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Effect of Series Resistance Simulation on Chalcogenide Solar Cells Using One-Dimensional AFORS-HET Program

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ABSTRACT:

In this work, the effect of chain resistance on the performance of the CZTS/CdS/i-ZnO/ITO solar cell has been examined by a one-dimensional program where the chainresistance is changed from (0-8) Ω.cm^2. The above cell arrangement shows the possibility to achieve an efficiency of 9.28%,with a thickness of 5 μm asthis result is consistent with the experimental research. Yet, the efficiency was 6.19% and increased to 8.90%. After optimization, by the change of theabsorbent layer thickness and replacing the absorbent layer with other layers such as (CIGS, CNTS, CdTe) under the same conditions as the original absorbent layer (CZTS). The best obtained layer is the (CIGS) layer (Eff- 8.43%, FF- 43.8%, J_{sc} - 33.1 mA/cm^2 and V_{oc} – 582 mV)onthe solar cell optimization.

Key Words: CZTS-Simulation solar cell; AFORS-HET; maximum efficiency; Effects (Rs); Quaternary chalcogenides

1 - Introduction:

The principle of solar cell work is based on convertingthe sunlight energy into electrical energy through the photovoltaic phenomenon, this takes place through devices called solar cells[1]. After conducting many experiments and research, energy was obtained but with low-efficiency and highly-cost processes, in addition to the fact that some of the materials from which the cells are made are toxic[2]. Therefore, the researchers' interest turned into obtaining better alternatives and suitable materials for this matter, the quaternary chalcogenide compounds, which are characterized by their low-cost and availability in the earth's crust [3], and their direct energy gaps close to the ideal values, which necessitated the need to search for them extensively.In this research, we study the quaternary chalcogenide compound (CZTS), whichis a semiconductor compound in the group (I-II-IV-VI), it is also available and inexpensive [4-5], the (CZTS) has a clear energy gap (1.5 eV), refractive index (2.07)[6], high absorption coefficient (10^4 cm^{-1}), and the conversion efficiency is suitable [7]. This research includes a study of the impact of the series resistance (Rs) on the solar cell used (p-CZTS (n-CdS/n-i-ZnO/n-ITO) under the effect of varying the concentrationandthickness of both the absorption and the buffer layers when the highest effect of the series resistance (8 Ω cm^2).Moreover, the change of the absorption layer with other absorption layers at the same conditions as the absorption layer (CZTS) has been also studies. In this work, the experimental cells are compared to the theoretical cells to get a highly efficient cell.The researchers havebegun working on, (Cu_2ZnSnS_4) (CZTS), A rapid increase in solar cell efficiency based on CZTS was obtained in 2009 by 6.7% to 2012 by 11.1%.The compound isCZTS is a potential candidate to thin film solar cells, as it is considered one of the lowest cost and least toxic compounds, and the highest efficiency of the CZTS cell that has been achieved so far is 12.7% [8].It is still far from theoretical calculations, and a complete understanding and control of the various manufacturing processes and reactions is still needed to get a high efficiency of CZTS. Various deposition techniques have been used such as vacuum and non-vacuum deposition techniques used in CZTS-based solar cell research, where the cell layers are processed through a two-step manufacturing process such as deposition step,after which comes a high-temperature process of annealing [9].However, there is a need for low pressure, as the annealing process prevents decomposition reactions occurring at high temperatures [10].We have implemented a simulation programAFORS-HET is a 1D digital simulation program used to model heterogeneous solar cells, and solve semiconductor equations such as (the transport and continuum equations for electrons and holes and Poisson equation), where a series of semiconductor layers and interface properties can be formed between one layer and another. Through which it is possible to study the optical and electrical properties to find the current-voltage relationship (IV) quantumefficiency (QE) and thecapacity-voltage (CV)[11]. The simulation program is an easy-to-use interface through which the basic parameters can be adjusted to suit the given measurements.

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2- Theoretical study:

2-1Continuity equation:

The equation that describes the diffusion, drift and recombinationof electrons and holes is called the continuity equation, and thus the continuity equation is given by [12]

$$\frac{\partial n(x)}{\partial t} = G_n(x) - U_n(x) + \frac{1}{q}\frac{dJ_e(x)}{dx} \quad (1)$$

$$\frac{\partial p(x)}{\partial t} = G_p(x) - U_p(x) - \frac{1}{q}\frac{dJ_p(x)}{dx} \quad (2)$$

2-2 Poisson's equation:

The charge density and electron voltage equation are related according to Maxwell's general equation

$$\frac{d}{dx}.D(x) = \rho(x) \quad (3)$$

and the amount $D(x) = -\frac{\varepsilon(x)d}{dx}.\Phi(x)$ (4)

