



## Simulation of CZTSSe single solar cells by AFORS-HET software

Buthina M. Jandary , Ayed N. Saleh

Physics Department , College of Education for pure science University of Tikrit , Iraq

<https://doi.org/10.25130/tjps.v25i2.238>

### ARTICLE INFO.

Article history:

-Received: 23 / 9 / 2019

-Accepted: 29 / 11 / 2019

-Available online: / / 2020

**Keywords:**  $\text{Cu}_2\text{ZnSn}(\text{SSe})_4$ , thin-film solar cell, numerical modeling, AFORS-HET software.

**Corresponding Author:**

**Name:** Buthina M. Jandary

**E-mail:** [buthina088@gmail.com](mailto:buthina088@gmail.com)

**Tel:**

### ABSTRACT

In this paper, this study simulated photovoltaic characteristics of single heterojunction solar cell with  $\text{Cu}_2\text{ZnSnS}_4$  and  $\text{Cu}_2\text{ZnSnSe}_4$  absorber layer numerically using the AFORS-HET program. n-CdS/ZnO double buffer layer is used for heterostructure interfaces with the absorber layer. The cell performance is investigated against variation of different absorption layer properties such as thickness, carrier concentration. The mixed zinc and cadmium sulphide ( $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ ) is hired as buffer layers and research of the effect its thickness. CdS was selected a buffer because it improves the interface with absorbent CZTSSe and has a lofty sending in the blue wavelength. at thickness =1  $\mu\text{m}$  and acceptor concentration ( $N_a=7.9 \times 10^{15} \text{ cm}^{-3}$ ), a maximum efficiency ( $\eta=11.9\%$ ) is provided with an open-circuit voltage ( $V_{oc}=688\text{mv}$ ), short-circuit current ( $J_{sc}=24.6 \text{ mA.cm}^{-2}$ ) and fill factor ( $FF=70.8$  of the CZTS solar cell, and  $V_{oc}=(597 \text{ mv})$ ,  $J_{sc}= (41.7\text{mA.cm}^{-2})$ ,  $FF = (81.2 \%)$  and  $\eta= (20.2\%)$  of the CZTSe solar cell.

### 1- Introduction

The photovoltaic (PV) system, known today as renewable, clean, and sustainable have attracted much interest because of the following advantages: First, photovoltaic systems able of converting sunlight directly into electrical energy. Second, theoretical efficiency of photovoltaic system is relatively higher than the energy sources other. Third, photovoltaic cell technique not contain moving parts, which prevents corrosion of the system resulting from mechanical movement were PV system work continuously without maintenance [1]. Today, researchers are interested in exploring and developing new, cost-effective and abundant materials in the earth, such as semiconductors  $\text{Cu}_2\text{ZnSnS}_4$  and  $\text{Cu}_2\text{ZnSnSe}_4$  [ $\text{Cu}_2\text{ZnSn}(\text{SSe})_4$  (CZTSSe)] ,whose compounds are widely studied as absorption layers for thin-film solar cells [2]. due to its potential as a future absorber material for high efficiency thin film solar cell technology. The properties such as environmentally benign and earth a bundant constituent elements, optimum direct bandgap (1-1.5eV) and high absorption coefficient ( $\alpha > 10^4 \text{ cm}^{-1}$ ), ( thickness of 1 micrometer is enough to absorbare most of the falling sunlight) , make CZTSSe a material of choice as an alternative to the existing solar photovoltaic thin film technologies [3] ,Where the process of production of this compound is cheaper

compared to the bsorption of CdTe and CIGS,as shown in Fig 1.

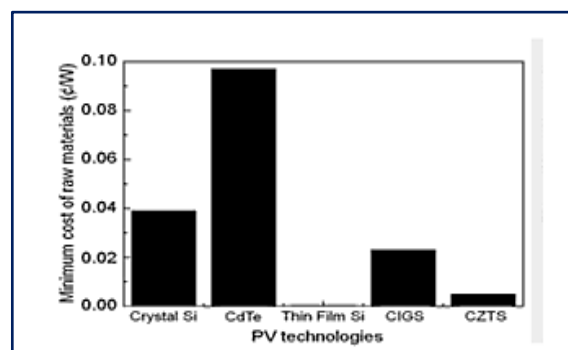


Fig 1: The cash cost of producing the absorption layers [4]

One of the greatest features of the  $\text{Cu}_2\text{ZnSn}(\text{SSe})_4$  compound is the possession of a direct band gap and easy to change which depends on the material composition by controlling the contents of S and Se [5]. Band gap varies with the ratio (S) and (S + Se) of about 1.0 eV in  $\text{Cu}_2\text{ZnSnSe}_4$  (CZTSe) to 1.5 eV in  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS). Recent research shows that the S / Se variation does not only result in variation of the band gap, but also changes the electronic structure, absorption coefficient, and other parameters such as electron affinity and dielectric permittivity, etc .

**2. Simulation Approach**

AFORS-HET (automat for simulation of Heterostructures) is a one dimensional numerical computer program for modelling multi layer homo- or Heterojunction solar cells as well as a variety of common characterization techniques have been implemented, like current-voltage (IV), internal quantum efficiency (IQE), impedance, capacitance (CV, CT) and photoluminescence (PL). A user-friendly interface allows to easily perform parameter variations, and to visualize and compare your simulation. The program solves the one dimensional semiconductor equations in steady-state and for a small sinusoidal ac-perturbations. has been developed since the year 2000 , and is free-on-demand. For more details,can be found in the developer’s guide provided with the software [6,7]. To model the electrical output precisely in most cell types, it is sufficient to solve the basic semiconductor equations, with the drift-diffusion approximation [8]:

$$1- -\nabla E = \nabla \cdot (\epsilon \nabla \psi) = -q(p - n + N_D^+ - N_A^-) \dots (1)$$

$$2\text{-Continuity equations : } \frac{\partial n}{\partial t} = \frac{1}{q} \nabla J_n + G - R_n, \frac{\partial p}{\partial t} = \frac{1}{q} \nabla J_p + G - R_p \dots (2)$$

$$3\text{- Transport(drift- diffusion): } J_n = -q\mu_n n \nabla \psi + qD_n \nabla n, J_p = -q\mu_p p \nabla \psi + qD_p \nabla p \dots (3)$$

Where  $\epsilon$  Electrical dielectric constant,  $\psi$  electrostatic voltage,  $n$  and  $p$  are electron and hole ensities.  $N_D^+, N_A^-$ , donor and acceptor concentration.  $J_n, J_p$  current density and holes,  $R_n(p), G$  is the recombination and generation rate).  $\mu_n, \mu_p$  Electron and hole mobility  $D_n (p)$  is the diffusivity of electron (hole). When simulating CZTS and CZTSe solar cells, the parameters in semiconductor transfer equations should be properly compensated which represent the properties of the semiconductor., such as band gap energy, case density, insulation constants, electron affinity etc. The measurement model iterates the specific data points to determine

the maximum power point (Impp), open –circuit voltage (Voc), short circuit current (Isc) and thus the fill factor (FF) .The efficiency of the solar cell was calculated as[9,10]:

