Optimization of simulations of thickness layers, temperature and defect density of CIS based solar cells, with SCAPS-1D software, for photovoltaic application

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In this paper, the performance of CIS Based solar cells was investigated, using a simulation program named SCAPS-1D Software (Solar Cells Capacitance Simulator). CIS cell structure is based on Cu(In, Ga), $(Se,S)_2$; which is a semiconductor compound as an absorber layer; un-doped Zinc Oxyd (i) ZnO as a window layer, and Sulfide Cadmium CdS as a Buffer layer, with an efficiency of η=15%. We studied the influence of different layers' thickness and their defect densities, working temperature and absorber carrier density on the CIS based solar cells. The photovoltaic parameters have been calculated, and we have obtained the optimal values of every constraint cited above. As a result, we obtained a new high efficiency value of 19.71%, under air mass (AM) 1.5 and 100 mW/cm2 illumination and the area of this device was 0.15 cm^2.

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*Keywords:*CIS, Defect density, Photovoltaic parameters, SCAPS-1D, Solar cells

1. Introduction

The Copper Indium Selenide (CIS) based solar cells ($CuInSe_2$), is a chalcopyrite semiconductor promoter for photovoltaic applications, because of its high absorption coefficient, in the range of the solar spectrum and its electrical and optical properties which are depending on the preparation conditions and the processing techniques. It is a material which belongs to the chain of chalcopyrite materials [12]. It was synthesized for the first time in 1953 by Hahn [5]; before being offered in 1974, for photovoltaic applications. A first review of this type of material was developed by Shay and Wernick [5].

In 1983, CIS has been developed as thin polycrystalline layers, and as an active layer. In Crystallography, CIS is a semiconductor that belongs to the group I-III-IV_2 and crystallizes into two allotropic structures: Sphalerite structure and chalcopyrite structure, with direct band gap (the band Gap of our material choosing here is 1.04 ev). This type of material is very promoter for the production of solar cells' batteries in thin layers. In our case, we will study the influence of high temperature, absorber layer thickness and its defect density, and buffer layer thickness and its carrier density, on the performance of CIS based solar cells thin films, using SCAPS-1D software (Solar Cells Capacitance Simulator) [1-2].Which is used to calculate the photovoltaic parameters at sunder standard illumination (AM1.5G, 100 mW/cm^2, 300K) [8]. The goal of these simulations is to optimize the high efficiency of this material (η=15% as sample solar cells before the simulation), in order to obtain a better efficiency of the said solar cells.

1.1. Literature overview

In 2011, Mohammed Istiaque et al, have studied the prospects of Indium Sulphide as an Alternative to Cadmium Sulphide Buffer Layer in CIS Based Solar Cells, using SCAPS with replace of CdS by In_2S_3 (buffer layer) and Effects of various layer thicknesses of In_2S_3 and effects of In_2S_3 layer bandgaps. In 2015, Alaine et al have charachterizeted Minority carriers' diffusion length determination in thin films CuInSe2 solar cells electro deposited on flexible substrate in Kapton using the same simulator. In 2017, T.BILAL et al have studied the same cells with replacing of CdS by (ZnO:F) and effect of doping in Absorber layer and in Buffer layer.

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1.2. Motivations and aim of study

In this paper, we study the influence of high temperature, thickness of absorbent layer and its defect density, and CdS buffer layer and its defect density on the performance of CIS based solar cells thin films. The goal of this simulation is to optimize the best high efficiency of CIS based solar cells, which would be made and used as photovoltaic solar cells. The Copper Indium Selenide (CIS) based solar cells ($CuInSe_2$), is a chalcopyrite semiconductor promoter for photovoltaic applications, because of its high absorption coefficient, in the range of the solar spectrum and its electrical and optical properties which are depending on the preparation conditions and the processing techniques. It is a material which belongs to the chain of chalcopyrite materials. It was synthesized for the first time in 1953 by Hahn [5]; before being offered in 1974, for photovoltaic applications. A first review of this type of material was developed by Shay and Wernick [5]. In 1983, CIS has been developed as thin polycrystalline layers, and as an active layer. In Crystallography, CIS is a semiconductor that belongs to the group I-III-IV_2 and crystallizes into two allotropic structures: Sphalerite structure and chalcopyrite structure, with direct band gap (the band Gap of our material choosing here is 1.04 ev). This type of material is very promoter for the production of solar cells' batteries in thin layers. In this work, we will study the influence of high temperature, absorber layer thickness and its defect density, and buffer layer thickness and its carrier density, on the performance of CIS based solar cells thin films, using SCAPS-1D software (Solar Cells Capacitance Simulator) [16]. Which is used to calculate the photovoltaic parameters at sunder standard illumination (AM 1.5G, 100 mW/cm^2, 300 K)[8]. The goal of these simulations is to optimize the high efficiency of this material (η =15% as sample solar cells before the simulation), in order to obtain a better efficiency of the said solar cells.

2. Material and methods

2.1. Presentation of SCAPS-1D Software

The structure of the CIS forms a complex junction made of materials of different types (hetero-junctions) of CIS(p)/CdS(n)/ZnO(n) type in the higher efficiency devices. In this structure, CIS is a p-type wide-band gap absorber layer, wich is deposited on the molybdenum coated back glass substrate. The other members of this junction is a buffer layer n-type (Zinc Sulfied thin films) and a window layer n-type (ZnO) (Fig. 1) [13].

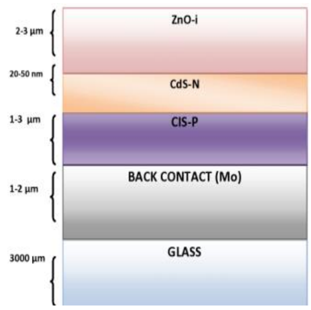

Fig.1. CIS Based Solar Cells section.