The (Poisson equation) is in the following form

$$\frac{d\ln(\varepsilon(x))}{dx}.\frac{d\Phi(x)}{dx} + \frac{d^2\Phi}{dx^2} = -\frac{\rho(x)}{\varepsilon(x)} \quad (5)$$

in a steady state ε. The (Poisson equation) is in the following form

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho(x)}{\varepsilon} \quad (6)$$

We usually use four variables to study the solar cell output:

1 - Short circuit current (I_{sc}): the current under the influence of voltage becomes [13]

$$I_d = I_0\left(\exp\frac{qv}{kT} - 1\right) (7)$$

I_d the injection current and it flows through the contact area under the influence of the applied voltage I_0 represents the saturation current for the carriers that can cross the barrier and are given by the relationship

$$I = I_0\left(\exp\frac{qv}{kT} - 1\right) - I_l (8)$$

$$I_0 = A\left[\frac{q\, D_n {n_i}^2}{L_n N_A} + \frac{q\, D_p {n_i}^2}{L_p N_D}\right] (9)$$

Here,(A) is the cross-sectional area, the load current (I),illumination current (I_L) and the potential difference on the load (V).In the case of a short circuit, the resistance of the load is equal to zero (the current passing is the short circuit current and compensated for (V = 0), theshortcircuitcurrentbecomes.[14]$R_l = 0$) (I_{sc})

$$I_{sc} = I$$

2- Open circuit voltage (V_{oc}):when the circuit is open, the load resistance is the greatest possible and the current is equal to zero [14]

$V_{oc} = \frac{kT}{q}\ln\left(\frac{I_{sc}}{I_0} + 1\right)(10)$

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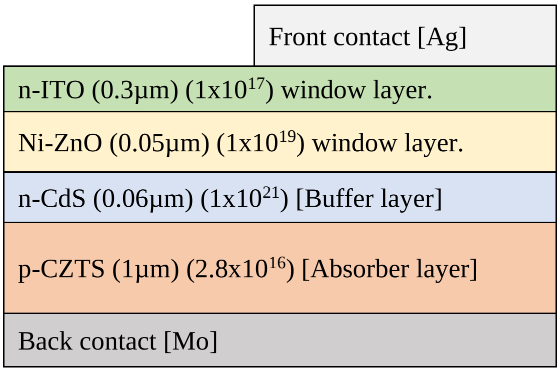
3- Fill factor (*FF*): It is a measure of the reference range of the output characteristics, and its value for cells with efficiency is between (70-85%) and it is defined according to the following relationship:

$$FF = \frac{V_{mp} I_{mp}}{V_{oc} I_{sc}} \quad (11)$$

4- Efficiency (Eff): It can be expressed by the following relationship:

$$\eta = \frac{p_m}{p_{in}} \times 100\%$$

$$\eta = \frac{I_m V_m}{p_{in}} \quad (12)$$



Thus, the conversion efficiency equation () can be written in the following form: -η

$$\eta = \frac{FF \times I_{sc} \times V_{oc}}{p_{in}} \times 100\% \quad (13)$$

where(Pin) is the total power of incoming light on the cell. The rate of solar energy conversion efficiency for commercial solar cells is usually between (12-14)% [15].

3- SolarCellStructures:

The solar cell used p-CZTS /n-CdS/n-i-ZnO/n-ITO consisted of different conductive layers which are respectivelyas shown in figure 1. The oxide (i-ZnO) is a transparent conductive oxide with a direct energy gap (3.37 eV) [16] and a thickness of (0.05) μm, preceded by a transparent window layer of titanium dioxide (ITO),titanium dioxide that has a large energy gap, high transparency (3.6 eV) [17], with a thickness of (0.3 μm), A layer of cadmium sulfide (CdS) with a thickness of (0.06 μm) and a relatively large energy gap (2.4 eV), followed by a layer of zinc-selenium (CZTS) with a thickness of (1 μm) and an energy gap (1.5 eV) [18], we usually use the molybdenum (Mo) back contact.In this cell, we used layers with relatively large energy gaps, due to their suitability in areas with strong thermal effect, such as (Iraq) atmosphere,as the efficiency of the solar cell is related to the energy gap, which is in turn determines the absorbed photons [19].

