SIMULATION OF THE EFFECT OF PARALLEL RESISTANCE ON CHALCOGENIDE SOLAR CELLS USING ONE-DIMENSIONAL AFORS-HET PROGRAM

Ziyad J. Yaseen
Dept of Physics, College of Science, University of Kirkuk, Iraq.
ziyad.jumaah55@gmail.com

Rafea.A. Munef [1]
Dept of Physics, College of Science, University of Kirkuk, Iraq.

Abstract:

In this work, the effect of parallel resistance on the performance of the CZTS/CdS/i-ZnO/ITO solar cell has been examined by a one-dimensional program. The parallel resistance is changed from (100-1400) Ω.cm^2. The above cell arrangement shows the possibility to achieve an efficiency of 10.64%,. This valu consistent with the experimental research. Yet, the efficiency was 6.75% and increased to 9.80%. After optimization. by the change of the absorbent 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 (CZTS) layer (Eff- 10.64%, FF- 62.74%, J_{sc} – 25.81 mA/cm^2 and V_{oc} – 657 mV).

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

1 - Introduction:

The principle of solar cell work is based on the conversion of sun light energy into electrical energy through the photovoltaic phenomenon, and this is achieved through devices called solar cells [1]. Conversion-efficiency, cost and reduced toxicity are among the factors which attracts researchers worldwide [2]. Quaternary Chalcogenide compounds, as alternative and suitable materials, characterized by their direct energy gap close to the ideal values, low cost and availability, attracted extensive research efforts [3]. In this research, we study the quaternary chalcogenide compound (CZTS), it is a semiconductor compound in the group (I-II-IV-VI), and it is available and inexpensive [4], has a direct energy gap of (1.5 eV), refractive index (2.07) [5], high absorption coefficient (10^4 cm^{-1}), and an acceptable conversion efficiency [6]. When researchers began working on solar cells based on (Cu2ZnSnS4) (CZTS), a rapid increase in the efficiency was obtained (6.7% in 2009 to 11.1% in 2012). The compound CZTS is a promising candidate for thin film solar cells, as it is considered one of the lowest costs and least toxic compounds. The highest efficiency of the CZTS cell that has been achieved so far is 12.7% [7]. It is still far from theoretical calculations, and a complete understanding and control of the various manufacturing processes and reactions is still required in order to obtain the required high efficiency. Various deposition techniques have been used including 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 including a deposition step which is followed by a high-temperature annealing process [8]. There is a need for low pressure, to prevent decomposition reactions that can occur at high temperatures [9]. This research includes a study of the effect of parallel resistance (Rp) on the solar cell structure: (p-CZTS (n-CdS/n-i-ZnO/n-ITO) under the influence of changing the thickness and concentration of both the absorption layer and the buffer layer. The highest effect of the parallel resistance (Rp) is at the highest value (1400 Ω. cm^2) covered by this study. Also, studying the change of the absorption layer with other absorption layers at the same conditions as the absorption layer (CZTS). We compared the experimental cells with the theoretical cells to obtain a highly efficient cell. We have a simulation program AFORS-HET which is a 1D digital simulation program used to model heterogeneous solar cells, and solve semiconductor equations such as (the transport and continuity 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 relationship between current - voltage (I-V) quantum efficiency (QE) capacitance - voltage (C-V) [10]. It has an easy-to-use interface through which the basic parameters can be changed to suit the given measurements.

2- Theoretical study:

2-1 continuity equation:

The continuity equation is given for electrons and holes [11]

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

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

2-2 Poisson's equation:

The charge density and displacement are related according to Maxwell's equation

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

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

The Poisson equation is in the following form [Reference if possible]

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

When ε is constant, Poisson equation reduces to

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

We usually use four variables to study what comes out of the solar cell, which are:

1 - Short circuit current (Isc): It is the largest flowing current in the solar cell, when the load is equal to zero (RL= 0). The solar cell voltage is equal to zero at the highest value (Isc) [12].

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

2- Open circuit voltage (Voc): It represents the greatest effort that can be obtained from the solar cell when the load resistance is infinite (RL = ∞). the flow is at its lowest level equal to (0), in the equation (8) below[81].

$$V_{oc}=\frac{nKT}{q}ln\left(\frac{I_L}{I_0}+1\right) at\ I=0 \quad (8)$$

Where Voc depends on the light current (I_L) and the saturation current (I_0). The saturation current (I_0) in solar cells. is given by the equation below [13].

$$I_\circ = A\left[\frac{qD_e ni^2}{L_e N_A}+\frac{qD_h ni^2}{L_h N_D}\right] \quad (9)$$

Where: (A) cross-section area, (D_h) and (D_e) fixed spread electrons and gaps, (ni^2) the real box of concentrations. (L_e) The length of the spread of electrons, (L_h) the length of the spread of gaps. Acceptable estimate of minimum saturation current density (I_0) as a function of the blocked gap of the equation below [13].