We will study some parameter optimization of solar cells, using SCAPS-1D software [17]. It is a one dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium [3 , 4]. Several researchers have contributed to it's development: Alex Niemegeers, Marc Burgelman, Koen Decock, Johan Verschraegen, Stefaan Degrave. A description of the program, and the algorithms it uses, is found in the literature [5 , 11].In first, we start by define the problem, on clicking on set problem, than we define the working point by specifing the parameters which are not varied in a measurement simulation, and which are relevant to that measurement, than we select the measurement (s) to simulate (I-V); (C-V); C- and Q(E)(λ). Finaly, we start the simulation by clicking button Calculate Single shot.

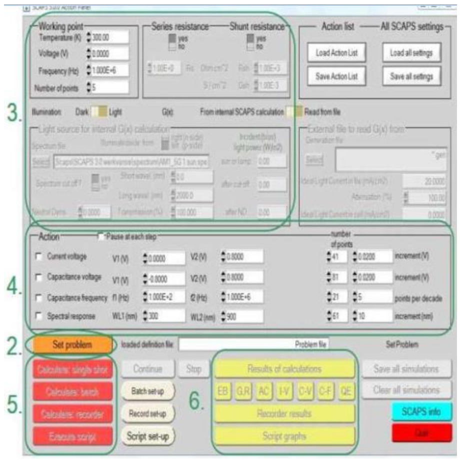

Fig.2.The SCAPS start-up panel: the Action panel or main panel.

1.Run SCAPS;
2.Define the problem, thus the geometry, the materials, all properties of your solar cell;
3.Indicate the circumstances in which you want to do the simulation, i.e. specify the working point;
4.Indicate what you will calculate, i.e. which measurement you will simulate;
5.Start the calculation(s);
6.Display the simulated curves.

2.2. Mathematical formalism of SCAPS-1D

The principle of SCAPS software is based on four equations namely:

2.2.1. The poisson equation

The Poisson's equation is derived from Coulomb'slaw and Gauss's theorem. It is a partial differential equation with broad utility in electro-statics, mechanical engineering, and theoretical physics. It has the following form:

$$\frac{d^2\psi(x)}{dx^2} = \frac{e}{\varepsilon_0\varepsilon_r}\left(p(x) - n(x) + N_D - N_A + \rho_p - \rho_n\right)$$

where: Ψ(x) is electrostatic potential, P(x) and n(x) are respectively electron and hole density; ε_0 and ε_r are respectively vacuum and relative permittivity, N_D and N_A are respectively charged impurities of donor and acceptor, ρ_n and ρ_p are respectively electron and hole distribution.

2.2.2. The continuity equations of electrons and holes

The continuity equation describes a basic concept, namely that a change in carrier density over time is due to the difference between the incoming and outgoing flux of carriers plus the generation and minus the recombination. They are "bookkeeping" equations that take into account all of theprocesses that occur within a semiconductor. Drift, diffusion, and recombination generation are constantly occurring in a semiconductor. Although we have studied these processes individually, they take place at the same time.

$$\frac{dj_n}{dx} = G - R \text{and} \frac{dj_p}{dx} = G - R$$

where J_n and J_p are respectivly electron and hole current densities, R is the recombination rate, and G is the generation rate.

2.2.3. The equations of carrier transport in semiconductors occurs by drift and diffusion

In semiconductor materials, current results from the displacement of electrons or holes, under the action of an external force. This force comes either an excitation by electric field (drift current), or by a concentration gradient in the semiconductor (diffusion current). The conduction current is carried out at two levels by: the electrons of the conduction band, which go up the applied electric field. The holes in the valence band which move in the same direction as the field electric. The diffusion current appears when the density of free carriers is modified locally inside the semiconductor, either by variations in temperature or light, or usually by an appropriate technology such as non-uniform doping hence a displacement of carriers from the region more populated to the less populated region (In physics of semiconductors, we can explain the phenomena of Transport, using these two equations below):

$$J_{p=D_p \frac{dp}{dx} + \mu_p \frac{d}{dx}} \text{ and } \qquad J_{n=D_n \frac{dn}{dx} + \mu_n \frac{d}{dx}}$$

where: μ_n and μ_p are respectively electron and hole mobility.

In this paper, we study the influence of high temperature, thickness of absorbent layer and its defect density, and CdS buffer layer and its defect density on the performance of CIS based solar cells thin films [15]. The goal of this simulation is to optimize the best high efficiency of CIS based solar cells, which would be made and used as photovoltaic solar cells [14].

3. Results and discussion

3.1. The influence of absorber carrier density on the CIS based solar cells:

In the theory of semiconductors, especially in PN Junction, we have a model that explains the influence of carrier density (N_A) on the characteristics of CIS Based solar cells; it is described by the following equations [7]:

$$\boldsymbol{I_0 = Aqn^2\left(\frac{D_e}{L_e N_A} + \frac{D_h}{L_h N_D}\right) \quad V_{OC} = \frac{KT}{q} \ln\left(\frac{I_L}{I_0} + 1\right)}$$

where: I_0 is the saturation current, A is the quality factor of the diode, q is the electronic charge, ni is the intrinsic concentration, D_e and D_h are respectively the diffusion coefficients of electron and hole, L_e and L_h are respectively diffusion lengths of electron and hole, N_A and N_D are respectively the acceptor and donor doping concentrations, K is the Boltzmann's constant, T is the temperature, I_L is the light generated current, and V_{OC} is the open circuit voltage [7].We can notice from these equations, that the saturation current density will be decreasing when the absorber carrier density N_A is increasing, with an increase in open circuit voltage V_{OC}. This can be explained by the fact that higher carrier densities will enhance the recombination process, which will reduce the probability of photon-generated electron's collection, with a reduction of the long wavelength photons. In the CIS layer, the photons of long wavelength will be deeply absorbed, therefore, the collected efficiency of the electrons created there, is more dependent on the diffusion effect [4].The optimization of CIS/CdS/ZnO heterojunction solar cell has been simulated based on the above listed properties of the absorbing and window layers in Table 1.