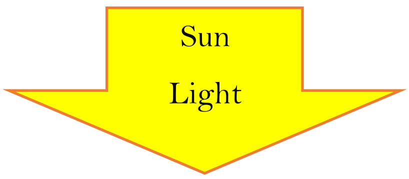


Fig.1. Cell Structure Composition: p-CZTS /n-CdS/n-i-ZnO/n-ITO

4- Results and Discussion:

4.1 Comparing the Results of the AFORS-HET Program with the Results of the Practical Research:

In this study we simulate a solar cell for (CZTS) [18], experimental research using thesimulation program AFORS-HET The goal is to compare the theoretical results with the experimental ones through the used program in order to find out their agreement with the practical results as the absorbing layer thickness (CZTS) (1 μm) and the concentration of doping (2.8 x 10^{16} cm^{-3}), buffer layer (CdS) thickness (60 nm) and concentration (1 x $10^{21}$$cm^{-3}$), and permeable layer (i-ZnO) thickness and concentration (50 nm)(1 x 10^{19} cm^{-3}), the transparent layer (ITO) thickness (300 nm) and concentration (1 x 10^{17} cm^{-3}) respectively, the values of series resistance and parallel resistance were (5.76 Ω cm^2) and (400 Ω cm^2) respectively.After starting work, we have noticed that there is a great match between the results of the experimental cell

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and the theoretical cell as in Table (1), and other basic parameters constituting the cell were taken from Published research as in Table (2). The open circuit voltage (V_{oc}) is roughly remain similar and the current is slightly reduced (I_{sc}) and increased, The value of each fill factor (*FF*) and efficiency (Eff) as in Table (1).

Table (1) Comparing the theoretical results with the practical results:

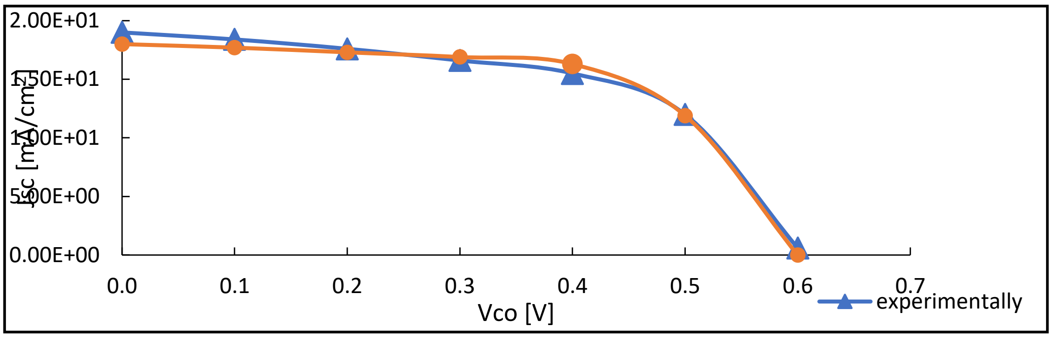

Fig. 2. (I-V) diagram prior to improvi

2- p-CZTS /n-CdS/n-i-ZnO/n-ITO theoretical	603.9	18.01	59.12	6.4

Table (2) shows the parameters of the solar cell used:

Parameters	**Symbol (unit)**	**p-CZTS**	**n-CdS**	**n-i-ZnO**	**n-ITO**
Thickness	**d (µm)**	1 [18]	0.06 [18]	0.05[18]	0.3 [18]
Dielectric permittivity	**Dk**	7 [20]	10 [24]	9 [11]	10 [27]
Electron Affinity	**χ (eV)**	4.3 [21]	4.2 [24]	4.4 [26]	4.1 [27]
Band gap	**(eV)**	1.5 [18]	2.4 [24]	3.37 [26]	3.6 [27]
Density of states in CB	**Nc (cm^{-3})**	$2.2x10^{18}$ [22]	$1.8x10^{19}$ [24]	$2.2x10^{18}$ [11]	$2.2x10^{18}$ [28]
Density of states in VB	**Nv(cm^{-3})**	$1.8x10^{19}$ [22]	$2.2x10^{18}$ [24]	$1.8x10^{19}$ [11]	$1.8x10^{19}$ [28]
Electron mobility	**µn (cm^2/Vs)**	100 [22]	100 [25]	100 [11]	100 [28]
Hole mobility	**µp (cm^2/Vs)**	25 [22]	25 [25]	25 [11]	25 [28]
Acceptor concentration	**Na (cm^2)**	$2.8x10^{16}$	0	0	0
Donor concentration	**Nd (cm^2)**	0	$1x10^{21}$	$1x10^{19}$	$1x10^{17}$
Thermal velocity of electron and hole	**υ (cm/s)**	$1x10^7$ [22]	$1x10^7$[11]	$1x10^7$ [11]	$1x10^7$ [11]
Layer density	**Rho (g*cm^{-3})**	2.328 [11]	2.328 [11]	2.328 [11]	2.328 [11]
Refractive index	**N**	2.85 [23]	File AFORS-HET	File AFORS-HET	1.827 [29]
Extinction coefficient	**K**	0.1 [23]			0.0031 [29]
Total trap density (defect)	**Nt (cm^{-3})**	$1x10^{14}$ [23]			
Characteristic Energy (defect)	**Et (eV)**	0.5 [23]			
Capture cross section electrons and hols (cm^2)	**δn ,δp**	$1x10^{-15}$ [22]			
Type Defect		Single/D			

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4.2Series Resistance Effect on the Cell (p-CZTS /n-CdS/n-i-ZnO/n-ITO)

There are three series resistance impact on the solar cells:

1 - Resistors of the constituent layers of the cellp-CZTS /n-CdS/n-i-ZnO/n-ITO, The resistance of the all layers.