3- Fill factor (FF): Its value can be found by dividing the largest capacity (which we find by multiplying the largest Imax current in the largest Vmax voltage), on the theoretical capability (found through voc output in Isc), as shown in equations (11) and (12) [14].

$$FF\% = \frac{P_{max}}{P_t} \quad (11)$$

$$FF\% = \frac{I_{mp}.V_{mp}}{I_{sc}.V_{oc}} \quad (12)$$

4- Efficiency (Eff): It can be defined as the ratio of energy coming out of the solar cell to the energy it enters. It is used to compare the operation of two solar cells, so the external energy of the solar cell is given the equation below.

$$P_m = I_m.V_m \quad (13)$$

Cell efficiency is known as the following equation:

$$\eta = \frac{P_m}{P_{in}} = \frac{I_m V_m}{P_{in}} = \frac{V_m^2 \, I_s \left(\frac{q}{KT}\right) \exp\left(\frac{qV_m}{KT}\right)}{P_{in}} \qquad (14)$$

$$\eta = \frac{\mathrm{FF} \times \mathrm{I_{sc}} \times \mathrm{V_{oc}}}{\mathrm{p_{in}}} \times 100\% \qquad (15)$$

The P_in: the sun's rays falling on the solar cell [14].

3- Solar Cell Structures:

The structure of the solar cell used is shown in Figure 1. It consists from a number of different layers; p-CZTS /n-CdS/n-i-ZnO/n-ITO as shown in the figure. The (i-ZnO) layer is a transparent conductive oxide with a direct energy gap (3.37 eV) [15], and a thickness of (0.05) µm, preceded by an (0.3 µm) thick transparent window layer of titanium dioxide (ITO) that has a large energy gap (3.6 eV), and high transparency [16]. A layer of (0.06 µm) thick cadmium sulfide (CdS) and a relatively large energy-gap (2.4 eV) follows the (ZnO)-layer, followed by a (1 µm) thick, (1.5 eV) [17]. energy-gap, layer of zinc-selenium (CZTS). Molybdenum (Mo) is used as the back-contact.

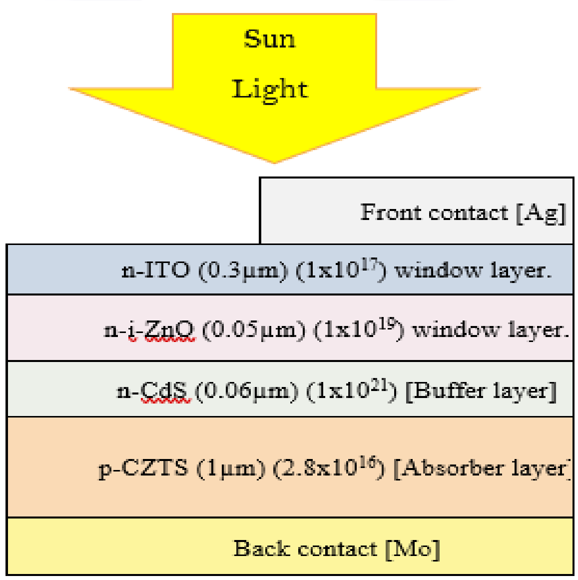

Fig. 1. The diagram of Solar Cell Structure: p-CZTS / n-CdS/ n-i-ZnO/ n-ITO

4- Results and Discussion:

4.1 Comparing Simulation with Experimental Result:

In this study, as a start, we used results of an experimental study by [17] for a (CZTS) solar cell in order to check with the simulation program (AFORS-HET). As shown in Table (1), there is a great match between results of the experimental cell and the theoretical cell. The open circuit voltage (Voc) is roughly the same, the short-circuit current-density (Isc) is slightly less, and the value of fill factor (FF) and efficiency (Eff) is slightly larger. The thickness and the doping-concentration of the layers were, respectively: absorbing layer (CZTS): (1 µm) and (2.8 x 10^{16} cm^{-3}), buffer layer (CdS): (60 nm) and concentration (1 x 10^{21} cm^{-3}), permeable layer (i-ZnO): (50 nm) (1 x 10^{19} cm^{-3}), and the transparent layer (ITO): (300 nm) and (1 x 10^{17} cm^{-3}). The value of series resistance (5.76 Ω cm^2) and parallel resistance (400 Ω cm^2), and other basic parameters constituting the cell were taken from Published works as in Table (2).

