quality factor FF, and cost-effectiveness n), double-layer connectors CdS, ZnS. Compare the results obtained to determine the best structure. After the comparison, we selected the cell with the best buffer layer and studied the doping effect, energy gap and thickness of the absorber (CIGS) and buffer layers (ZnS) to obtain the best solar cell with the best buffer layer.

2. Thin film solar cell

In principle, a thin film is a thin layer of a material deposited on another material, called "substrate", one of whose dimensions, called the thickness, has been greatly reduced so that it varies from a few "nm" to a few "µm" (typically these are layers of 10 ... 100 nanometres thick). In the field of thin films, there are three main channels:

- The amorphous and microcrystalline silicon pathway noted TFSi (Thin-Film Silicon).
- The CdTe (Cadmium Telluride) process.
- The Cu(In, Ga)Se2 (Copper-Indium/Gallium-Selenium) process, noted CIGS.

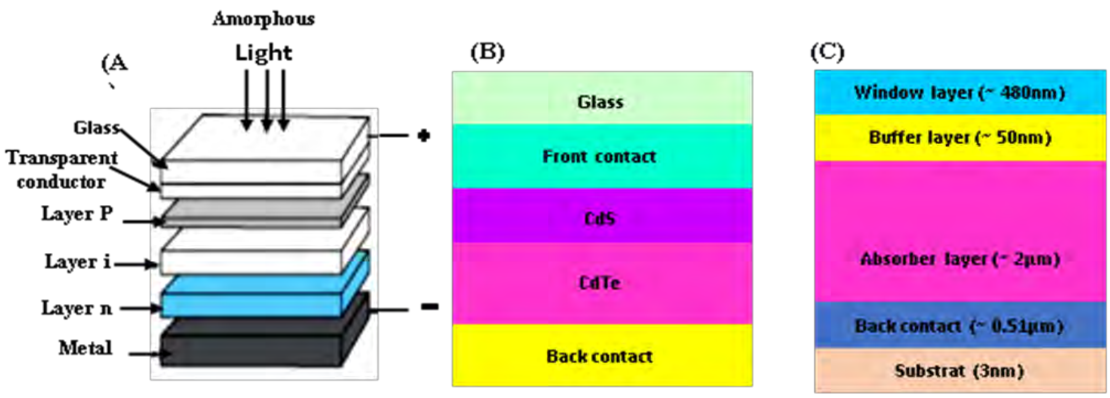

Fig.1. (A) Amorphous silicon solar cell [7] (B) Cadmium telluride solar cell [8], (C) Schematic of a CdS/CIGS solar cell simulated in APSYS [9].

3. Operating principle of a photovoltaic cell

The operation of any photovoltaic cell is based on the existence of an internal field to separate the electron-hole pairs generated by the absorption of light.

This potential barrier can be created by [8]:

- A p-n junction with a single semiconductor, which is called a homojunction
- A p-n junction with two different semiconductors, called a heterojunction
- A metal/semiconductor Schottky contact.

The operating principle of a p-n junction cell with a homojunction is described in figure 2