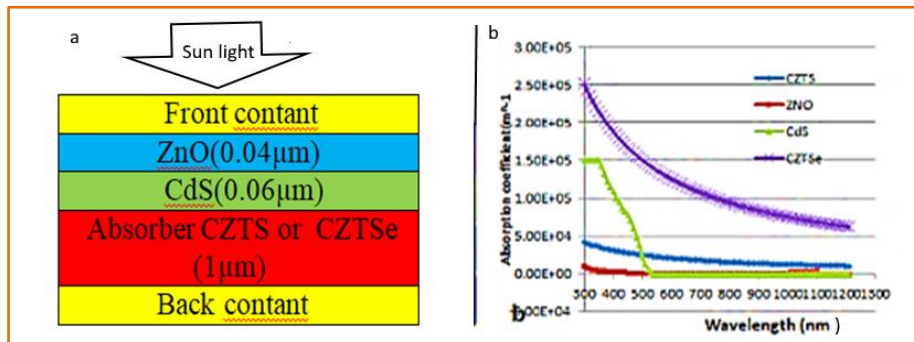
$$FF = \frac{V_{max} I_{max}}{V_{oc} I_{sc}} \dots (4)$$

$$\eta = FF \frac{V_{oc} I_{sc}}{\text{Illumination power}} \dots (5)$$

CZTS(Se) solar cells show that relatively low conversion efficiency compared to those in other photovoltaic technology fields, such as CIGS solar cells with a standard capacity of more than 20% [11]. Therefore, it is necessary to conduct a complete search of the thickness effect and concentrations of defects of the absorption layer, as well as the effect of the thickness and concentration of defects of the buffer layer. The results obtained in this research may be useful for the design of high-performance solar cells based on CZTS (Se).

**3- Device Structure**

In this work, AFORS-HET is used for simulation to determine the current voltage wher it's used the Shockley–Read–Hall sample to describe the recombination currents in the cell layers . The total current and voltage passing through the solar cell (the sum of the electron and hole current at a boundary grid point) is then calculated. This can be done in the dark or under illumination. Efficiency of solar cells is improved through appropriate selection of layers, carrier concentrations, resistivity, thickness and absorption layers of CZTSSe. Is a heterojunction of CZTS or CZTSe / CdS/ i-ZnO thin film solar cells have been designed, and analyzed by AFORS-HET simulation. The structure of the studied cell ,shown in Fig.2 a. ZnO is a window layer and CdS layer acts as the buffer layer from n-type, making a hetero structure p-n junction with absorption layer, coefficients for different layers are used can be seen in Fig .2 b .



**Fig. 2: a) Solar cell structure. b) The absorption coefficients of different materials**

For studied cell, defect distributions: donor defects are assigned to the p-type materials (CZTS, CZTSe layers) and acceptor defects to the n-type materials (ZnO, CdS).The study used the Fermi level pinning , characterized by density ( $1 \times 10^{16} \text{ cm}^{-3}$ ) of donor

defects located at 0.5 eV below the absorber conduction band and it capture crosssections  $\sigma_n = \sigma_p = 10^{-15} \text{ cm}^2$ , the thermal velocity  $= 1 \times 10^7 \text{ cm} \cdot \text{s}^{-1}$  ( $S_n, S_p$ ) for electrons and holes. The properties of the materials are up in Table 1.

Table 1: Material parameters

parameters	Symbol (unit)	i-ZnO	CdS	CZTS	CZTSe
Thickness	d (μm)	0.04	0.06	1	1
Dielectric permittivity	dk	9 [12,13]	10 [12,13]	7 [15]	13.6 [14]
Electron Affinity	χ (eV)	4.4 [14, 17]	4.2 [14]	4.3 [15]	4.35 [14]
Bandgap	E <sub>g</sub> (eV)	3.37 [13]	2.42 [13]	1.5	1
Density Of States in CB	N <sub>c</sub> (cm <sup>-3</sup> )	2.2×10 <sup>18</sup> [16]	1.8×10 <sup>19</sup> [16]	2.2×10 <sup>18</sup> [17]	2.2×10 <sup>18</sup> [18]
Density Of States in VB	N <sub>v</sub> (cm <sup>-3</sup> )	1.8×10 <sup>19</sup> [16]	2.2×10 <sup>18</sup> [13]	1.8×10 <sup>19</sup> [17]	1.8×10 <sup>19</sup> [18]
Electron mobility	μ <sub>n</sub> (cm <sup>2</sup> .Vs <sup>-1</sup> )	100 [17]	100 [17]	100 [13]	100 [17]
Hole mobility	μ <sub>p</sub> (cm <sup>2</sup> .Vs <sup>-1</sup> )	25 [17]	25 [17]	25 [13]	25 [17]
Acceptor concentration	N <sub>a</sub> (cm <sup>-3</sup> )	0	0	8×10 <sup>15</sup>	2×10 <sup>16</sup>
Donor concentration	N <sub>d</sub> (cm <sup>-3</sup> )	1×10 <sup>19</sup>	1×10 <sup>17</sup>	0	0
n		File AFORS-HET		2.85[19]	2.45[20]
k				0.1 [19]	0.6 [20]

4- Result and Discussion

4-1 Thickness of the Absorption Layer

Ordered defect compound (ODC) layer that lies between the absorber and buffer layers. Where it is improving of the CZTSSe cells by lowering the valence band maximum with respect to the Fermi level, thus leads to reduces the interface recombination rate. it observes in Fig.3, the schematic solar power scheme of a CZTS-based energy cell (Se).cells with a large (cliff-like) onset are of low efficiency, whereas most high-efficiency cells have (spike-like) or semi-planar. The large cliff in the band

structure at heterointerface lowers the open circuit voltage and spike type heterostructure reduces the short circuit current density (Jsc) of the cell . specially when the absorber layer conduction band is higher than that of the buffer layer [17] . Control of inter diffusion can to creator the best band alignment in CZTS/CdS solar cells., but it can be bad in CZTSe/CdS solar cells. The band alignment at the heterointerface is critical for the cell performance. That is why the optimization of heterostructure interface is necessary for enhanced performance.