2 - Each layer's constituent elements.

3-The front and rear contactResistance.

The keyeffect series resistance is reducing the fill factors. Yet, a very high value could also be a reason for the reduction of the short-circuit current (I_{sc}) [30].We have studied the effect of series resistance from (0-8).$\boldsymbol{\Omega}$.cm^2, where it was found that the rise of the series resistance reduces the short circuit current (I_{sc}) curve, as shown in Figure (3). The reason for the decrease in the short circuit current (I_{sc}), with the increase in the series resistance is due to the decrease in the conductivity of the carriers, decreasing in the value of the current. This affects the efficiency of the solar cell, as the efficiency value (Eff) decreases, while the open circuit voltage (V_{oc}) stays usually constant, because the current is equal to zero, will not affect the voltage, as shown in Figure (3).

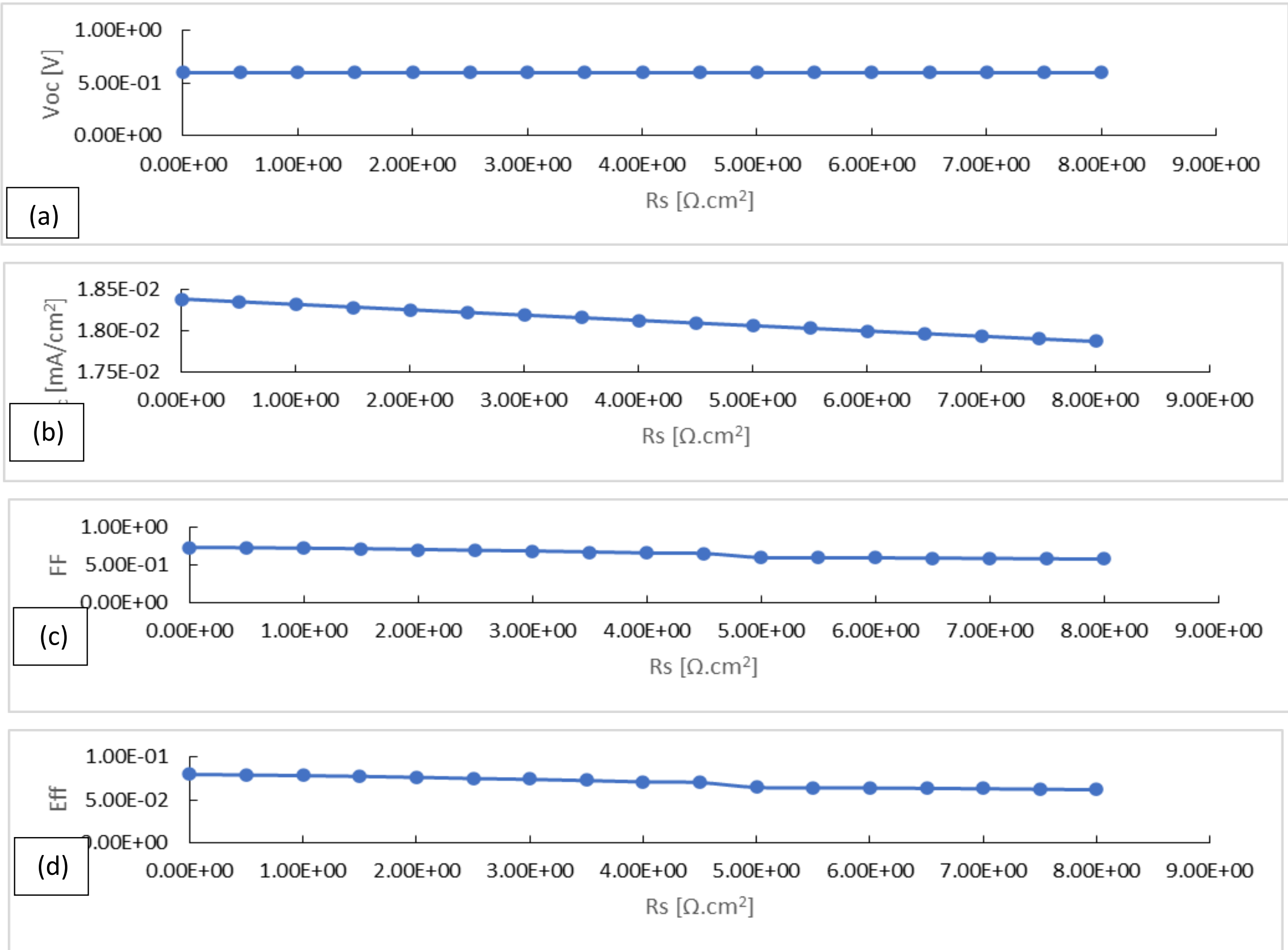

Fig. 3. Series resistance effect on the cell:(p-CZTS /n-CdS/n-i-ZnO/n-ITO)