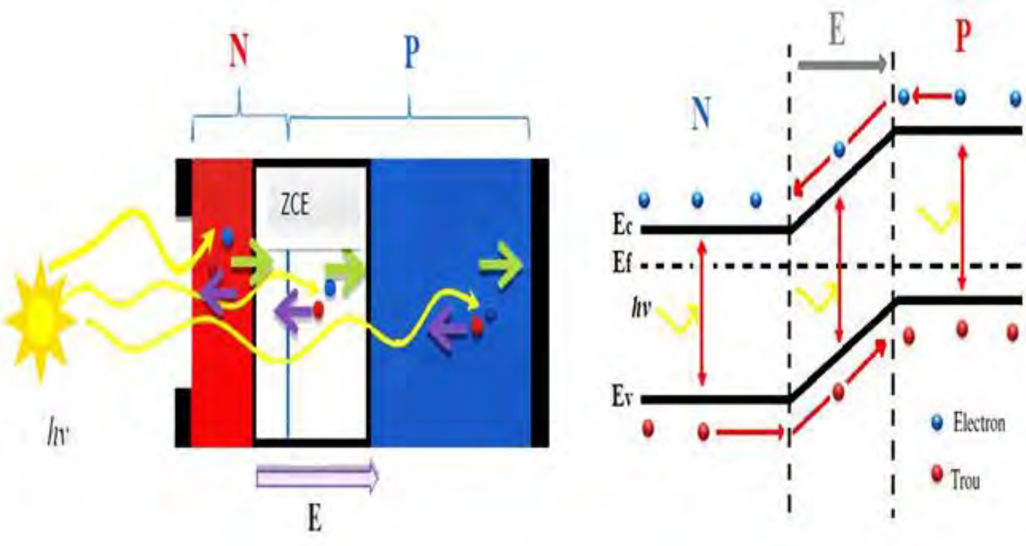

Fig.2. Structure and band diagram of a solar cell.

Incident photons create electron-hole pairs in the n and p regions and in the space charge region [8-9]:

- If a pair is generated in an electrically neutral region (p or n), the carriers diffuse. If the minority carriers reach the space charge region, then they are propelled by the electric field into the region where they become majority carriers. These carriers thus contribute to the current by their diffusion and a diffusion current is created.
- If an electron-hole pair is generated in the space charge region, the electron and hole are separated by the electric field, and each is propelled into the region where it is a majority carrier (region n for the electron and region p for the hole). These carriers give rise to a generation current [10].

4. I (v) characteristic and equivalent diagram of a solar cell

The I(V) characteristic corresponds to the subtraction of the photo-current and the diode current in the dark by [10]:

$$I(V) = I_{obs}(V) - I_{ph} = I_s(exp(\frac{qV}{KT}) - 1) - I_{ph} \quad (1)$$

With Iph the photo-current, $Iobs$ the dark current, Is the saturation current of the diode, q the elementary charge, K the Boltzmann constant and T the temperature.

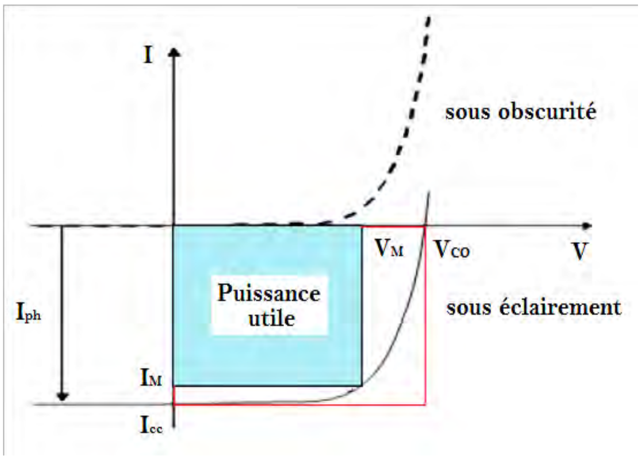

Fig.3. Dark and illuminated I(V) characteristics of a photovoltaic cell.

The characteristic of a cell in the dark is identical to that of a diode. In figure 3 we have shown the two current-voltage characteristics of a solar cell in the dark as a dashed line, and under illumination as a solid line.

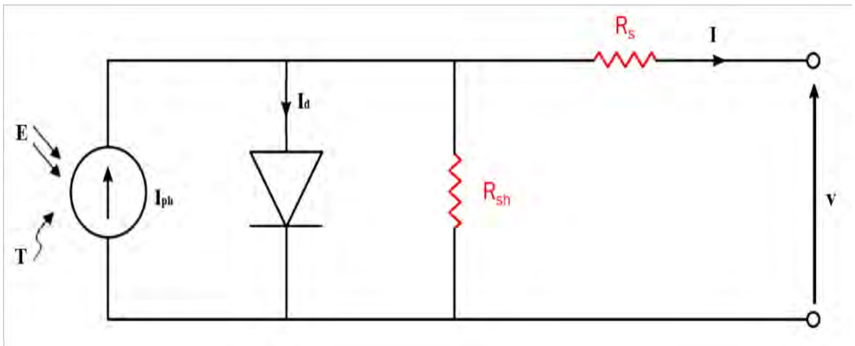

Fig.4. the equivalent electrical circuit of the solar cell.