Table 1. Optical and electrical parameters of CIS based solar cells.

Parameters	***i-ZnO***	***CdS***	***CIS***
Thickness (µm)	0.200	0.100	2.000
Band Gap (eV)	3.300	2.420	1.040
Electron Affinity (eV)	4.100	4.10	4.300
Dielectric Permittivity (relative)	9.000	10.000	10.000
CB Effective Density of States (cm^{-3})	4.000E+18	3.000E+18	1.000E+19
VB Effective Density of States (cm^{-3})	1.000E+19	1.800E+19	1.000E+19
Electron Thermal Velocity (cm/S)	1.000E+8	1.000E+7	1.000E+7
Hole Thermal Velocity (cm/S)	1.000E+8	1.000E+7	1.000E+7
Electron Mobility (cm^2/V.S)	1.000E+2	1.000E+2	1.000E+2
Hole Mobility (cm^2/V.S)	2.500E+1	2.500E+1	2.500E+1

3.2. The effect of thickness on CIS based solar cells

3.2.1. The influence of thickness absorber layer

We study the effect of thickness of the absorber layer on cell performance, by changing this parameter from 2000 nm to 3800 nm, and keeping the other material parameters of different layers unchanged. Fig. 1 below shows the cell performance with variable absorber layer of CIS. We can notice that the short current density (J_{sc}), Open circuit voltage (V_{OC}), Fill factor (FF) and High efficiency (η) are increasing with an increasing thickness of CIS layer. This can be explained by the high absorption degree of the thicker absorber layer, which will absorb more photons with longer wavelengths [21], and will also contribute to the generation of electron-hole-pairs. Also, we can notice from the graph in Figure 1 that J_{sc} decreases linearly when the CIS layer thickness is less than 2800 nm. This can be explained by an incomplete absorption of the incident photons with an increasing recombination of photo-generated carriers at the back contact [4]. It can be found that the efficiency is increasing with the increase of CIS thickness, but when the layer is over 3400 nm, the efficiency has a much slower increasing rate (+0.07%); that is this value of thickness is enough to absorb most of the incident photons [21].

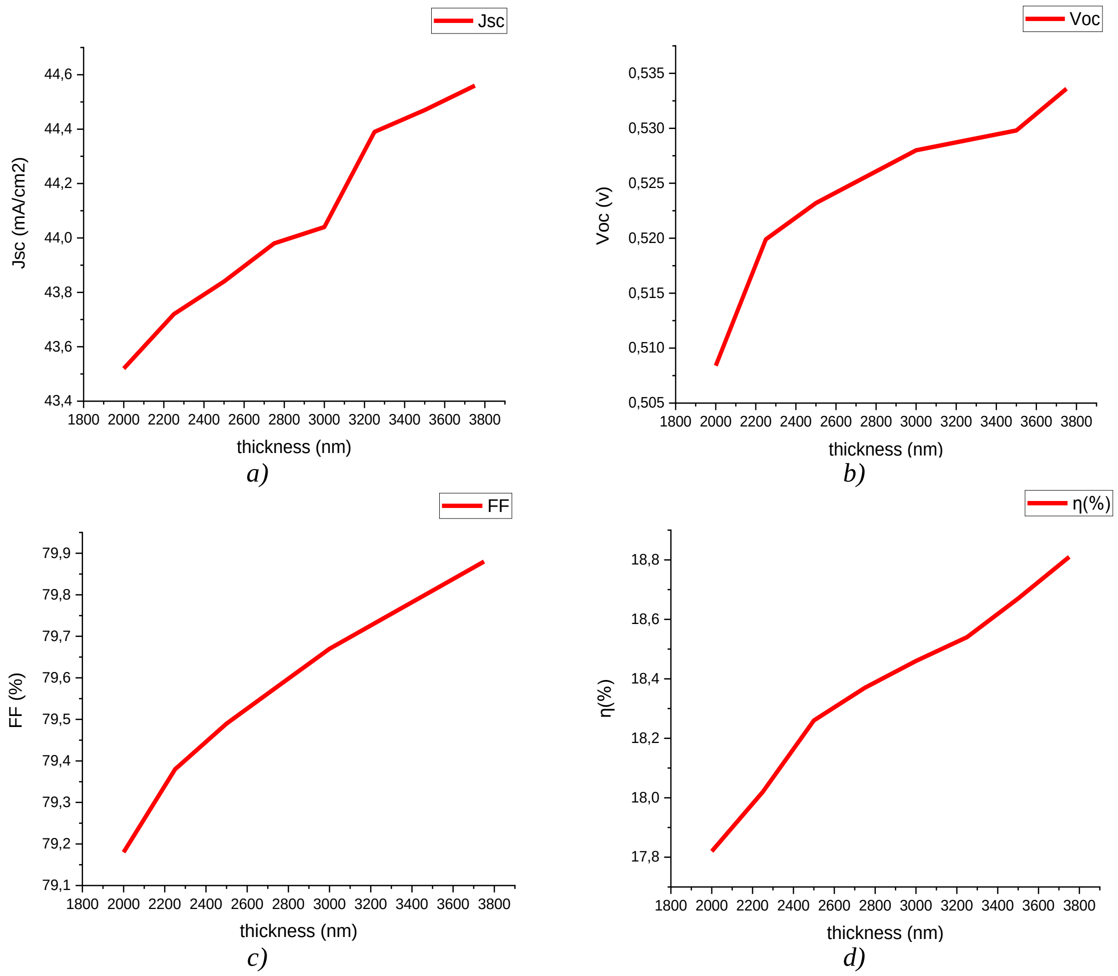

Fig. 3.The effect of CIS layer thickness on solar cells' performance:
a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