Table (1) Comparison between theory and practice:

	Cell	Voc (mV)	Jsc (mA/cm^2)	FF%	Eff%
1-	p-CZTS /n-CdS/ni-ZnO/n-ITO experimentally	603	19	55	6.2
2-	p-CZTS /n-CdS/n-i-ZnO/n-ITO theoretical	603.9	18.01	59.12	6.4

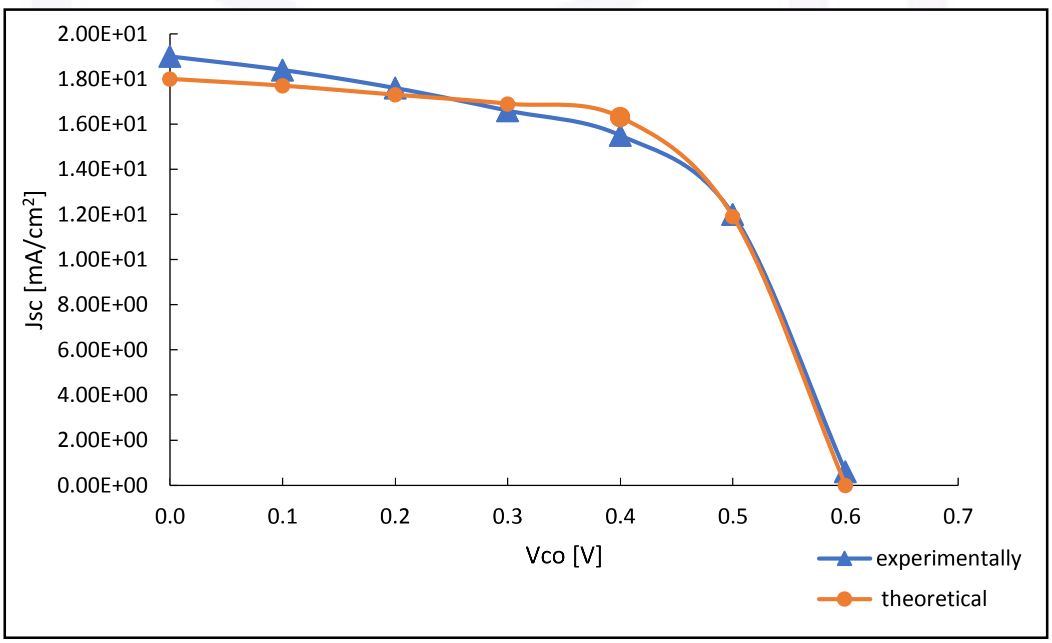

Fig. 2. (J - V) graph of the CZTS Solar Cell.

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Table (2) parameters used in the search:

Parameters	Symbol (unit)	p-CZTS	n-CdS	n-i-ZnO	n-ITO
Thickness	d (µm)	1 [17]	0.06 [17]	0.05[17]	0.3 [17]
Dielectric, permittivity	.dk	7 [18]	10 [22]	9 [10]	10 [25]
Electron, Affinity	χ (eV)	4.3 [19]	4.2 [22]	4.4 [24]	4.1 [25]
Band gap	(eV)	1.5 [17]	2.4 [22]	3.37 [24]	3.6 [25]
Density, of states in CB	Nc (cm-3)	2.2x1018 [20]	1.8x1019 [22]	2.2x1018 [10]	2.2x1018 [26]
Density of states, in VB	Nv(cm-3)	1.8x1019 [20]	2.2x1018 [22]	1.8x1019 [10]	1.8x1019 [26]
Electron, mobility	µn (cm2/Vs)	100 [20]	100 [23]	100 [10]	100 [26]
Hole mobility,	µp (cm2/Vs)	25 [20]	25 [23]	25 [10]	25 [26]
Acceptor, concentration	Na (cm2)	2.8x1016	0	0	0
Donor concentration	Nd (cm2)	0	1x1021	1x1019	1x1017
Thermal velocity of electron and hole	υ (cm/s)	1x107 [20]	1x107[10]	1x107 [10]	1x107 [10]
Layer density	Rho (g/cm-3)	2.328 [10]	2.328 [10]	2.328 [10]	2.328 [10]
Refractive index	N	2.85 [21]	File AFORS-HET	File AFORS-HET	1.827 [27]
Extinction coefficient	K	0.1 [21]			0.0031 [27]
Total trap density (defect)	Nt (cm-3)	1x1014 [21]			
Characteristic Energy (defect)	Et (eV)	0.5 [21]			
Capture cross section electrons and hols (cm^2)	δn , δp	1x10-15 [20]			
Type Defect		Single/D			

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

Parallel resistance causes significant loss of power, usually as a result of manufacturing defects and leaks at the edges of the cell, and reduced parallel resistance (Rp) causes a significant loss of power in the solar cell by displacing the path of the light-generated current, such deviation reduces the current that flows through the solar cell link as well as reduces cell voltage [28]. To study the effect of parallel resistance (Rp) on the cell used (p-CZTS./n-CdS /n-i-ZnO /n-ITO), the value of

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parallel resistance (Rp) has changed (100_ 1400) Ω. cm^2 . We note that there is an increase in both the open circle volts (Voc), the short circuit current (Isc), the filling factor (FF) and the efficiency of the cell (Eff) as in the form (3).