Its equivalent diagram is represented by an ideal diode connected in parallel with a current source (figure 4). The series resistance, R_s, is related to the impedance of the electrodes and the base, so the voltage V across the cell is different from the voltage across the junction. The shunt resistance, R_{sh}, which corresponds to the losses in the surface and losses due to defects in the material, it results that part of the current I_{ph} will be shunted by this resistance and cannot be delivered to the load [11].

- The current I can be written:

$$I = I_{ph} - I_d - I_{sh} \quad (2)$$

According to the equivalent diagram of a solar cell in figure 4, we have:

$$I = I_{ph} - I_d - (\frac{V+I.R_S}{R_{sh}}) \quad (3)$$

$$I = I_{ph} - I_s[exp\ (\frac{V+I.R_S}{A.U_T}) - 1] - (\frac{V+I.R_S}{R_{sh}}) \quad (4)$$

With A: Quality factor

$$U_T = (\frac{K.T}{q}) \quad (5)$$

5. Parameters of a solar cell

The characteristic I=f(V) also noted "I-V" is a function that describes the behaviour of the solar cell, and from which several parameters related to the cell can be calculated.

The short-circuit current Icc: corresponds to the intensity of the short-circuit current, i.e. V=0

A. The open-circuit voltage Vco: corresponds to the open-circuit voltage, i.e. I=0

B. The maximum power Pm: This is the maximum output power corresponding to the point at which the product of the voltage and the current is maximum:

$$P_m = V_m.I_m \quad (6)$$

C. The form factor FF: It is the ratio between the maximum power delivered by the cell and the product between Icc and Vco corresponding to the ideal maximum power

$$FF = \frac{V_m.I_m}{V_{co}.I_{oc}} = \frac{P_m}{V_{co}.I_{oc}} \quad (7)$$

D. Efficiency: measures the energy conversion rate

$$\eta = \frac{P_{out}}{P_{in}} = \frac{I_{sc}.V_{oc}.FF}{P_{in}} \quad (8)$$

E. The peak power Pin: the maximum electrical power output under standard conditions (STC: Standard Test Condition), an irradiance of 1000W/m2, a temperature of 25°C and a spectrum AM1.5.

F. Quantum efficiency QE: This is the number of electron-hole pairs photo-generated by the number of photons incident on the cell. It is measured as a function of wavelength.

The short circuit current can be calculated from the quantum yield.

$$I_{cc} = \int_0^{\infty} QE(\lambda).\varphi(\lambda)dE \quad (9)$$

6. Digital simulation of the CIGS/(CdS/ZnS)/ZnO cell on SCAPS-1D.

We introduce the concept of numerical simulation of semiconductors, especially the application on CIGS-type solar cells using the SCAPS-1D calculation software, developed especially for the simulation of CIGS-based cells.

Table 1. Simulation Parameters

Settings	Absorbent, p-CIGS	Buffer Layer		Window Layer ZnO	ZnO: Al
		n-CdS	n-ZnS		
Thickness (nm)	3500	50	50	0.2	0.2
Permittivity	13.9	10	8.32	9	9
Gap energy (eV)	1.15	2.4	3.68	3.3	3.3
Affinity (eV)	4.8	4.5		4.1	4.1
Densities of states in BC, Nc (cm^{-3})	$2.2 \times 10^{+18}$	$2.2 \times 10^{+18}$		$2.2 \times 10^{+18}$	$2.2 \times 10^{+18}$
Densities of states in the BV, Nv (cm^{-3})	$1.8 \times 10^{+19}$	$1.8 \times 10^{+19}$		$1.8 \times 10^{+19}$	$1.8 \times 10^{+19}$
electron thermal velocity (cm/s)	1.0×10^{7}	1.0×10^{7}		1.0×10^{7}	1.0×10^{7}
hole thermal velocity (cm/s)	1.0×10^{7}	1.0×10^{7}		1.0×10^{7}	1.0×10^{7}
Electron mobility, µn (cm^2/V.s)	100	100		100	100
Hole mobility, µp (cm^2 /V.s)	25	25		25	25
Doping concentrations (cm^{-3})	0	$1\times 10^{+18}$		$1\times 10^{+18}$	$1\times 10^{+18}$
Density of defects (cm^{-3})	$2 \times 10^{+16}$	0		0	0
EA, ED (eV)	Milieu gap	Milieu gap		Milieu gap	Milieu gap
WG (eV)	0.1	0.1		0.1	0.1
Electron capture section (cm^2)	5×10^{-17}	10^{-17}		10^{-12}	10^{-12}
Hole capture section (cm^2)	10^{-13}	10^{-12}		10^{-15}	10^{-15}

The absorption coefficients of CIGS and CdS are taken from reference [12] and those of ZnO: Al and ZnO-i are taken from reference [13].