(a) V_{oc} (b) I_{sc} (c) FF (d) Eff

4.3Change the Thickness of the Absorbent Layer (CZTS)

The absorbent layer thickness has been changed (CZTS) from (1 µm) to (5 µm) at a concentration of (2.8 x $10^{16}cm^{-3}$) and the highest effect of the series resistance (Rs) on the cell used (8 Ω cm^2), and the results were obtained as in Figure (4), As we can see from the open circuit voltage (V_{oc}) its value increases slightly with the increase in this thickness (CZTS), the short circuit current (Isc) increases with the growth of the thickness of the absorption layer (CZTS) and the reason for the increase in I_{sc} and V_{oc} is that by increasing this thickness, additional photons are absorbed which in turn will contribute to the generation of electron-hole pairs, thus increasing the J_{sc} and V_{oc}[11] based on equation (10). The fill factor (*FF*), it decreases with the rise in the thickness of the absorption layer (CZTS) according to equation (11), and as shown in Figure (4).The efficiency of the cell used (Eff), there was a noticeable rise in the efficiency with the increase in the the absorption layer thickness (CZTS)) and that the increase in the efficiency of the cell is due to the generation rise rate of pairs (electron-hole) [11], and the increase in this thickness led to a higher in the value of (J_{sc}, V_{oc}, Eff) and the decrease in the fill factor (*FF*) according to equation (13).