(a)
(b)
(c)
(d)

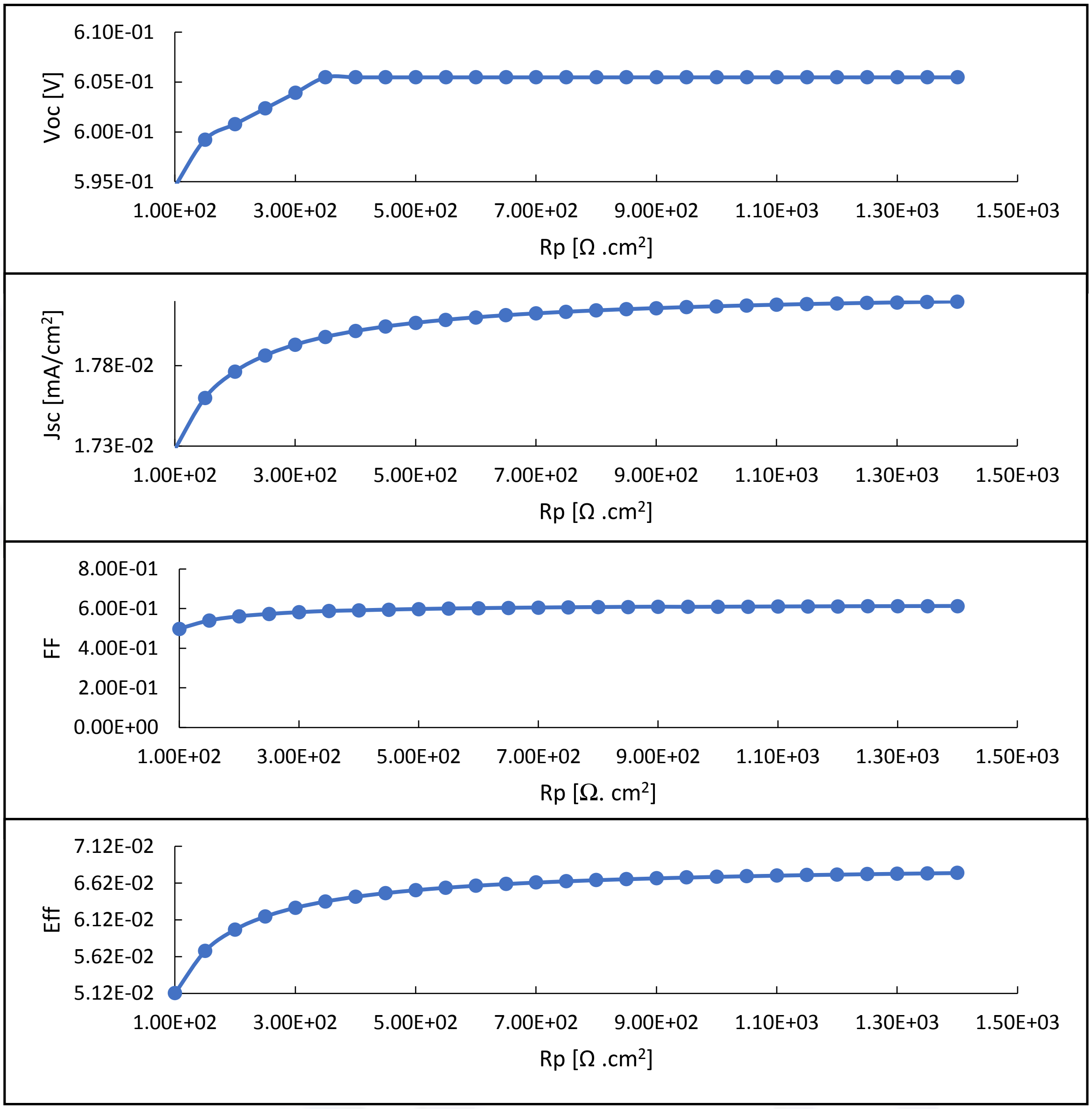

Fig. 3. Parallel resistance. effect on the cell.: (p-CZTS /n-CdS/n-i-ZnO/n-ITO)

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

4.3 Effect of the thickness of the absorbent layer (CZTS)

The thickness of the absorption layer (CZTS) has been varied from (1 µm) to (5 µm) at a concentration of (2.8 x 10^{16} cm^{-3}) and the highest effect of the

parallel resistance (Rp), on the cell used (1400 Ω. cm^2), and the results are shown in Figure (4). With increasing thickness, the open-circuit voltage (Voc) increases slightly, the short-circuit

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current (Isc) also increases by equations (8,9). as well as the increased value of cell efficiency (Eff), due to the fact that by increasing the thickness of the absorption layer (CZTS), there will be absorption of more photons which in turn will contribute to the generation of pairs electron – gap thus increasing the current and voltage Jsc, Voc and Eff [10]. The filling factor (FF) decreases slightly with increased absorption layer thickness (CZTS), in accordance with equation (12).