6.1 The cell used, ZnO/CdS(n)/CIGS(p)/Mo:

We propose to simulate the essential properties of a CIGS-based cell with a structure composed of a transparent conducting oxide (CTO) of the n-ZnO type, a buffer layer of the n-CdS type and an absorbing layer of the p-CIGS type (Figure 5).

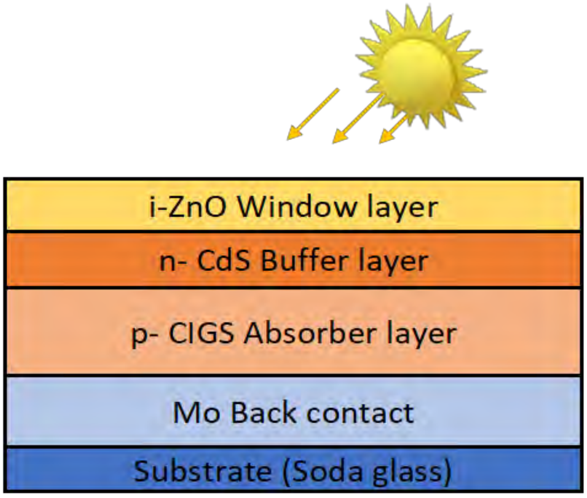

Fig.5. The ZnO/CdS(n)/CIGS(p)/Mo cell

6.2 Simulation results of the CdS/CIGS solar cell

After simulating the CdS/CIGS solar cell with the above parameters and a surface area of 0.5 cm^2 considering the AM 1.5 solar spectrum with a power density of 100 mW/cm^2, we obtained the results shown in Figure 6

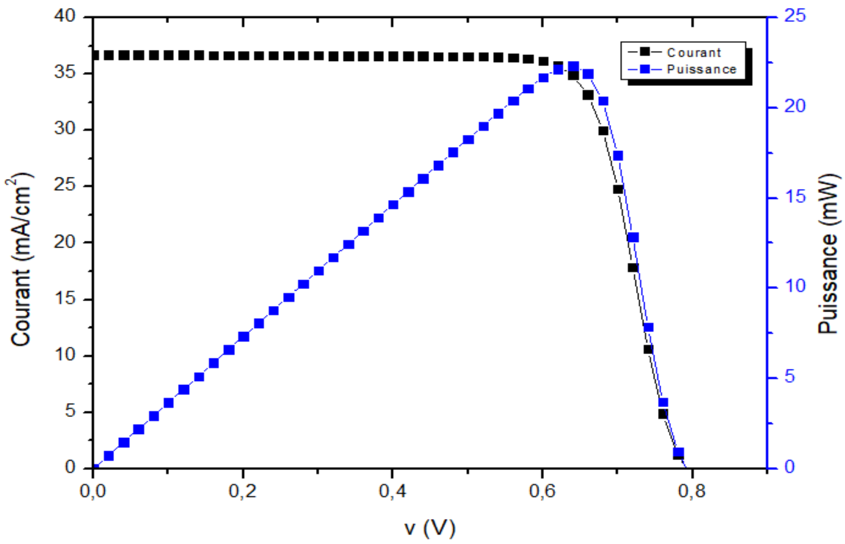

Fig 6. Simulated I(V) and P(V) characteristics of a CIGS/CdS solar cell.

An open circuit voltage Vco=0.7901 V, a short circuit current Joc= 36.712 mA/cm^2, a form factor FF=76.97% and a conversion efficiency η=22.32%.

Table 2: Comparison of simulated and experimentally obtained photovoltaic parameters of CdS/CIGS solar cells.