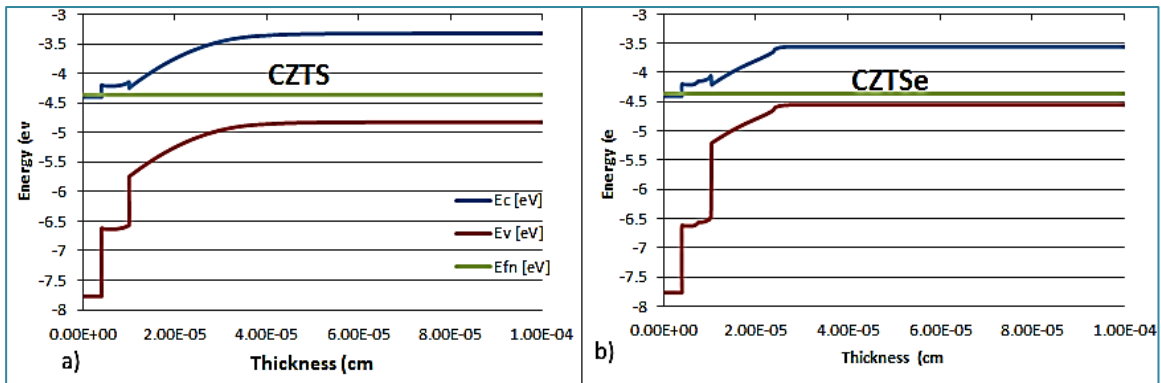


Fig.3 : Band alignments at CZTS and CZTSe cells.

The simulated J-V curves are shown in Fig.4 at different thickness of the CZTS and CZTSe absorption layer , it observes the change of curves as the thickness of the absorption layer increases. This

trend is easy to understand as longer wavelength radiation have lower absorption coefficient, so with a thicker absorber layer more of the longer wavelength radiation will be absorbed.

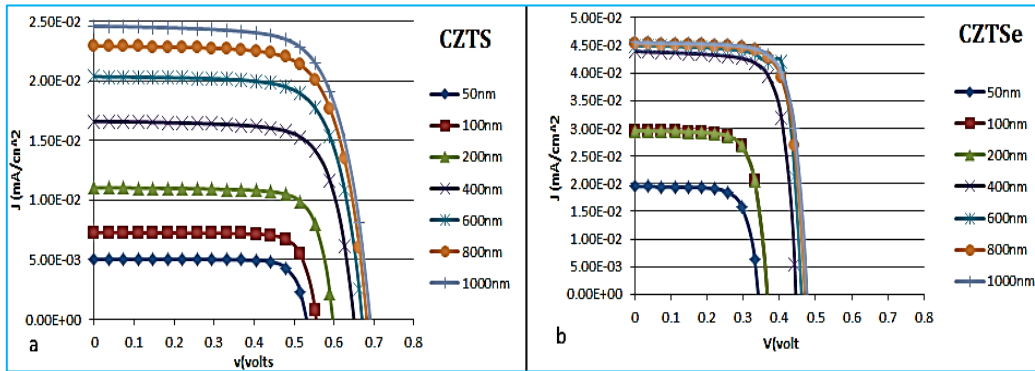


Fig. 4. Current -voltage characteristic curves of the CZTS, CZTSe cells, Due to the difference in the thickness of the absorption layer.

Note the thickness effects of the absorption layer on the electrical properties of the cells, where all the parameters increase as the thickness of the CZTS and CZTSe increases and more photons will be absorbed and generate more pairs electron- hole,resulting into the excess photogenerated carriers and thus, improved device efficiency . this is can be seen in Fig. 5. The properties of other layers are maintained constant with a change in the thickness of the absorber layer. Note that  $V_{oc}$  and  $J_{sc}$ , become almost constant for the thickness exceeding  $2 \mu m$  (The nature of variation of the estimated  $J_{sc}$  with increased thickness of the absorberlayer, tends to reach a

saturation) [21]. According to Beer's law the thickness of the absorption layer is preferably sufficient to absorb most of the photons of the solar spectrum, where about 90 percent of the photons can be absorbed when the absorption layer thickness is greater than 1 micron. The highest value obtained during this simulation before becoming almost constant for CZTS ( $V_{oc} = 680mv$  at thicness= $1.47\mu m$  , $J_{sc}=27.8 mA.cm^{-2}$  at thickness= $2.24 \mu m$  and  $E_{ff} =13.1%$  at thickness= $1.31\mu m$ ). for CZTSe ( $V_{oc}=494mv$  at thickness= $0.711\mu m$ , $J_{sc}=45.8mA/cm^2$  at thickness= $1.32\mu m$  and  $E_{ff}=16.9%$  thickness= $1.17\mu m$ ) .

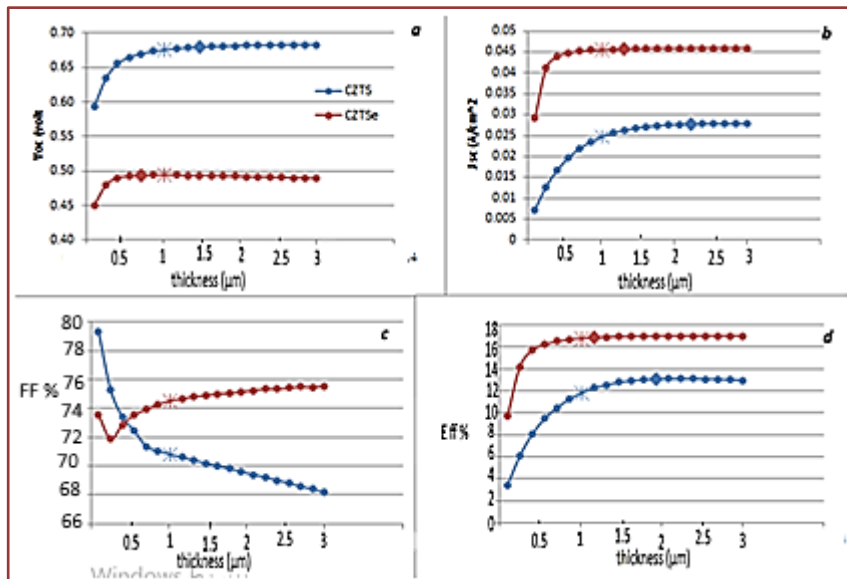


Fig.5 (a)  $V_{oc}$ ; (b)  $J_{sc}$  (c) FF (d)  $E_{ff}$  ; of CZTS and CZTSe solar cells for different thickness of the absorber layer