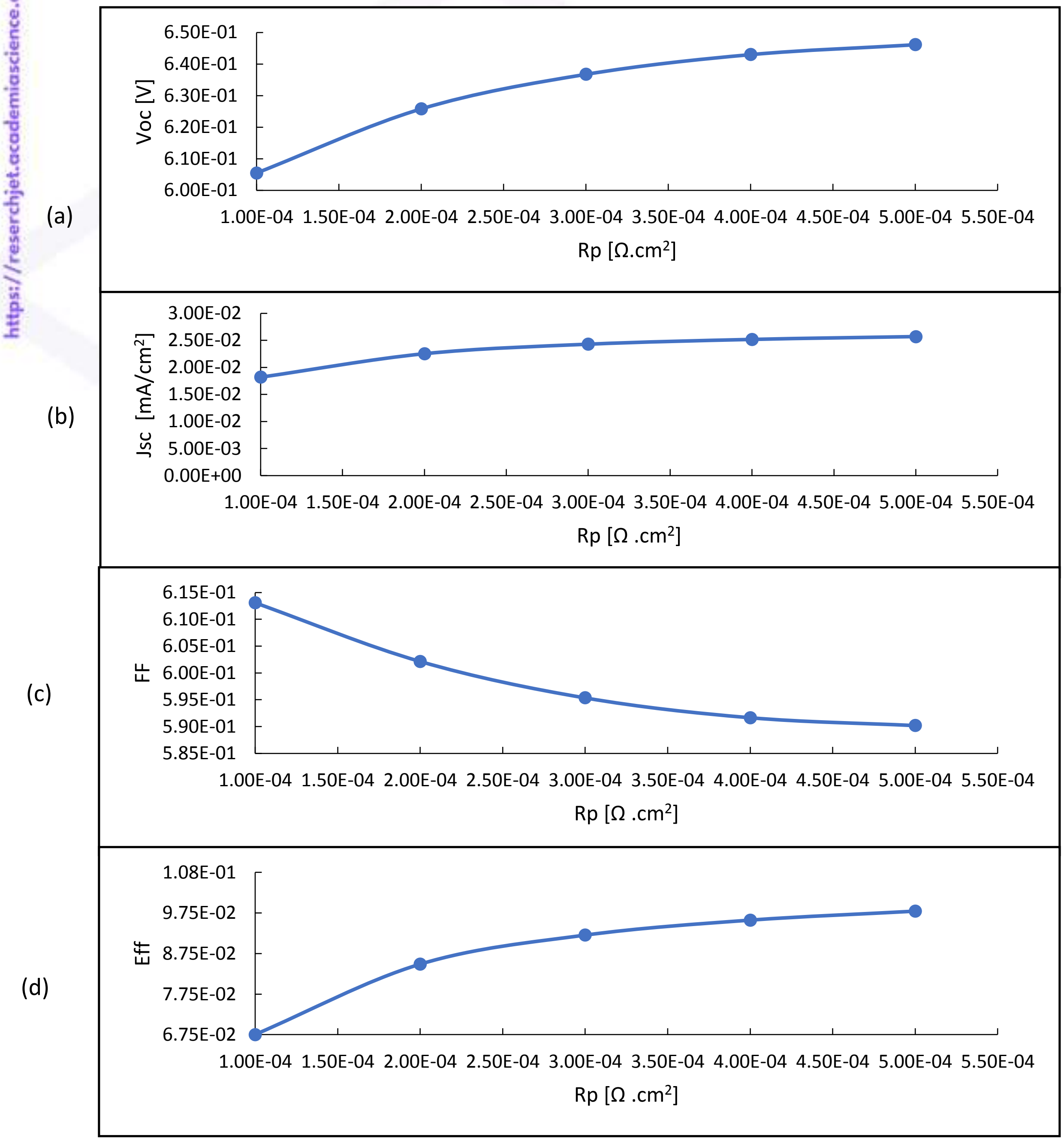

Fig. 4; Changing the thickness of the cell absorbent layer impact.: (p-CZTS /n-CdS/n-i-ZnO/n-ITO)