3.2.2. The effect of window layer thickness

We study in this part, the influence of the window layer thickness (ZnO), on the performance of CIS based solar cells. We change the thickness of window layer from 40 nm to 200 nm and keep the other material parameters unchanged. We can notice from the graphs in Figure 2 below that the Fill Factor is constant when ZnO thickness increases, with a relative decrease in open circuit voltage (from 0.51701 V to 0.5166 V). Physically, this can be explained by the fact that the increase in TCO thickness induces an increase in the optical absorption in the layer of the incident light at the front side of the cell [20]. The longer light and longer path-length will be proportional to the thickness, when the optical absorption is linked in the internal scattering .As a summary concerning the effect of ZnO layer thickness on the efficiency of solar cells, we can say that the highest value of efficiency is 17.97% for 40 nm of ZnO layer thickness, with a continuous decrease of this performance to reach 17.84% for 200 nm of ZnO thickness. This loss of efficiency is explained by the decrease in number of photons crossing through the ZnO layer with the thickness, because of the decrease of current density participating in the photovoltaic process. From this simulation, we can conclude that the increase in window layer thickness decreases the cell performance [20].

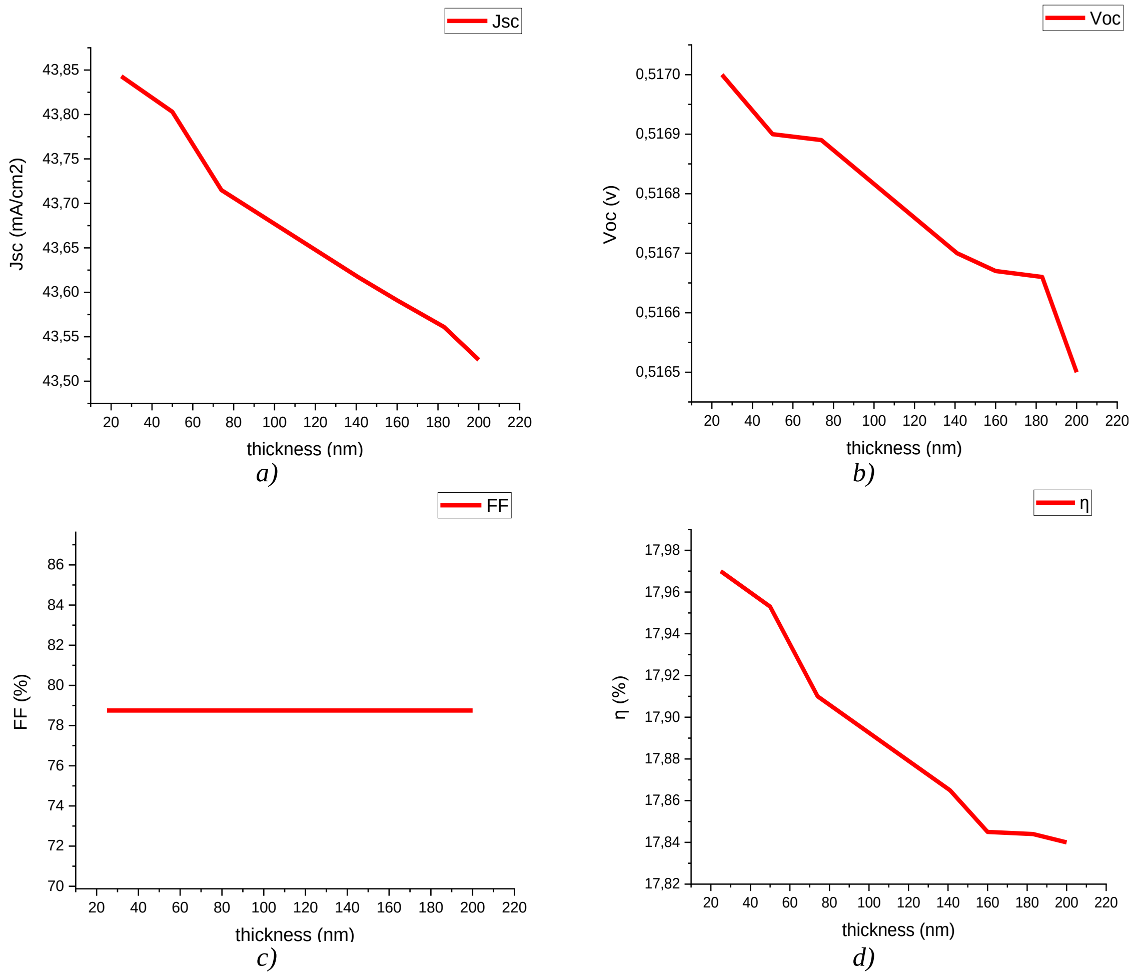

Fig. 4.The effect of ZnO thickness on solar cells' performance:
a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

3.2.3. The effect of buffer layer thickness

The logical criteria to select a buffer layer are specific; it must be n-type, or i-type to make a good junction partner with the absorber layer, and its resistivity must be the highest to reduce the possibility of shunting of a junction [2]. In this part, we change the buffer layer thickness from 35 nm to 100 nm. Fig. 3 shows the effect of CdS buffer layer thickness on solar cells' performance. As we can notice, on one side the short current density Jsc decreases with an increase in buffer layer thickness. On the other side, we can also notice that the open circuit voltage and Fill Form are relatively decreasing (from 0.516v to 0.517v for V_{co} and from 79.28% to 79.40% for FF). This can be explained by the fact that the quantity of photons that reach the absorber layer should decrease, due to the increase of the absorption in the CdS layer. When the CdS thickness increases, the material absorption increases too, however, the electron-hole pairs proceeded from these absorbed photons recombine in the CdS and are not collected [5]. Another effect of the buffer layer thickness is the increase of series' resistance; which is proportional to the buffer layer thickness.