It can see in Fig.5a.  $V_{oc}$  of the CZTS solar cell is larger than the  $V_{oc}$  of the CZTSe solar cell, due to the increase in majority carriers of with increased absorption as the thickness increases and the energy gap widens for the CZTS cell. Fig.5b. Note that  $J_{sc}$  for the CZTSe cell largest of  $J_{sc}$  for the CZTS cell for same thickness. That maximize the photovoltaic response can be observes when the thickness is above  $1.5\mu m$ . This complies with Beer-Lamberts law, suggesting that higher absorption produces an

increase in current carriers and thus increases cell efficiency Fig.5d. The generation rate of electron-generated electron hole pairs seem to be low for the CZTS, CZTSe thick layer. The increasing the thicknes of CZTS led to increase majority carrier due to the bigger energy gap compared to CZTSe. The fill factor (FF) of the CZTS cell is process begins to increase and decrease because this cell absorption of the long wavelengths. As for the CZTSe cell, the FF is increased depending to the absorption of the short

wavelengths as stated by Fig .5 c. This result can be explained in of stated by scheme of external quantum efficiency EQE of thin absorber layers in Fig. 6. The CZTS absorbs short wavelengths, while the CZTSe absorbs long wavelengths where the analysis external quantum efficiency (EQE) spectra gives an indication

about the absorption of solar radiation. The EQE depends on optical absorption and internal quantum efficiency (IQE). It was reported that the IQE of the cells can be close to unity [22]. The main electrical properties of the CZTS and CZTSe cells at the same thickness (1 $\mu\text{m}$ ) can be summarized in Table 2.

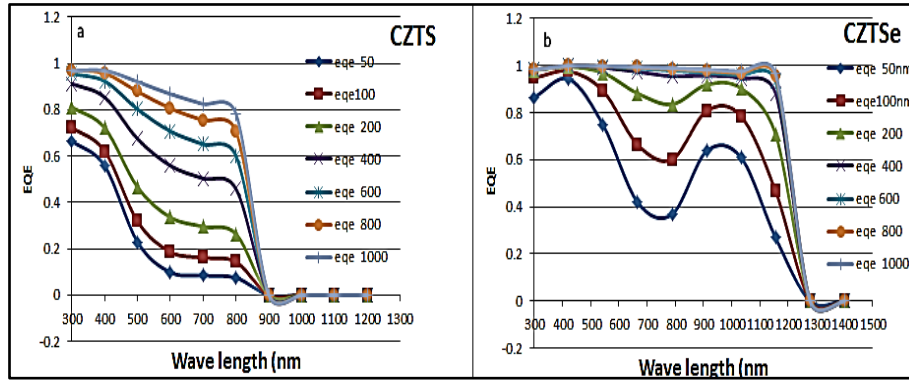


Fig. 6 :EQE for CZTS and CZTSe at different thickness

Table 2 : The electrical properties of the CZTS and CZTSe cells (at 1 $\mu\text{m}$ ).

Thickness=1 $\mu\text{m}$	Voc (mv)	Jsc (mA.cm <sup>-2</sup> )	FF %	E ff %
CZTS	691.7	24.59	70.02	11.91
CZTSe	475.2	45.5	75.53	16.33

4-2 absorber layer concentration.

CZTS(Se) is a type of absorption substance, where the concentration of the carrier (Na) depends on the defects in the composite materials of this material. In the current work the value of Na range from (1 $\times 10^{13}$ –1 $\times 10^{16}$ ) cm<sup>-3</sup> for the absorption layer. Open circuit voltage (V<sub>OC</sub>) for CZTS solar cell, Fig. 7a, increases rapidly to 688 mv, with increased carrier concentration. Before declining rapidly at (Na=7.9E<sup>15</sup>), while (CZTSe) solar cell reaches the voltage of 572 mv. The calculated results correspond to the fact that increasing the Na should lower the life time of the minority carriers. The increase of the Voc is rapid with doping at first and then decreases because of the compensatory nature of the donor type. Therefore, that maximum power can be reached when determining the optimal carrier concentration. The depletion width towards the absorption layer, which affects the effective separation of the charge

vectors resulting from the image and causes a small increase in Jsc as stated by Fig.7 b. Efficiency increases with increased concentration of carriers as stated by Fig. 7d. The maximum efficiency calculated with these carrier densities is about 11. 9% and ~ 20%, for the CZTS and CZTSe solar cell, respectively. The study notes that the efficiency of the CZTSe cell is higher than that of the CZTS cell, because of its high absorption coefficient as shown in the Fig 2b, it has the ability to absorb short and long wave lengths.The best results can be recorded with the same acceptor concentration (Na =7.9 $\times 10^{15}$ cm<sup>-3</sup>) of the two cells CZTS, CZTSe in the Table 3:

Table 3: The electrical properties of the CZTS and CZTSe cells at 7.9 $\times 10^{15}$ cm<sup>-3</sup>

Na=7.9E15 (cm <sup>-3</sup> )	Voc (mv)	Jsc (mA.cm <sup>-2</sup> )	FF %	E ff %
CZTS	688	24.6	0.708	11.9
CZTSe	597	41.7	0.812	20.2

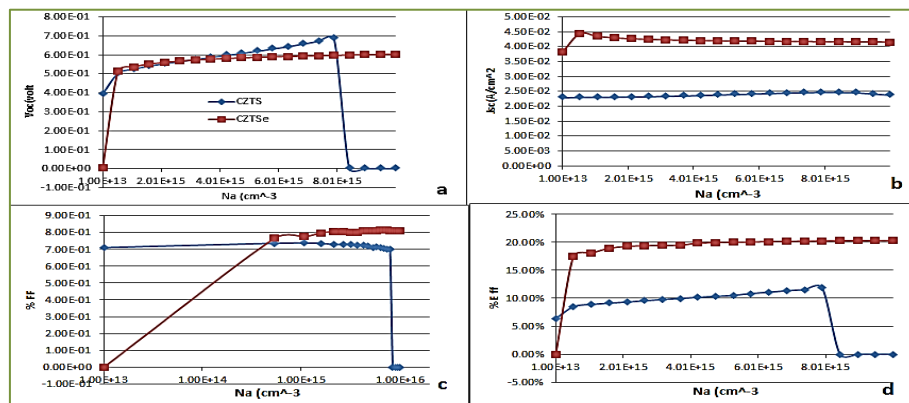


Fig 7: Solar cell parameters as a function of Na for CZTS and CZTSe solar cells



**4-3 Mole fraction (x) of CZTS<sub>x</sub>Se<sub>1-x</sub> solar cells :**

The gradual substitution of (S) by (Se) in CZTS<sub>x</sub>Se<sub>1-x</sub> affects its electronic, and optical properties. In this search it has chosen to describe Eg of CZTS<sub>x</sub>Se<sub>1-x</sub> material by equations of ref [19] . When x varied gradually from (0 to 1) the composition of the alloy varied linearly from CZTS to CZTSe . When x varied from (0 to 1) the Eg of CZTS<sub>x</sub>Se<sub>1-x</sub> from 1.5 to 1 eV , which is utilized to tailor and optimize the solar cell.[23,24]. Can be used to find different of solar cells that differ in the Eg, electron Affinity (χ) and other parameters of interpolation scheme for CZTSSe be given by [15]. (see Table 4)

$$CZTSSe = x CZTS + (1-x) CZTSe \dots\dots(6)$$

$$\frac{\epsilon(CZTSSe) - 1}{\epsilon(CZTSSe) + 2} = x \frac{\epsilon(CZTS) - 1}{\epsilon(CZTS) + 2} + (1-x) \frac{\epsilon(CZTSe) - 1}{\epsilon(CZTSe) + 2} \dots\dots(7)$$