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

4.4 Effect of Changing the Absorber Layer Concentration (CZTS)

In the simulation, the concentration of (Na) acceptor in the absorption layer (CZTS) was varied in the range ($1 \times 10^{14} – 1 \times 10^{16}$) cm^{-3} while the thickness of the (CZTS) layer was fixed at (5μm) and the parallel resistance (Rp) was fixed at (1400 Ω. cm^2).The increase in the doping concentration led to an increase in the open-circuit voltage (Voc), a slight decrease in the short-circuit current (Isc), an increase in the value of the fill-factor (FF) and an increase in the efficiency (Eff) as shown in Figure (5). Because the increase in the concentration of doping leads to an increase in the density of the carriers, so the open circuit voltage (Voc) increases as in equation (8), due to the decrease in the saturation current of the cell, which also leads to a decrease in the short circuit current (Isc). Longer wavelength photons have less energy and are deeply absorbed into the p-CZTS layer [29]. Figure 6 shows the power chart of the best cell obtained, which shows (Spike) between the absorption and reflection layer and (Cliff), between the absorption layer, alignment and permeability, which increases the efficiency of the solar cell .

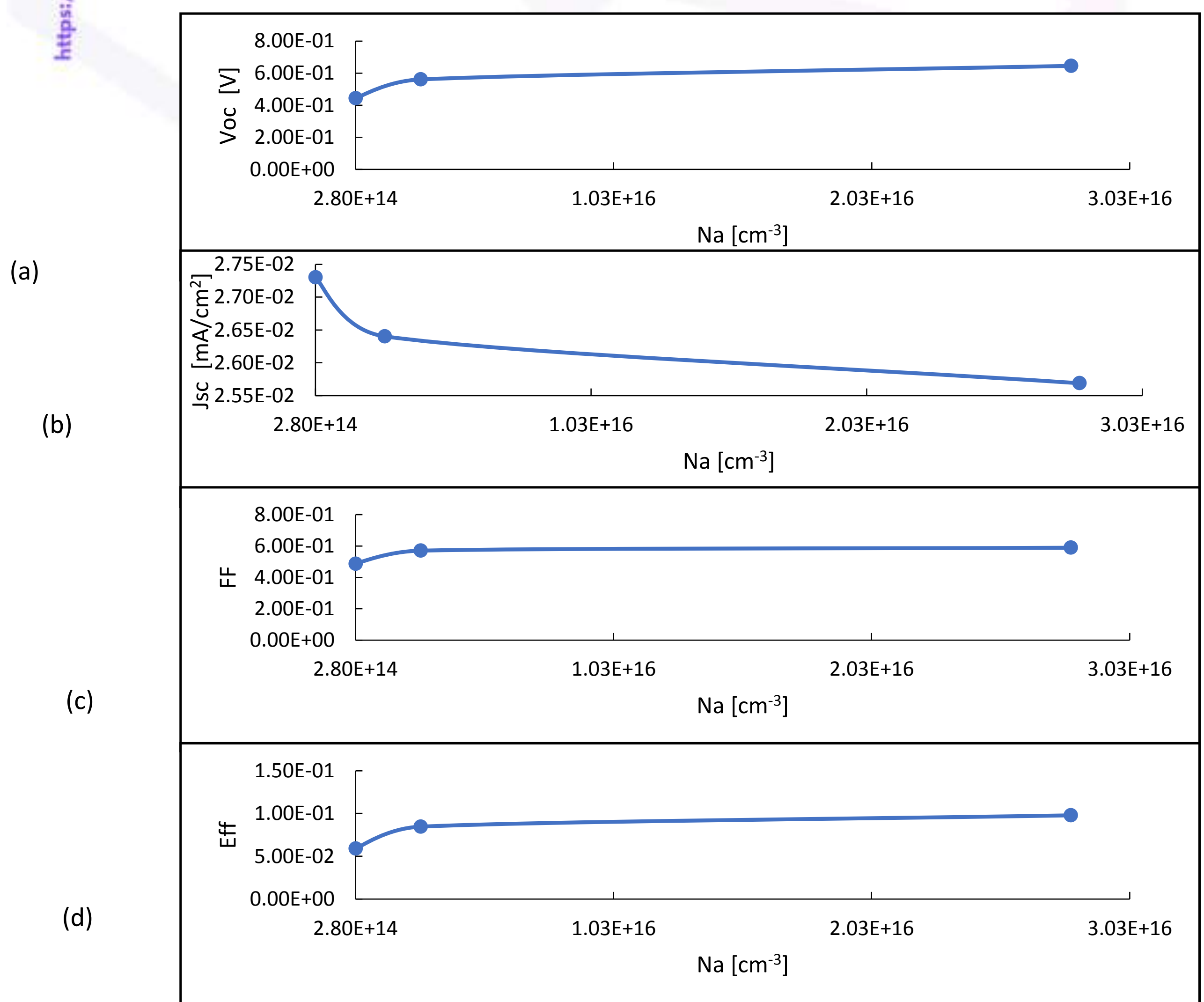

Fig. 5; Effect of changing the absorber layer concentration (CZTS) on the cell: (p-CZTS /n-CdS/ni-ZnO/n-ITO) V_{oc} (b) I_{sc} (c) FF (d) Eff