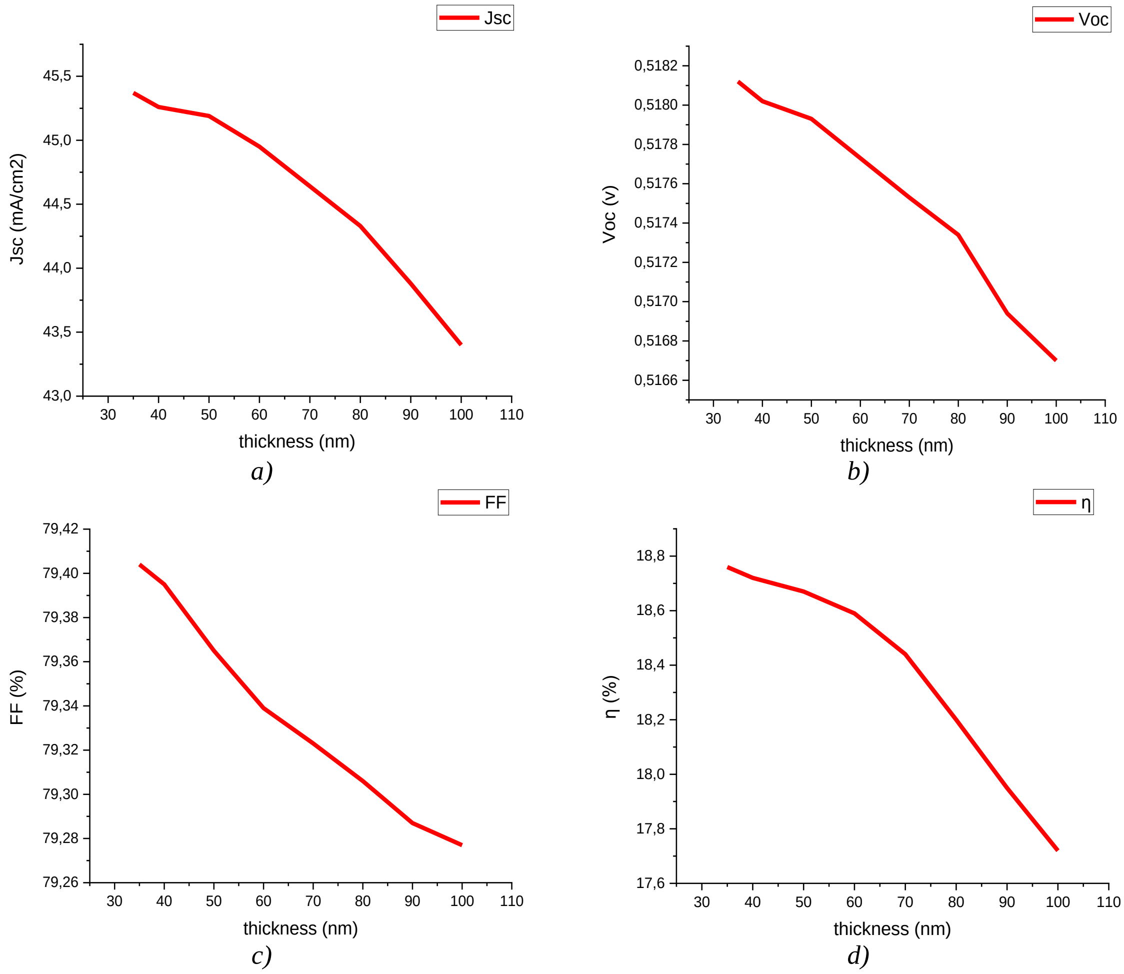

Fig. 5. The effect of CdS thickness on solar cells performance:
a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

3.3. The effect of temperature on CIS- based solar cells' performance

Usually, the solar cell panels are installed outdoor, where the sunlight will cause the heating of these solar panels, and therefore an increase in the temperature. In this part of the article, we study the influence of the operating temperature on the CIS based solar cells' performance, by changing the temperature values from 300 K to 390 K. The simulation results illustrate that the different performance parameters of solar cells are decreasing with an increase in temperature. This can be explained by the dependence between the temperature and the reverse saturation current or reverse Leakage current [18]. However, this increase in the current due to an increasing temperature will also decrease the open circuit voltage. The increase in operating temperature gives an additional energy to the electrons in solar cells. This makes them unstable at higher temperatures, and more likely to be recombined with the holes before reaching the depletion region and finally be collected [19].