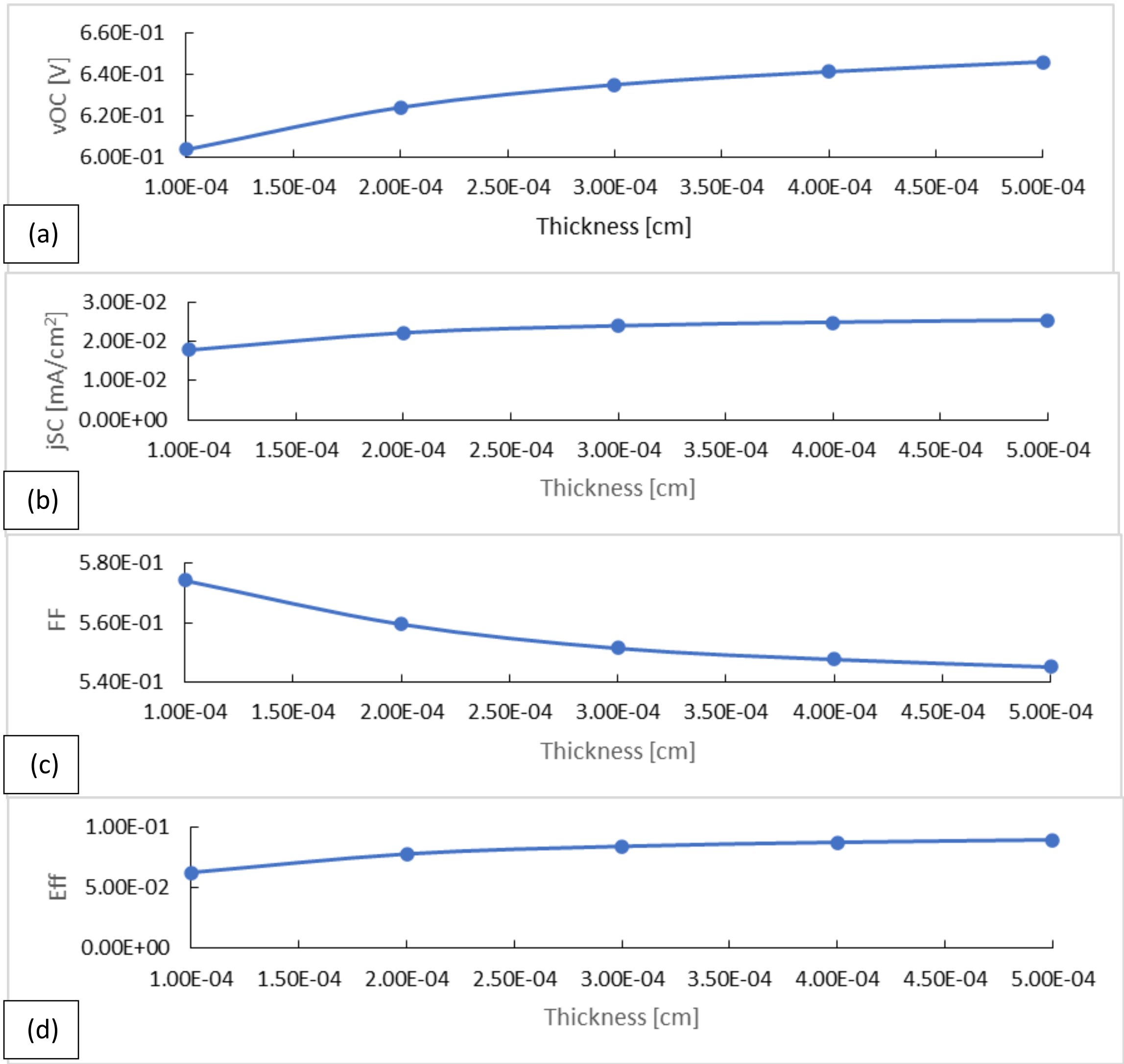

Fig. 4. Changing the thickness of the cellabsorbent layer impact: (p-CZTS /n-CdS/n-i-ZnO/n-ITO)

(a) V_{oc} (b) I_{sc} (c) FF (d) Eff

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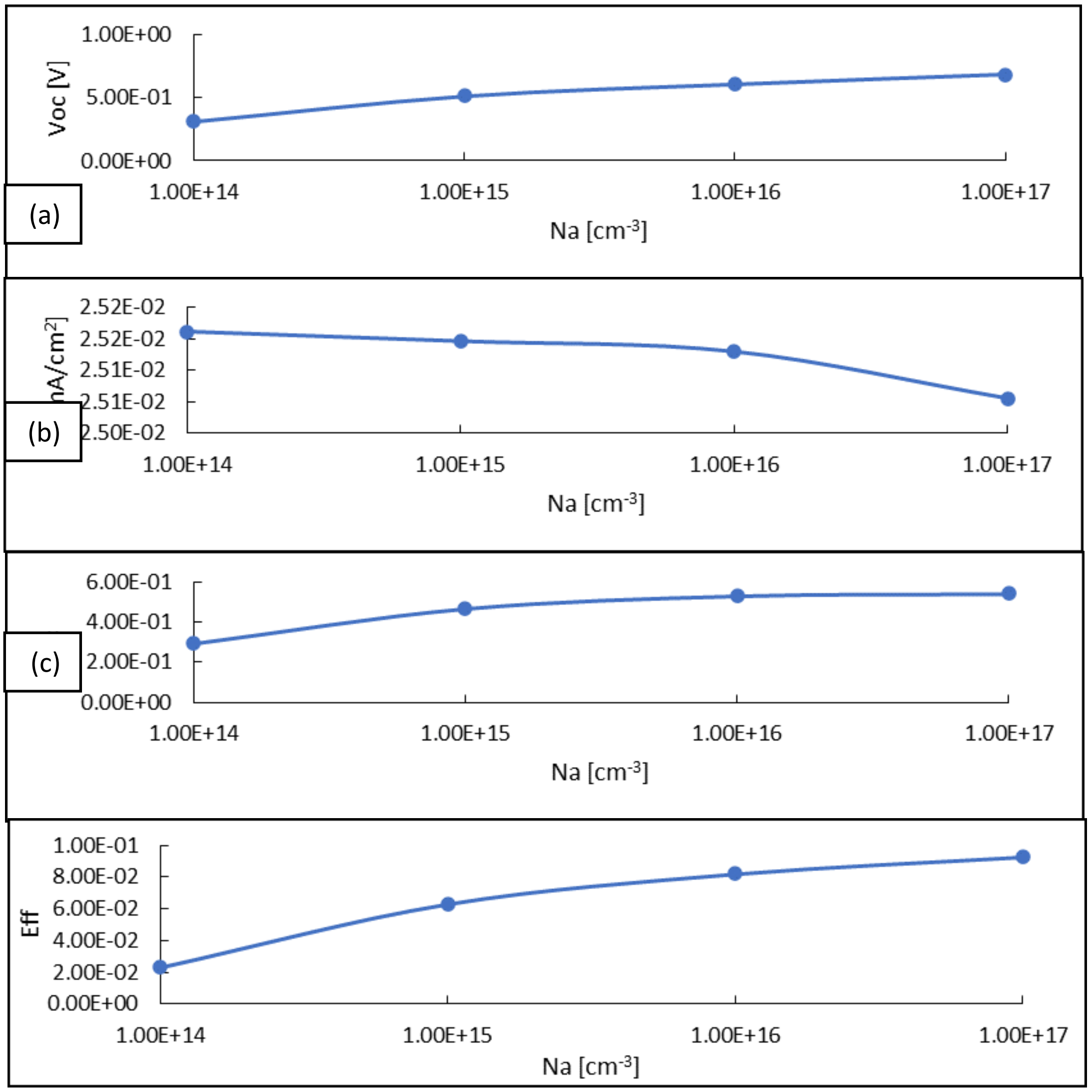
4.4Effect of Changing the Absorber Layer Concentration (CZTS)