	Jsc (mA/cm^2)	Vco (V)	FF (%)	η (%)
Experimental solar cell [14]	37.8	0.741	80.6	22.6
Cell simulated by Silvaco-Atlas [15]	34.3	0.803	82.08	22.6
SCAPS-1D simulated cell	36.721	0.7901	76.97	22.32

The CdS/CIGS solar cell causes environmental and health problems due to the toxicity of the cadmium (Cd) material contained in cadmium sulphide (CdS). Zinc sulphide (ZnS) materials have been found to be more suitable for replacing cadmium sulphide (CdS) [16-17]. They are free of toxic elements and the band gap of ZnS (3.68 eV) is higher than that of CdS (2.42 eV), which allows the transmission of higher energy photons than the CIGS absorbing layer. It is a material that exists in abundance in nature and at low cost, for these reasons we have replaced the CdS material by the ZnS material in the following work.

6.3 The cell used, ZnO/ZnS(n)/CIGS(p)/Mo:

We took a ZnS/CIGS solar cell with the same structure as the CdS/CIGS solar cell described in the previous paragraph (Figure.5), the CdS layer was substituted by the ZnS layer.

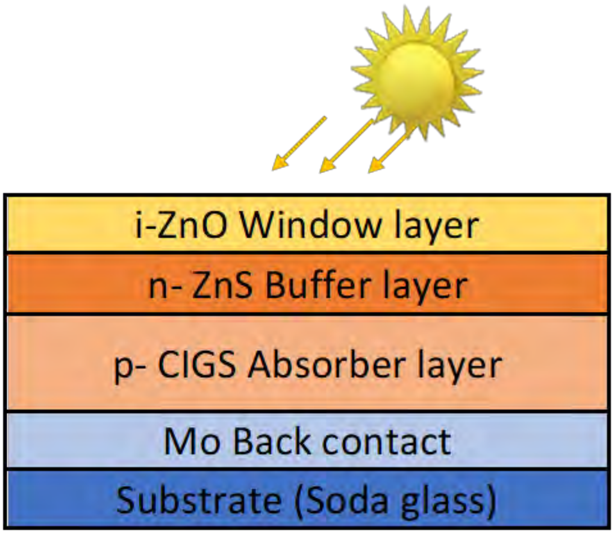

Fig 7. The ZnO/ZnS(n)/CIGS(p)/Mo cell

6.4 Simulation results of the ZnS/CIGC solar cell

ZnS/CIGS solar cell under illumination by AM 1.5 solar spectrum and power density 100 mW/cm^2 and surface area 0.5 cm^2 that we simulated gives as results: The short circuit current density Jsc = 39. 28 mA/cm2, the open circuit voltage Vco = 708.1 mV, the form factor FF = 83.13% and the conversion efficiency η = 23.12%.

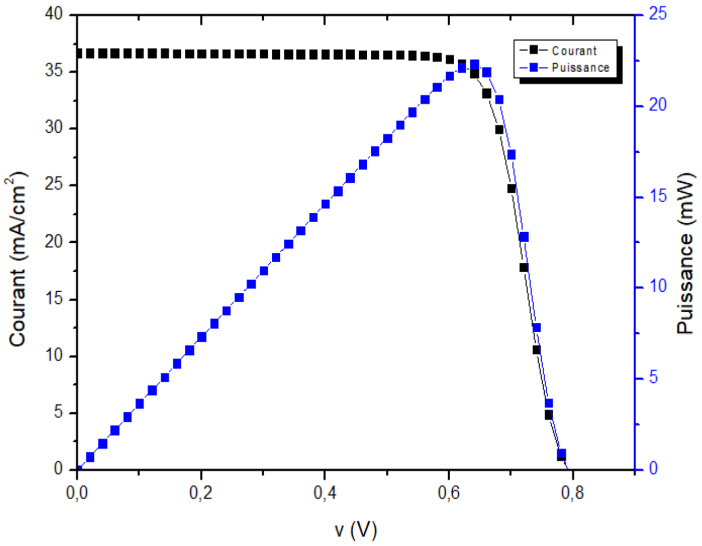

Fig 8. Simulated I(V) and P(V) characteristics of a CIGS/ZnS solar cell.