The electron or hole effective mass me(h) can be written as:

$$\frac{1}{m_{e(h)}(CZTSSe)} = \frac{x}{m_{e(h)}(CZTS)} + \frac{1-x}{m_{e(h)}(CZTSe)} \dots\dots(8)$$

It can observe in Fig .8, the properties of the solar cell versus x. an efficiency of 20.41% for (CZTS<sub>0.4</sub>Se<sub>0.6</sub> cell) is obtained for x = 0.4 and Eg = 1.2 eV, ( Fig. 8d) . At higher values x > 0.4, the efficiency of cells drops much due of spectral distribution.

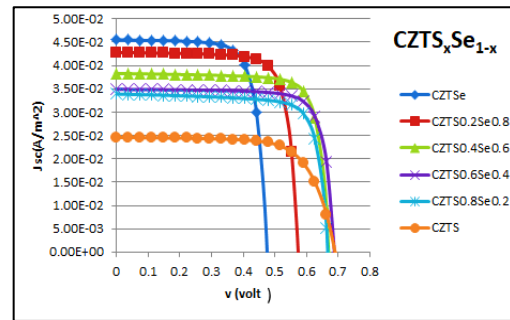
**Table 4: factor x and properties of Cu<sub>2</sub>ZnSn(S<sub>x</sub>Se<sub>1-x</sub>)<sub>4</sub> solar cells.**

x	Eg(ev)	χ (eV)	dk	m	Solar models cell	Voc(mv)	Jsc(mA.cm <sup>-2</sup> )	FF %	Eff %
0	1	4.35	13.6	0.07	CZTSe	475.2	45.5	75.53	16.33
0.2	1.1	4.34	11.56	0.079	CZTS <sub>0.2</sub> Se <sub>0.8</sub>	574.2	42.81	77.63	19.08
0.4	1.2	4.33	10.02	0.09	CZTS <sub>0.4</sub> Se <sub>0.6</sub>	671.5	38.3	79.36	20.41
0.6	1.3	4.32	8.806	0.11	CZTS <sub>0.6</sub> Se <sub>0.4</sub>	691.1	34.9	78.93	19.04
0.8	1.4	4.31	7.81	0.13	CZTS <sub>0.8</sub> Se <sub>0.2</sub>	668.6	33.9	76.67	16.61
1	1.5	4.3	7	0.18	CZTS	691.7	24.59	70.02	11.91

The FF (fill factor) curve shows a behavior similar to the efficiency curve and takes the same direction of increase and decrease as stated by Fig .8 c,d. J<sub>SC</sub> decreases and V<sub>OC</sub> increases with x , (see Fig. 8a,b) because, The carrier recombination rate depends on two basic parameters. First, the carrier concentration is an exponential function of the band gap. Second, the lifetime of the carrier. wher reflects the low lifetime of the carrier as the band gap increases. Therefore, the increase in energy band gap lead decrease in saturation current of minority carrier increasing in Voc refer to:

$$Voc = \frac{nkT}{q} \ln \left( \frac{I_L}{I_0} + 1 \right) \dots(9)$$

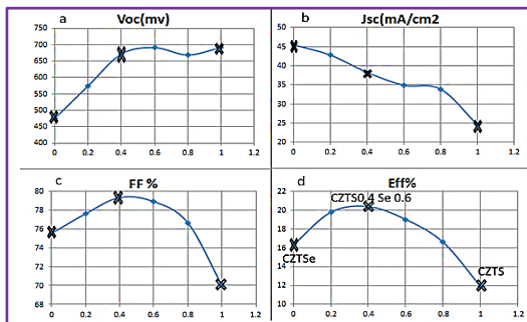
Where the I<sub>L</sub> is photo current of the cell and I<sub>0</sub> is the saturation current. We can observe the current drop and the voltage increase with the increase of the X coefficient of the compound CZTS<sub>x</sub>Se<sub>1-x</sub> from (0 to 1), through the J-V curve shown in Fig 9.



**Fig. 9: curve J-V for CZTS<sub>x</sub>Se<sub>1-x</sub>**

**4-4 Effect of Buffer Layer**

The main role of buffer layer at the intersection of covariance is to form an interface with the absorption layer, allowing the maximum quantity of light to pass into the absorption layer [25]. This layer must have the least amount of loss of absorption and must be able to output the photo generated carriers with the least quantity of recombination losses and transfer to the outer circuit with minimal electrical resistance. For high photovoltaic with minimal resistance loss, the Eg of the buffer layer must be high energy gap to keep low series resistance . Although CZTS and CZTSe a good choice as absorption material for solar cell, the buffer layer should also be improved because it aligns the gap between the CZTS or CZTSe and the ZnO layer [26] CdS layer can be used because it's improved interface with the absorption layer and has transmission in the blue wavelength zone . CdS has Eg =2.42 ev and can absorb photons with wavelength over than 500 nm [27]. It has good electrical properties and good optical permeability, making it an ideal material for manufacturing solar cells [28]. It can be used an other buffer layer like ZnS ,wher it



**Fig. 8: The electrical properties of the CZTS<sub>x</sub>Se<sub>1-x</sub>.**

has a higher energy gap ( $E_g=3.5$  ev) from CdS, resulting in lower absorption of low wavelength photons [29].  $Cd_{1-x}Zn_xS$  is an Electron Transport Layer and Interface of CZTSSe Solar Cell .The molarity or x variation in  $Cd_{1-x}Zn_xS$  results in variation in the  $E_g$  and electron affinity ( $\chi$ ),  $Cd_{1-x}Zn_xS$  can also be used as another buffer layer with  $E_g$  for CdS= 2.42 ev and  $E_g$  for ZnS = 3.5 ev for ZnS layer. The  $Cd_{1-x}Zn_xS$  range gap can be

calculated to configure a different Zn (x) using the Vegard law [30]:

$$E_g(Cd_{1-x}Zn_xS)=2.566+0.041X+1.086 X^2 \dots\dots\dots(10)$$

Many solar cells, which uses different types of buffer layers such as CdS, ZnS and ( $Cd_{1-x}Zn_xS$ ), numerically using AFORS-HET to obtain solar cell performance parameters, a decrease in  $V_{OC}$ ,  $J_{sc}$ , FF and Eff values was observed for each of the cells CZTS, CZTSe as shown in Table 5:

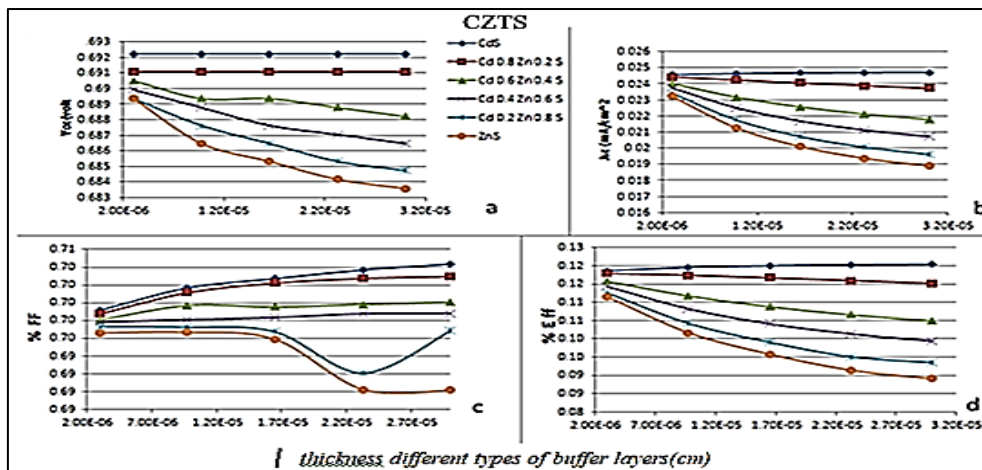
**Table 5: properties of different types of buffer layers**

x	Eg (ev)	buffer layers $Cd_{1-x}Zn_xS$	CZTS(1 $\mu$ m)				CZTSe(1 $\mu$ m)			
			Voc(mv)	Jsc (mA.cm <sup>-2</sup> )	FF %	Eff %	Voc (mv)	Jsc (mA.cm <sup>-2</sup> )	FF %	Eff %
0	2.42	CdS	691.7	24.59	70.02	11.91	475.2	45.5	75.53	16.33
0.2	2.58	$Cd_{0.8}Zn_{0.2}S$	691.1	24.34	70.01	11.78	475.2	45.24	75.49	16.23
0.4	2.76	$Cd_{0.6}Zn_{0.4}S$	689.9	23.6	69.9	11.38	474.6	44.5	75.44	15.93
0.6	2.98	$Cd_{0.4}Zn_{0.6}S$	689.4	23.13	69.81	11.13	474.1	44.03	75.44	15.74
0.8	3.29	$Cd_{0.2}Zn_{0.8}S$	688.2	22.57	69.73	10.83	474.1	43.41	75.33	15.52
1	3.5	ZnS	688.2	22.27	69.68	10.68	473.5	43.2	75.34	15.41

**4-5 Thickness of Buffer Layers**

To study effect of thickness buffer layer, the thickness was taken from 30 to 300 nm with a constant 1000 nm for CZTS. Fig.10 Shows the difference of solar cell parameters when the thickness of the buffer layer increases. The ZnS layer has a higher band gap than the other buffer layers. The change in Jsc and Voc is shown in Fig. 10 a,b. where there is a descending curve of the ZnS buffer. On the other hand, the CdS and ( $Cd_{0.8}Zn_{0.2}S$ ) buffer curves are almost flat. The ZnS has a lower Jsc value than other layers because photons doesn't have energy to absorb photons that possess high wavelength and

produce an electron-hole when the material band gap becomes larger, resulting in a decrease in Jsc. FF for ZnS layer decreases (in Fig. 10c) due to rising in series resistance. Finally, Fig.10, illustrates the efficiency curves of the buffer types that follow the Jsc and Voc behavior. Efficiency of the ZnS buffer layers decreases to approximately 10.68 %, Low efficiency is due to the effect of Voc, Jsc and the FF. The same behavior can be observed for the CZTSe solar cell in Fig 11. Where the efficiency of the ZnS buffer layers decreases to approximately 14 % ,this agrees with the reference [31].



**Fig 10: solar cell parameters versus thickness of buffer layers(cm) for CZTS absorber solar cells.**

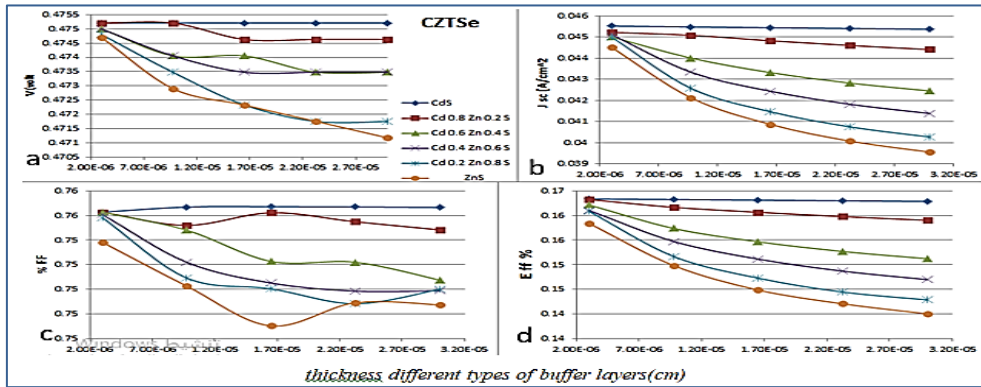


Fig 11 : solar cell parameters versus thickness of buffer layers(cm) for CZTSe absorber solar cells.

It can be seen that the best layer is CdS and the best thickness of this layer was 60 -80nm, a thick insulating layer will absorb bit of the solar radiation, thus reduces the amount of photons that can reach the absorption layer, it is leading to the degradation of the cell parameters, ie, Voc, Jsc, FF and Eff.

**4-6 Concentration of CdS Buffer Layer:** As stated by Fig.12 the characteristics parameters of cells

change slightly when doping concentrations increase the dielectric layer (Nd) of  $10^{17} \text{ cm}^{-3}$ , it notes that the open circuit voltage Voc. is not affected by the change the doping concentrations (Nd) of the CdS buffer layer as in Fig. 12a. It can be said that a simple change in concentrations of the buffer layer does not significantly affect the cell output.