On the increase in the value of the series resistance which led to a decrease in the efficiency of the cell, the the cellefficiency has to grow. Weused p-CZTS /n-CdS/ni-ZnO/n-ITO to change the concentration of (Na) absorption layer (CZTS) by increasing the concentration of receptors ($1 \times 10^{14} - 1 \times 10^{17}$) cm^{-3} when the absorbing layer thickness (CZTS) was fixed at (5µm) as the best thickness and the highest value of the series resistance was established (8 $\Omega.cm^2$). It was noticed that the increase in concentration increased the open circuit voltage (V_{oc}), a slight decrease in the short circuit current (I_{sc}), an the value of the filling factor (*FF*) growth and the efficiency of the cell (Eff) rise in Figure (5), because the concentration of doping rise increases in the density of the carriers, so the open circuit voltage (V_{oc}) increases as in equation (10), due to the rise in the saturation currents of the cells, which also leads to a decrease in the short circuit current (I_{sc}). Photons with longer wavelength have lower energy and are extremely absorbed in the p-CZTS layer [31]. The energy diagram of the cell when light falls through the simulation program AFORS-HETT the craters and bulges appearing in the diagram because of the contacts of the surfaces of the various layers in Figure (6).



(d)

Fig. 5. Effect of changing the absorber layer concentration (CZTS) on the cell: (p-CZTS /n-CdS/ni-ZnO/n-ITO)

(a) V_{oc} (b) I_{sc} (c) FF (d) Eff

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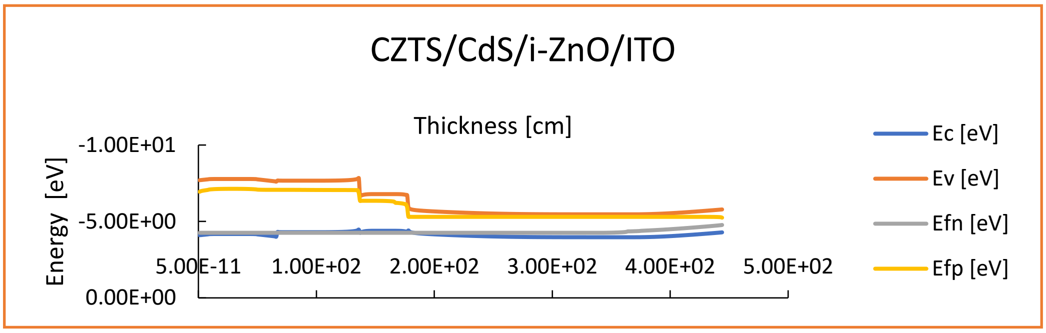

Fig. 6.The cell energy of (CZTS/CdS/ i-ZnO/ITO)

4.5Effect of Changing the Absorption Layer to Other Absorption Layers (CNTS, CIGS, CdTe):

To study cell improvement (p-CZTS /n-CdS/n-i-ZnO/n-ITO), and to obtain a cell with a higher efficiency, we have changed the absorption layer (CZTS) with other absorption layers such as (CNTS (defect), CIGS (defect), CdTe (defect), Taking into account the same conditions for the original absorption layer (CZTS) both thickness value (5 µm) and concentration ($2.8x10^{16}$ cm^{-3}), the highest value of the series resistance (8 Ω cm^2),defects (Nt = $1x10^{14}$), table (3) shows the results that were obtained after changing the absorption layer of the cell used through the simulation program, and table (4) shows the basic parameters of the absorption layers that are useful in studying the improvement of the cell through the simulation program. and the results showed that the best cell is (CIGS/CdS/i-ZnO/ITO) with efficiency reached 8.43%, and then the CNTS/CdS/i-ZnO/ITO cell also had an efficiency of 7.86%. Figure (10) shows curve (V-I) of changing the absorption layer to other absorption layers.

Table (3)The effect of changing the absorption layer to other absorbent layers (CIGS, CNTS, CdTe)

Cell	Voc [mV]	Jsc [mA/cm^2]	FF [%]	Eff [%]
CZTS/CdS/i-ZnO/ITO (defect)	614	25.5	52.9	8.29
CIGS/CdS/i-ZnO/ITO (defect)	582	33.1	43.8	8.43
CNTS/CdS/i-ZnO/ITO (defect)	660	21.6	55.2	7.86
CdTe/CdS/i-ZnO/ITO (defect)	508	25.4	47.0	6.07