We notice that the short-circuit current density (Jsc) of the ZnS cell is higher than that of the CdS cell because the light absorption for short wavelengths by the CdS material is higher than that of the ZnS material ($EgZnS > EgCdS$). On the other hand, the open circuit voltage (Vco) of the CdS cell is almost the same as that of the ZnS cell (Table 3).

Table 3: Comparison between CdS and ZnS cells.

	Jsc (mA/cm^2)	Vco (V)	FF (%)	η (%)
CIGS/ZnS/ZnO simulation cell	39.28	0.7081	83.13	23.12
CIGS/CdS/ZnO Simulated cell	36.72	0.7901	76.97	22.32

The comparison between the two solar cells made of CdS and ZnS indicates that the ZnS solar cell has a better performance than the CdS solar cell.
In the following we will study the effect of doping and thickness of ZnS and CIGS layers on the parameters of the CIGS solar cell to optimize our ZnS/CIGS solar cell.

7. Results and discussion

7.1 Effects of ZnS and CIGS layers on solar cell performance

7.1.1 Effect of ZnS layer doping

For a ZnS (30 nm) and CIGS (3.5 µm) layer, we calculated the solar cell parameters for different values of ZnS doping concentration Nd between 1×10^{15} cm^{-3} and 1×10^{17} cm^{-3}

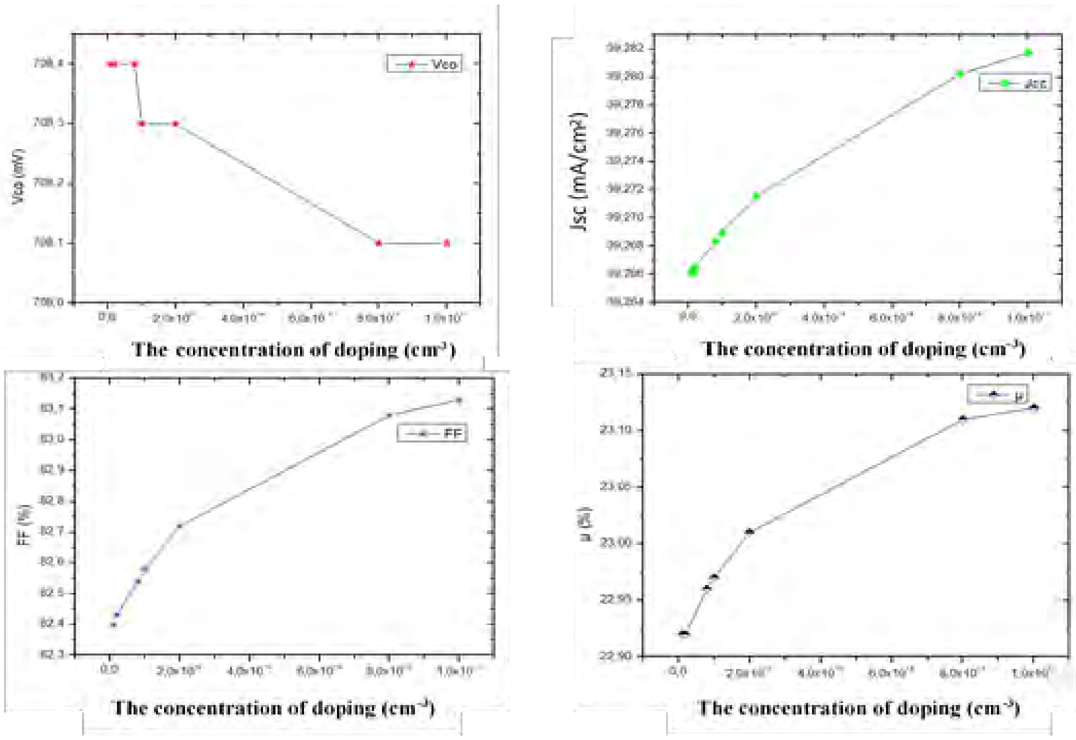

Fig 9. The effect of ZnS layer doping concentration on the parameters (Jsc, Vco, FF, η) of the solar cell.

7.1.2 Effect of CIGS layer thickness

The thickness of the CIGS layer is varied from 2µm to 4µm. The effect of the CIGS layer thickness on the solar cell is shown in Figure 10.