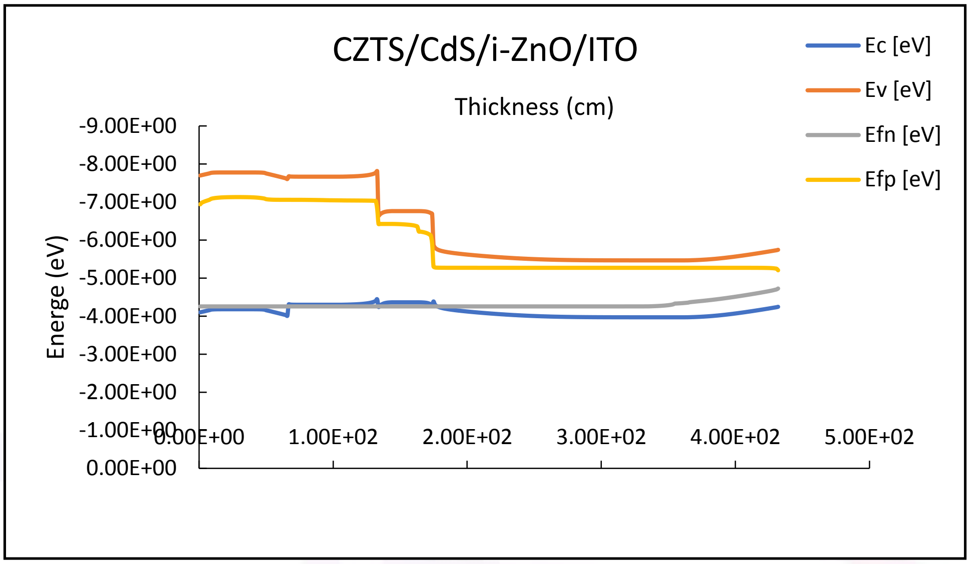

Fig. 6; The energy diagram of the cell. (CZTS /CdS / i-ZnO /ITO)

4.5. Effect of changing the type of the absorption layer (CNTS, CIGS, CdTe):

To investigate improvement of the cell (p-CZTS /n-CdS/n-i-ZnO/n-ITO), and to obtain a higher efficiency, we replaced the original absorption layer (CZTS) with other absorption layers such as (CNTS (defect), CIGS (defect), CdTe (defect). The same conditions as for the original absorption layer (CZTS) were used; thickness value (5 µm), doping-concentration ($2.8x10^{16}$ cm^{-3}), parallel-resistance (1400 Ω. cm^2), and defects density (Nt = $1x10^{14}$). All the other layers were kept the same. Table (4) shows the basic parameters of the absorption layers that are used in the study, and Table (3) shows the results as obtained from the simulation program. The results shows that the best cell is (CIGS/CdS/i-ZnO/ITO) its efficiency reached 10.39%, and that the CNTS/CdS/i-ZnO/ITO cell had an efficiency of 9.02%. Figure (10) shows (V-I)- curves of the cells..

Table (3) Effect of changing the type of the absorption layer (CIGS, CNTS, CdTe)

Cell	V_{oc} [mV]	J_{sc} [mA/cm^2]	FF [%]	Eff [%]
CZTS/CdS/i-ZnO/ITO (defect)	657	25.81	62.74	10.64
CIGS/CdS/i-ZnO/ITO (defect)	575	34.16	53.82	10.39
CNTS/CdS/i-ZnO/ITO (defect)	646	21.60	64.68	9.02
CdTe/CdS/i-ZnO/ITO (defect)	496	25.80	53.19	6.90