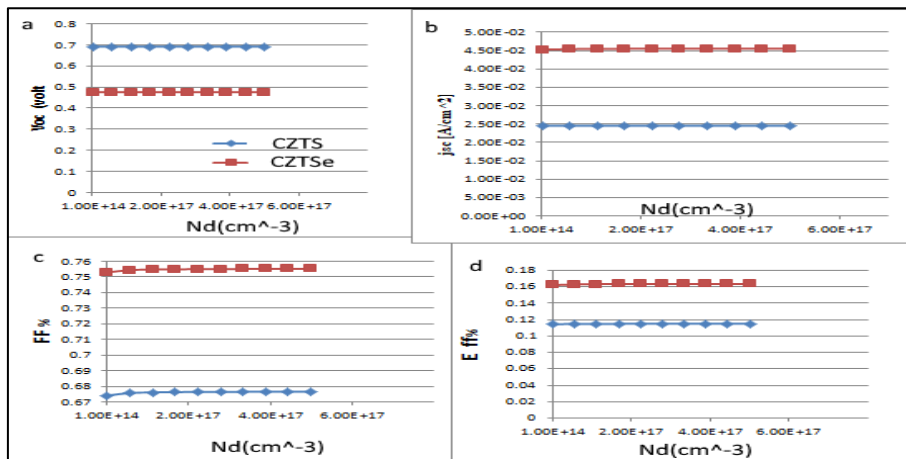


Fig. 12 : Parameters of the solar cell as a function of CdS buffer doping concentrations (Nd)

**5- Conclusions**

The results of this research had described solar cell devices based on the CZTS and CZTSe absorption cells using the AFORS-HET simulation program. Simulations were performed of the solar cells when the thickness of the absorption layer is changed from 100 to 3000 nm. The Efficiency increases in both cells, and reaches the saturation state after the thickness of 1  $\mu\text{m}$ . The results show that the efficiency( Eff = 11.91% ) CZTS is lower than the efficiency of the CZTSe (Eff = 16.33 %) cell with the same thickness of the absorption layer. In contrast, the open circuit voltage of CZTS (Voc = 691.7 mv) is higher than CZTSe (Voc = 475.2 mv) than the same thickness of the absorption layer.As noted, the Na increases the efficiency of the cell (CZTSe) and reaches (20.2%). Cell CZTS 0.4Se 0.6, which has

reached efficiency of 20.41%, As noted, the concentration of the receptor increases the efficiency of the cell (CZTSe) and reaches (20.2%). Depending on the mole fraction from 0 to 1 was used different buffer layers among them CdS buffer layer used in solar cells wicth showed higher efficiency. The increase in the thickness of the CdS buffer layer reduces the efficiency of each CZTS, CZTSe cells by a small percentage and there is no any change in the Voc of each cell. Empirically (To compare results) was obtained the best CZTSSe absorbers (sulfur around 1%) absorber was prepared by sputtering on a CZTS target followed by selenization under Ar carried H<sub>2</sub>Se gas, The highest efficiency of 9.6% achieved at the optimal temperature of 560 °C [32] and CZTSSe solar cells was fabricated with a maximum efficiency of 8.97% [33].



## References

- [1] Minlin, J. and Xingzhong, Y. (2014). Cu<sub>2</sub>ZnSnS<sub>4</sub> Thin Film Solar Cells Present Status and Future Prospects. *Solar cells Research and application perspectives* , **9(5100)**: 107-146.
- [2] Stephan, A.(2013). Non-vacuum processed next generation thin film photovoltaics: Towards marketable efficiency and production of CZTS based solar cells. *Solar Energy*,**94** : 37–70.
- [3] Yang, K.J. et al. (2016). A band-gap-graded CZTSSe solar cell with 12.3% efficiency. *Journal of Materials Chemistry A*, **4(26)** : 10151-10158.
- [4] Wadia, W.; Alivisatos, A.P. and Daniel, M.K. (2009). Materials availability expands the opportunity for large-scale photovoltaics deployment. *Environmental Science and Technology*, **43(6)**: 2072-2077.
- [5] Fang, Q.Z. et al. (2016). Fabrication of earthabundant Cu<sub>2</sub>ZnSn(S, Se)<sub>4</sub> light absorbers by a sol-gel and selenization route for thin film solar cells. *Royal Society of Chemistry (RSC)* ,**6 (8)** : 6562-6570.
- [6] Stangl, R.; Froitzheim, A.; Kriegel, M.; Elstner, L. and Fuhs, W. (2003). AFORS-HET, a computer Program for the Simulation of Heterojunction Solar Cells to be Distributed for Public Use. In: 3rd World Conference on Photovoltaic Energy Conversion, 11-18 May 2003, Osaka, Japan: 279-282.
- [7] Stangl, R.; Haschke, J. and Leendertz, C. (2009). Numerical Simulation of Solar Cells and Solar Cell Characterization Methods: the open-source on demand program AFORS-HET, version 2.4. *Solar Energy*,**1(191)** : 432.
- [8] Roosbroeck, W.V. et al (1950). Theory of the flow of electrons and holes in germanium and other semiconductors. *The Bell System Technical Journal* **29(4)** : 560–607.
- [9] Green, M.A. (1982). Solar Cells, Operating Principles, Technology and System Application . *Prentice-Hall* , **85823( 5803)** : 274.
- [10] Jha, A.R. (2019) . Deployment of Rare Earth Materials in Microwave Devices, RF Transmitters, and Laser Systems. *Solar Cells Technology and Applications*. *CRC Press, Taylor & Francis Group*: 180 pp
- [11] Wanda, M.D.; Ouédraogo, S.; Tchoffo, F.; Zougmore, F. and Ndjaka, J. (2016). Numerical investigations and analysis of Cu<sub>2</sub>ZnSnS<sub>4</sub> based solar cells by SCAPS-1D. *International Journal of Photoenergy* , **21(5201)** :1-9 .
- [12] Doo, Y.L.; Byung, T.K. and Hoon, Y.J. (2003). Effect of First-Stage Temperature On Cu(In,Ga)Se<sub>2</sub> Solar Cells Using The Evaporation Of Binary Selenide Compounds. *Solar Energy. Materils. Solar Cells*.**75(1-2)** :73-79.
- [13] Uday, S. and Kawsar, A. (2017). Proposition and computational analysis of a kesterite/kesterite tandem solar cell with enhanced efficiency. *Royal Society of Chemistry (RSC)* , **7 (4806)** : 4806-4814 .
- [14] Brammertz, G. et al. (2014). Spectral current–voltage analysis of kesterite solar cells. *Journal of Physics D: Applied Physics*, **47(17)** :1-4.
- [15] Sadao, A. (2015). Earth-Abundant Materials for Solar Cells: Cu<sub>2</sub>-II-IV-VI<sub>4</sub> Semiconductors, Earth-Abundant Mater. *Solar Cells Cu<sub>2</sub>-II-IV-VI<sub>4</sub> semiconductors*. Library of Congress Cataloging-in-Publication data applied for ISBN: 9781119052777, *India* : 462 pp.
- [16] Courel, M.; Pulgarn, F. A.; Andrade, J. A. and Vigil, O.G.(2016). Open-circuit voltage enhancement in CdS/Cu<sub>2</sub>ZnSnSe<sub>4</sub>-based thin film solar cells, A metal-insulator-semiconductor (MIS) performance. *Solar Energy Mater. Solar Cells*, **149(23)** : 204-212.
- [17] Mahbub, R.; Saidul Islam, M.; Anwar, F.; Satter, S.S. and Mahmud Ullah, S. (2016). Simulation of CZTS thin film solar cell for different buffer layers for high efficiency performance. *South Asian Journal of Engineering and Technology*, **2(52)** : 1-10.
- [18] Simya, O.; Mahaboob batcha. A. and Balachander, K.(2015). A comparative study on the performance of Kesterite based thin film solar cells using SCAPS simulation program. *Superlattices and Microstruct*, **82(3)** : 248-261.
- [19] Islam, S. et al. (2015) . Optical, Structural and Morphological Properties of Spin Coated Copper Zinc Tin Sulfide Thin Films. Received: *International Journal of Thin Films Science and Technology* , **4 (3)** :155-161 .
- [20] Amal, M. I. and Kim. K. H. (2012). Optical Properties Of Selenized Cu<sub>2</sub>ZnSnSe<sub>4</sub> Films From A Cu-Zn-Sn Metallic Precursor. *Materials Science and Engineering* , **9(8)** : 345 – 353.
- [21] Iftiqar, S.M. and Junsin, Y. (2016). Numerical simulation and light trapping in perovskite solar cell. *Journal of Photonics for Energy*, **6(2)** :1-7.
- [22] Burschka, J. et al. (2013). Sequential deposition as a route to high-performance perovskite-sensitized solar cells. *Journal of Nature*, **499 (13)** : 316–319.
- [23] Wang, K. G. et al. (2010). Thermally evaporated Cu<sub>2</sub>ZnSnS<sub>4</sub> solar cells. *Applied Physics Letters*, **97(14)** : 480-484.
- [24] Marlein, J.; Decock, K. and Burgelman, M. (2009) . Analysis of electrical properties of CIGSSe and Cd-free buffer CIGSSe solar cells. *Thin solid films*, **517( 7)** : 2353-2356.
- [25] Candles, M. and Hegedus, B.S. (1991). Influence of CdS window layer on Thinfilm CdS/CdTe solar cell performance. Proceedings of 22<sup>nd</sup> IEEE photovoltaic specialists conference, 7–11 October 1991, Las Vegas, Nevada, USA : 967-972.
- [26] Eisele, W. et al. (2003). TEM and NRA investigations of Zn(Se, OH)/Zn(OH)<sub>2</sub> films on Cu(In, Ga)(S, Se)<sub>2</sub> substrates for highly efficient solar cells. *Solar Energy Mater. Solar Cell*, **7(1–2)**: 17–26.
- [27] Nguyen, M. et al. (2015). ZnS buffer layer for Cu<sub>2</sub>ZnSn(SSe)<sub>4</sub> monograin layer solar cell. *Solar Energy*, **111(15)** : 344–349.