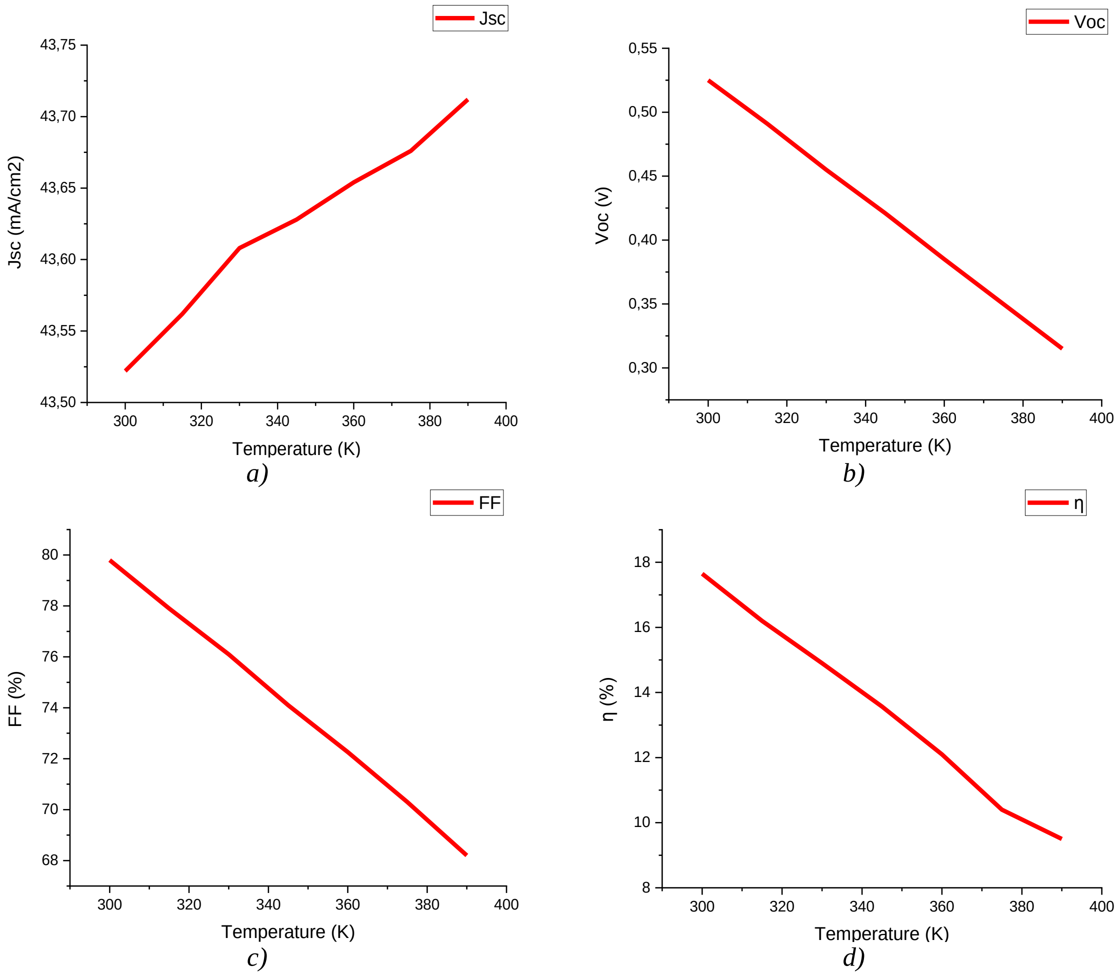

Fig.6. The effect of temperature on CIS-based solar cells' performance:
a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

3.4. The defect density effect on CIS-based solar cells' layers

The Defect density is one of the criteria used to determine the electronic properties of semiconductors. These defects are subdivided into four important categories: donors and acceptors, which play an important role to produce a p-n junction, defects as recombination centers that limit the lifetime of minority carries and hence the efficiency of these cells, the third group is responsible for carrier scattering or recombination, and the last group has defects which trap carriers and influence the space charge that determines the carrier transport. They represent: generation, recombination, and transport process inside the absorber layer [4]. In this part of the article, we study the effects of defect density on CIS-based solar cells, in the different layers of the photovoltaic device. To understand more this simulation, we have varied the defect density of one layer while keeping it constant for the other layers.

3.4.1. The defect density effect of absorber layer

In this step, we have varied the CIS layer defect density from 10^{14} cm^{-3} to 10^{19} cm^{-3}, while keeping the buffer layer (CdS) and window layer (ZnO) defects constant. Figure 7 below shows the defect density effect on CIS solar cell's performance. We can notice that when the value of defect density increases from 10^{14} cm^{-3} to 10^{17} cm^{-3}, the open circuit voltage, fill form and efficiency increase, with a small decrease in short current density. However, after a value of 10^{17} cm^{-3}, all the parameters will be degraded, except the open circuit voltage which keeps increasing with the increase of CIS defect density [22]. The reason behind the decrease of J_{sh} is the creation of a current named “Leackage Current”, which is a result of the recombination with localized energy levels, created by the defects [22]. As a principal result of that, we can see a dropping in the values of high efficiency (from 17.84 % to 3.61%).