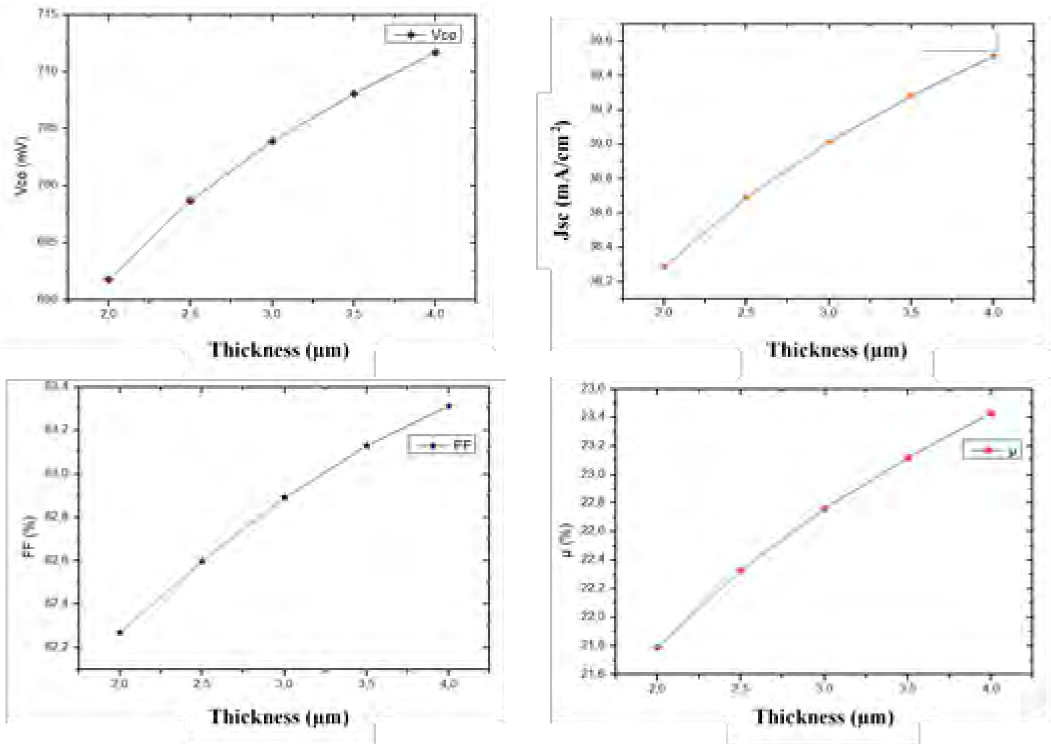

Fig 10.The effect of CIGS layer thickness on the parameters (Jsc, Vco, FF, η) of the solar cell.

1. Effect of Eg gap energy of CIGS layers

The gap energy of the CIGS layer is varied from 1.25eV to 1.3eV. The effect of the gap energy of the CIGS layers on the solar cell is shown in figure 11.