- [28] Roy, P. and Srivastava, S. K.(2006) . Hydrothermal Growth of CuS Nanowires from Cu-Dithiooxamide, a Novel Single-Source Precursor. *Journal of applied central science(ACS)* , **6 (8)** : 1921-1926.
- [29] Gunavathy, K.V.; Parthibaraj,V. ; Rangasami, C. and Tamilarasan,K. (2016). Prospects of alternate buffer layers for CZTS based thin films solar cells from numerical analysis—a review. *South Asian Journal of Engineering and Technology(SAJET)* , **2(16)** : 88–96.
- [30] Ferdaous, M.T.; Islam, M.F.; Haque, K.A and Amin, N.(2015). Numerical analysis of ultra-thin high efficiency Cd<sub>1-x</sub>Zn<sub>x</sub>S/Cd<sub>1-x</sub>Zn<sub>x</sub>Te solar cell. *Electron Enrgy*, **5(A)** : 14–18.
- [31] Farjana, A.J; Marshia .Z.S and Mohammad ,J.R. (2019) . Towards high efficiency CZTS solar cell through buffer layer optimization. *Materials for Renewable and Sustainable Energy* **8(6)** : 1-7.
- [32]Sun, D.Z. et al. (2018). CZTSSe solar cells with 9.6% efficienizing Cu-Zn-Sn-S precursor sputtered from a quaternary target. *Solar Energy Materials and Solar Cells*, **174(7)** : 42-49.
- [33] Yaowei, W. et al .(2019).An investigation on the relation ship between open circuit voltage and grain size for cztsse thin film solar cells fabricated by selenization of sputtered precursors. *Journal of alloys and compounds* ,**778(30)** : 689-697.

## محاكاة الخلية الشمسية المنفردة CZTSSe<sub>4</sub> باستخدام برنامج

بثينة محمود جنداري ، عايد نجم صالح

قسم الفيزياء ، كلية التربية للعلوم الصرفة ، جامعة تكريت ، تكريت ، العراق

### الملخص

في هذا البحث، قمنا بمحاكاة الخصائص الكهروضوئية للخلية الشمسية غير المتجانسة المفردة مع طبقة امتصاص Cu<sub>2</sub>ZnSnS<sub>4</sub> و n-CdS / ZnO. يتم استخدام الطبقة النافذة وطبقة الموائمة. يتم تعيين الزنك المختلط وكبريتيد الكاديوم (Cd<sub>1-x</sub>Zn<sub>x</sub>S) كطبقات عازلة وإعادة البحث عن تأثير سمكه. وقد تم اختيار المركب CdS كطبقة موائمة لأنه يعمل على تحسين السطح البيني مع طبقة الامتصاص CZTSSe ولديه إرسال عالي في منطقة الطول الموجي الأزرق لتحسين كفاءة الخلية الشمسية. تم الحصول على كفاءة (η = 11.9%) عند سمك 1 ميكرون وتركيز الناقل (Na=7.9 × 10<sup>15</sup> cm<sup>-3</sup>) مع جهد الدائرة المفتوحة (V<sub>OC</sub> = 688mv) ، تيار الدائرة القصيرة (J<sub>sc</sub> = 24.6 mA.cm<sup>-2</sup>) ، عامل الملء (FF = 70.8%) للخلية الشمسية CZTS ، و Voc = 597 mv و Jsc = 41.7 و η = 20.2% والكفاءة و FF = 81.2% و ( mA.cm<sup>-2</sup> ) للخلية الشمسية CZTSe.