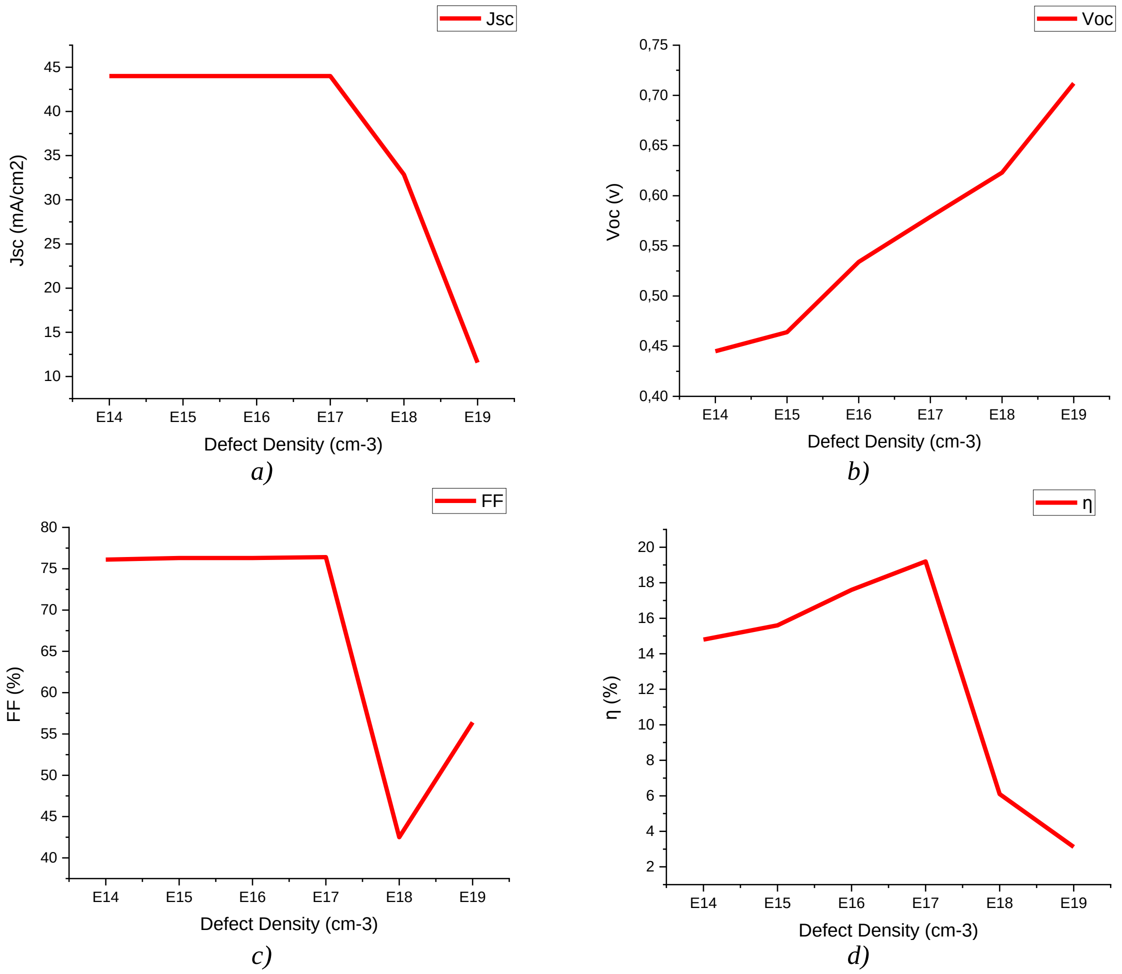

Fig. 7.The effectof absorber layer defect density on solar cells’ performance:
a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

3.4.2. The defect density effect of buffer layer

The defect density effect of buffer layer (CdS) has been studied here, by changing the defect density values from 10^{13} cm^{-3} to 10^{19} cm^{-3}, while keeping the window layer (ZnO) and absorber layer (CIS) defects constant. From Fig. 8 below, we can notice that the short current density J_{sh} decreases from 44.2327 mA/cm^2 for 10^{13} cm^{-3}, to 42.8177 mA/cm^2 for $10^{19}cm^{-3}$; therefore a decrease of 3.2%. The open circuit voltage also decreases from 0.5176 v for 10^{13} cm^{-3} to 0.5162 v for 10^{19} cm^{-3}; therefore a decrease of 0.27%. The Fill Form increases from 77.24% for $10^{13}cm^{-3}$ to 79.37% for 10^{19} cm^{-3}; therefore an increase of 2.13%. The efficiency curve has two importantzones: the first zone is where η increases to its maximal value (17.92% for $10^{16}cm^{-3}$), and the second one is where η decreases with an increase of buffer layer defect density (from 17.92% for 10^{16} cm^{-3}, to 17.54% for 10^{19} cm^{-3}). From these results, we can say that the CdS defect density can increase the efficiency of CIS based solar cells, for values fewer than 10^{16} cm^{-3}.We can observe that the defect density in Buffer layer has little effect in η, FF and J_{sh}, with unchanging values of V_{OC} [23].