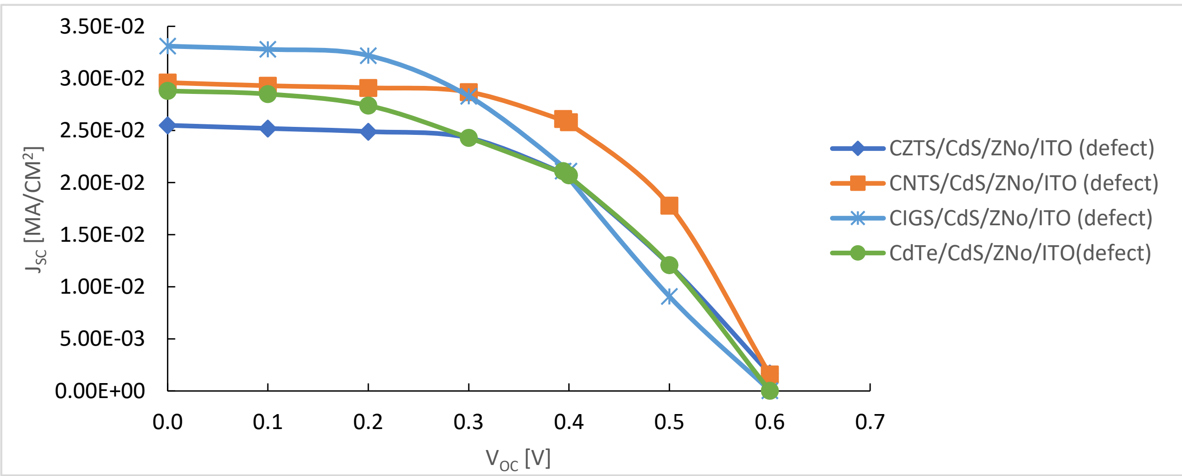

Fig. 7. Curve (I - V) Effect of changing the absorption layer to other absorption layers (CIGS, CNTS, CdTe)

Table (4) Basic parameters of absorbent layers:

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Parameters	**Symbol (unit)**	**p-CZTS**	**p-CIGS [34]**	**p-CNTS [32]**	**p-CdTe [35]**
Thickness	**d (µm)**	1 [18]	5	5	5
Dielectric permittivity	**dk**	7 [20]	13.6	9	9.4
Electron Affinity	**χ (eV)**	4.3 [21]	3.89	3.87	4.3
Band gap	**(eV)**	1.5 [18]	1.2	1.4 [33]	1.45
Density of states in CB	**Nc (cm^{-3})**	$2.2x10^{18}$ [22]	$2.2x10^{18}$	$2.2x10^{18}$	$1.3x10^{19}$
Density of states in VB	**Nv(cm^{-3})**	$1.8x10^{\backslash 19}$ [22]	$1.8x10^{19}$	$1.8x10^{19}$	$7.6x10^{18}$
Electron mobility	**µn (cm^2/Vs)**	100 [22]	300	11	50
Hole mobility	**µp (cm^2/Vs)**	25 [22]	30	11	30
Acceptor concentration	**Na (cm^{-3})**	$2.8x10^{16}$	$1x10^{16}$	$1x10^{16}$	$1x10^{16}$
Donor concentration	**Nd (cm^{-3})**	0	0	0	0
Thermal velocity of electron and hole	**υ (cm/s)**	$1x10^7$ [22]	$1x10^7$	$1x10^7$	$1X\ 10^7$
Layer density	**Rho (g*cm^{-3})**	2.328 [11]	2.328 [11]	2.328	2.328
Refractive index	**N**	2.85 [23]	2.85	2.77 [33]	2.76 [36]
Extinction coefficient	**K**	0.1 [23]	0.1	0.03 [33]	0.13 [36]
rap density	**Nt (cm^{-3})**	$1x10^{14}$ [23]	$1x10^{14}$[23]	$1x10^{14}$	$1x10^{14}$
Characteristic Energy	**Et (ev)**	0.5 [23]	0.5 [23]	0.5 [23]	0.5
Capture cross section electrons and hole (cm²)	**δn ,δp**	$1x10^{-15}$ [22]	$1x10^{-15}$ [22]	$1x10^{-15}$ [22]	$1x10^{-15}$
Type Defect		Single/D	Singie/D	Singie/D	Singie/D

5 – Conclusions:

This study simulated CZTS / CdS / i-ZnO / ITO cell by the AFORS-HET program while compared tothe experimental results.The effect of series resistance (Rs) have been optimized by increasing its value, it was noted that increasing the value of Rs significantly affected the efficiency of the cell. In order to overcome the effect of Rs. We changed both thickness and concentration of the absorbent layer (CZTS).A higher efficiency obtained of the cell Eff 8.29%. We also changed the absorption layer with other absorption layers (CIGS, CNTS, CdTe) under the same conditions as the original absorption layer (CZTS). It was found to be as follows; Eff- 8.43%, *FF*- 43.8%, J_{sc} - 33.1 mA/cm^2 and V_{oc}–582 mV which were belong to CIGS absorb layer. We can conclude that the best cell obtained result in this study is from CIGS absorption layers.

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