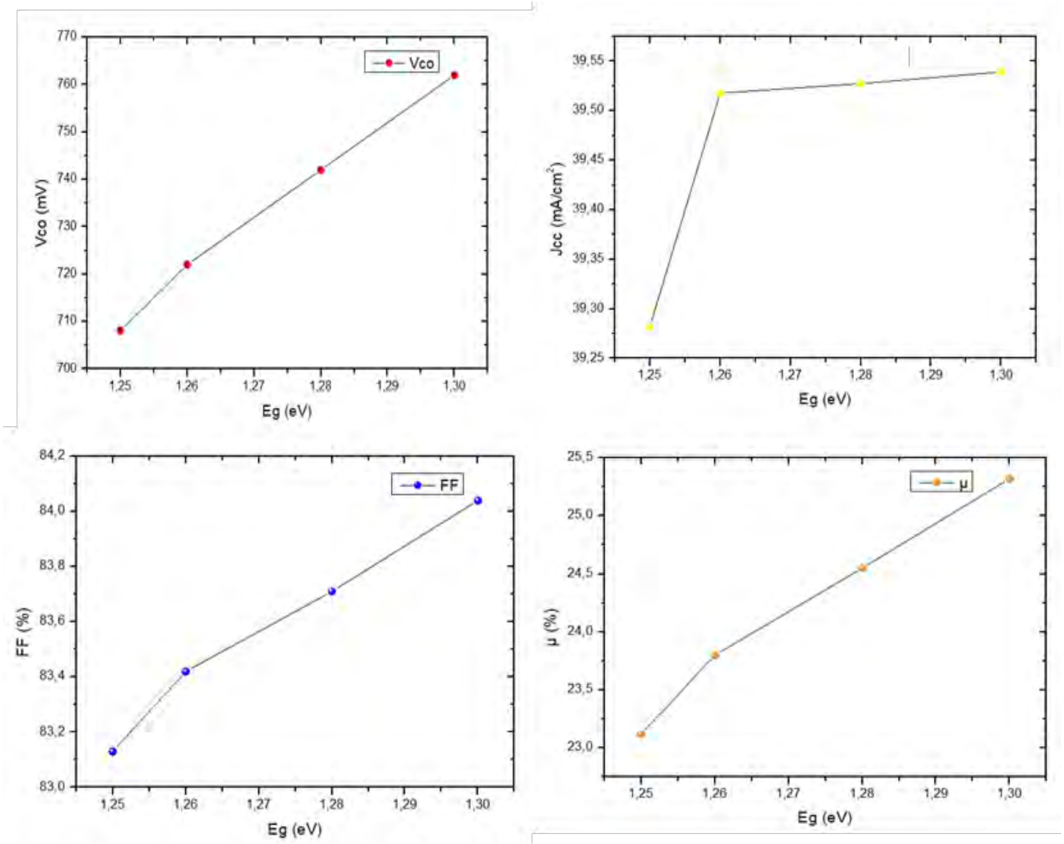

Fig 11. The effect of layer Eg gap energy in CIGS on the parameters (Jsc, Vco, FF, η) of the solar cell

The results of the study indicate that the best doping level for the ZnS layer was 1×10^{17} cm^{-3}, and the optimal thickness was 30 nm. Doping refers to the intentional introduction of impurities into a material to modify its electrical and optical properties. In this case, doping the ZnS layer with a specific concentration of impurities likely improved its ability to pass charge carriers (electrons or holes) to the adjacent layer, which could be the CIGS layer. The best energy (or bandgap) for the CIGS layer was found to be 1.3 eV, and the optimal thickness was 4 µm. The bandgap energy of a material determines which wavelengths of light it can absorb and convert into electrical energy. In photovoltaic cells, it's important to choose a material with a bandgap energy that matches the solar spectrum, so that the maximum amount of sunlight can be converted into electricity. The optimal thickness of the CIGS layer likely allowed for efficient absorption of light while minimizing losses due to recombination of charge carriers within the layer. The statement also indicates that the combination of these optimized parameters resulted in an electrical efficiency of 25.32%, which is a measure of how much of the sunlight that hits the cell is converted into usable electrical energy. This is a relatively high efficiency for a photovoltaic cell, which suggests that the optimized combination of layer parameters is effective at converting sunlight into electricity.

Table 4. Optimum parameters that gave η=25.32 %.

ZnS		CIGS			η (%)	FF (%)	Voc (mV)	Jsc (mA/cm^2)
Nd (cm^{-3})	Thickness (nm)	Nd (cm^{-3})	Thicknes s (μm)	Gap energy (eV)	25.32	84.04	762.0	39.53
1 x 10^{17}	30	1 x 10^{15}	4	1.3				

8. Conclusion

The simulation of two solar cells with structures: ZnO/CdS(n)/CIGS(p)/Mo and ZnO/ZnS (n)/CIGS(p)/Mo using SCAPS-1D software show that the solar cell with ZnS buffer layer gives the best efficiency η=23.12% compared to the solar cell with CdS buffer layer, η=22.32%. Secondly, we optimized the ZnS/CIGS solar cell by studying the effect of doping and thickness of the ZnS and CIGS layers. The optimal efficiency obtained is 25.32% for ZnS and CIGS layer thicknesses of the order of 30 nm and 4 μm respectively and doped by concentrations of the order of 1×10^{17} and 10^{15} cm^{-3} respectively.

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