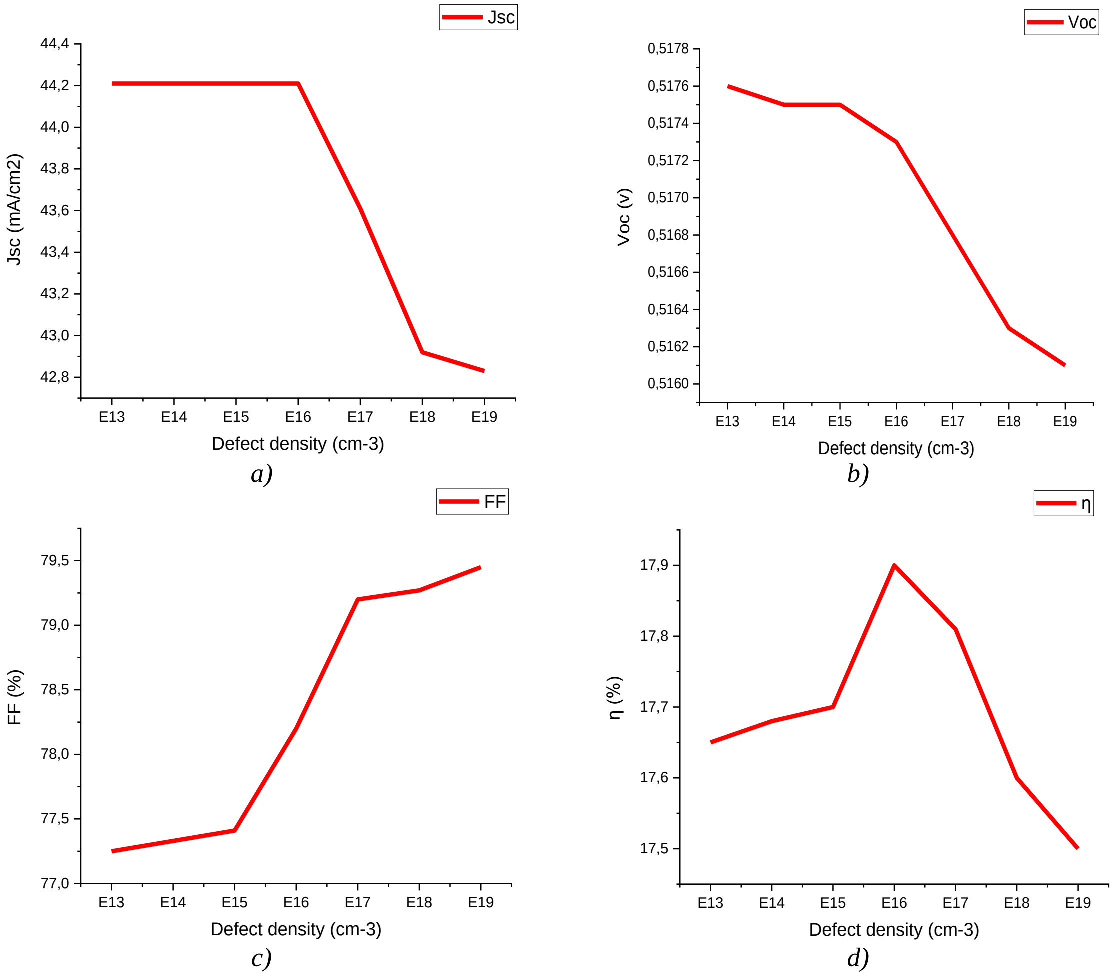

Fig. 8.The effect of buffer layer defect density on solar cells' performance:
a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

3.4.3. The defect density effect of window layer

We changed in this part of the simulation, the defect density of the window layer from 10^{13} cm^{-3} to 10^{19} cm^{-3}, while keeping the defect densities of buffer layer and *absorber layer constant*. *Fig.* 9 below shows that the photovoltaic parameters stay relatively the same with an increase of window layer's (ZnO) defect density. As a result, the rise of defect density in the ZnO layer has little impact on the performance parameters of CIS Based solar cells.

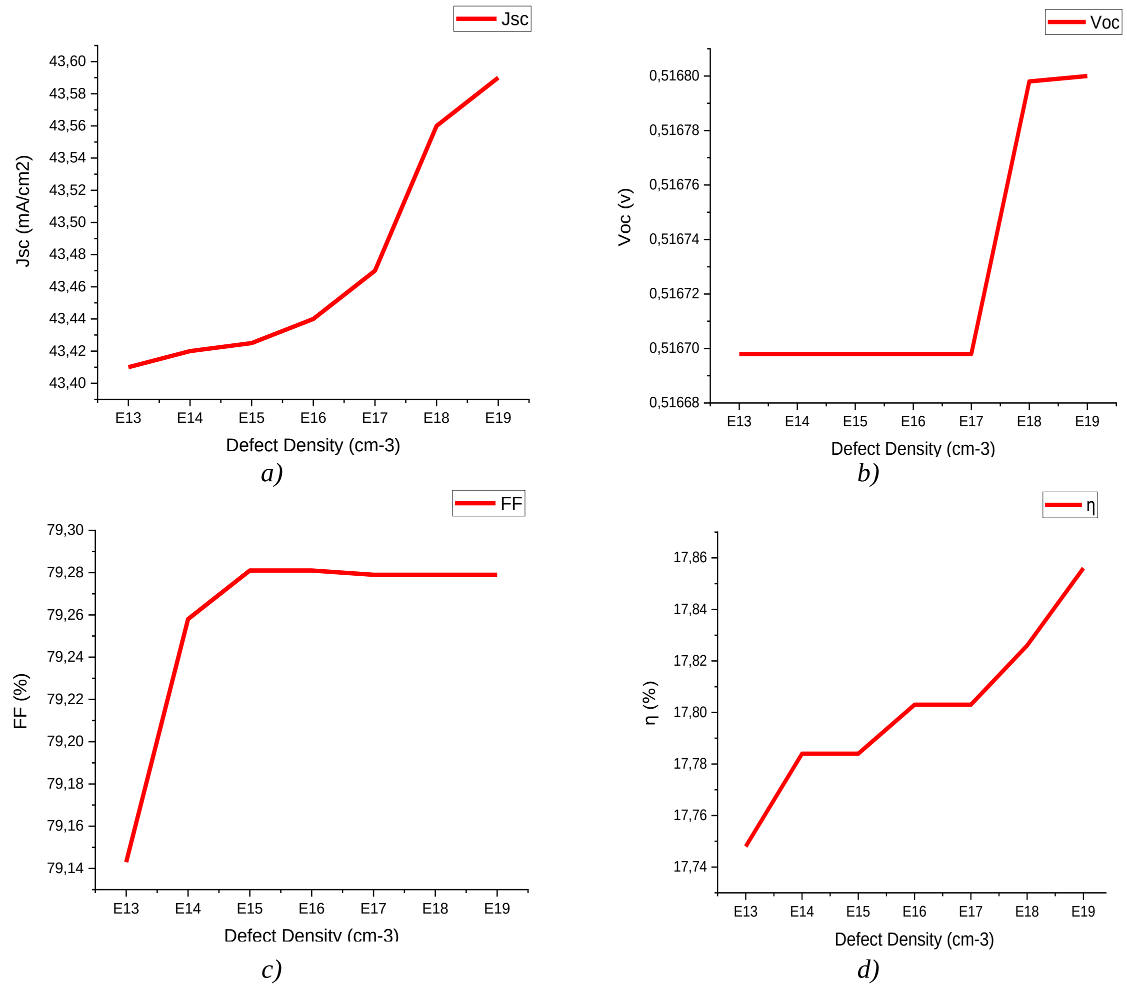

Fig. 9. The effect of window layer defect density on solar cells' performance: a) Short current density, b) Open circuit voltage, c) Fill Form, d) Efficiency

4. Conclusions

We analyzed the variations of, absorber layer thickness, absorber holes, and defects densities on CIS based solar cells. We have shown the following facts, using SCAP-1D package, and we found that the electrical parameters are affected significantly [19].

The CIS-based Solar Cells have been studied, after optimizing the values of all parameter performance, we found that the value of solar cells efficiency is 20.45%, with values of : 80.37%, 46.80855 mA/cm^2 and 0.5435 v for Fill Form, short current density and open circuit voltage respectively.

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