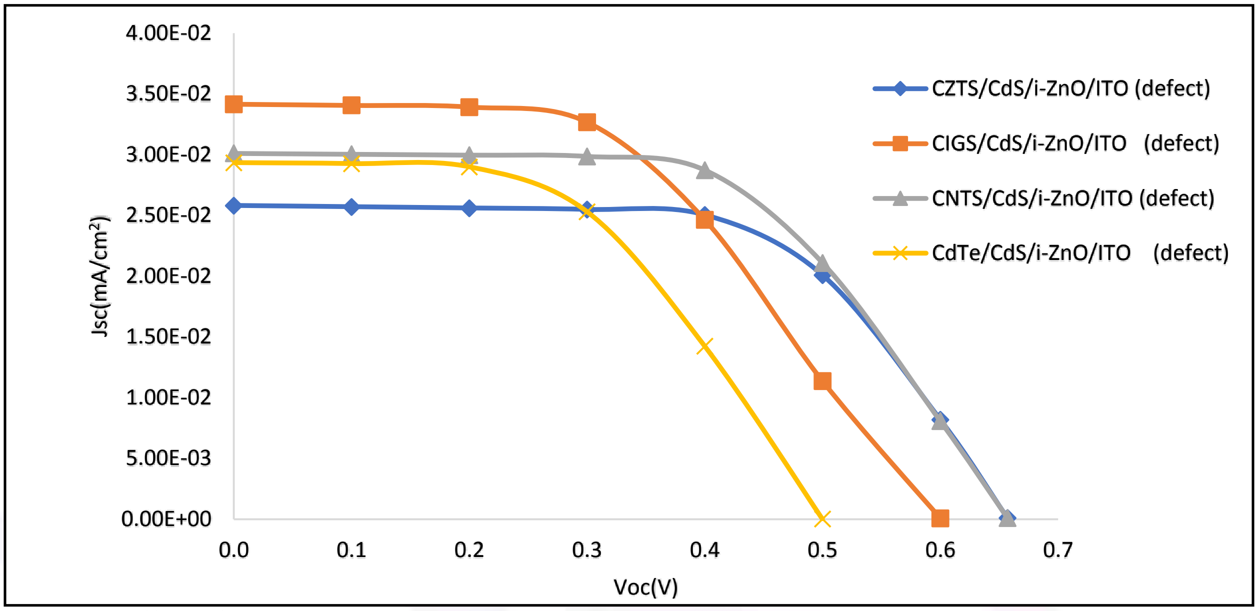

Fig. 7. Effect of changing the type of the absorption layer (CIGS, CNTS, CdTe) on the (I - V)- curve.

Table (4) Basic parameters of absorbent layers:

Parameters	**Symbol (unit)**	**p-CZTS**	**p-CIGS [31]**	**p-CNTS [29]**	**p-CdTe [32]**
Thickness	**d (μm)**	**1 [17]**	**5**	**5**	5
Dielectric permittivity	.dk	7 [18]	13.6	9	**9.4**
Electron Affinity	**χ (eV)**	**4.3 [19]**	**3.89**	**3.87**	4.3
Band gap	(eV)	1.5 [17]	1.2	1.4 [30]	**1.45**
Density of states in CB	**Nc (cm-3)**	**2.2x1018 [20]**	**2.2x1018**	**2.2x1018**	1.3x1019
Density of states in VB	Nv(cm-3)	1.8x1019 [20]	1.8x1019	1.8x1019	**7.6x1018**
Electron mobility	**μn (cm2/Vs)**	**100 [20]**	**300**	**11**	50
Hole mobility	μp (cm2/Vs)	25 [20]	30	11	**30**
Acceptor concentration	**Na (cm-3)**	**2.8x1016**	**1x1016**	**1x1016**	1x1016
Donor concentration	Nd (cm-3)	0	0	0	**0**
Thermal velocity of electron and hole	**υ (cm/s)**	**1x107 [20]**	**1x107**	**1x107**	1X 107

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Layer density	Rho (g/cm-3)	2.328 [10]	2.328 [10]	2.328	**2.328**
Refractive index	**N**	**2.85 [21]**	**2.85**	**2.77 [30]**	2.76 [33]
Extinction coefficient	K	0.1 [21]	0.1	0.03 [30]	**0.13 [33]**
Total trap density	**Nt (cm-3)**	**1x1014 [21]**	**1x1014[21]**	**1x1014**	1x1014
Characteristic Energy	Et (eV)	0.5 [21]	0.5 [21]	0.5 [21]	**0.5**
Capture cross section electrons and hole (cm²)	**δn , δp**	**1x10-15 [20]**	**1x10-15 [20]**	**1x10-15 [20]**	1x10-15
Type Defect		**Single/D**	**Singie/D**	**Singie/D**	Singie/D

5 – Conclusions:

Simulation of cell performance using software program (AFORS-HET), for an experimental solar cell (CZTS / CdS / i-ZnO / ITO), showed parameter values of: Eff- 6.4%, FF- 59.1%, Jsc – 18.01 mA/cm^2 and Voc – 603.9 mV which are close to those reported experimentally. The study of varying the parallel-resistance (Rp) from (100 Ω. cm^2) to (1400 Ω.cm^2), shows that it affects the efficiency significantly. We changed the thickness and concentration of the absorbent layer (CZTS), which counter the effect of (Rp), we obtained an efficiency of Eff 10.64%. We also changed the type of the absorption layer with other absorption layers (CIGS, CNTS, CdTe) under the same conditions as the original absorption layer (CZTS). It was found that the best cell is with absorption-layer (CZTS) with cell parameters: Eff- 10.64%, FF- 62.74%, Jsc – 25.81 mA/cm^2 and Voc – 657 mV.

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