Research Article

Simulation and improvement the solar cell Cu2CdSnS4 and study the effect of absorption layer defect

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Abstract: In this research, a quadruple cell was built from the bilayer cell, which is the basis for it, where a permeable layer was added to the binary cell, which is ZnO, to become the CCTS/CdS/ZnO cell, and then another permeable layer was added, which is AZO, to become a cell with four layers similar to the practical cell. The work is focused on increasing the efficiency from 1.80% to 7.7%, meaning that we have combined the high-efficiency binary cell and the low-efficiency quadruple cell, and then we learned to improve it by taking the best thickness for all layers, and the thickness values were as follows for the absorbent layer (5µm) For the buffer layer CdS is 0.2µm and the thickness of the permeation layers is ZnO and AZO is 0.2µm, the concentrations were for the absorption layer $10^{15}cm^{-3}$, the fitting layer is $10^{19}cm^{-3}$ and the first window layer is $10^{19}cm^{-3}$ and the second window layer is $10^{20}cm^{-3}$ and the outputs were The quadruple cell after optimization is as follows: (Voc=0.597V, Jsc=23.668mA/cm^2, FF=52.48%, eta=7.43%).to make the cell closer to practical reality, defects were added to the interface, the defect type is neutral, and the values of the interface defects are as follows (the energy level for the reference, which is the valence band equal to 0.6eV), (the defect density Nt equal to $1.0\times10^{13}cm^{-2}$), (the cross-sectional area for capturing the gaps and electrons $1.0\times10^{15}cm^2$) ,Then the defects were added to the CCTS absorbing layer of the defect type (donor, acceptor, and neutral) with fixing the interface defects at neutral and the values of the absorption layer defects as follows (energy level relative to the reference valence band equals 0.6Ev), (the defect density Nt equals $1.0\times10^{15}cm^{-2}$), (the cross-sectional area for capturing gaps and electrons is $1.0\times10^{15}cm^2$) and the results are close to the practical reality of the cell, which is the defect of the accepter absorbing surface (Voc=0.594V, Jsc=22.29mA/cm^2, FF=52.28%, eta=6.94%) ,In this last part of the optimization process, five BSL back reflection layers were added which are (Cu2O, ZnTe, SnS, MoSo2,Cu2Te). The best back reflection layer was Cu2O, where the final cell outputs after the optimization were as follows: (Voc=0.638V, Jsc= 25.47mA/cm2,FF=47.32%,eta=7.69%).

1. Introduction

The concept of Cu_2CdSnS_4 thin-film solar cells is based on the following principles. The compound semiconductor Collecting two necessary conditions for efficient (solar cells) is the direct nature of the hight band gap and the other is its width within a certain optimal range for photovoltaic cells. Because the pre-factor of absorption coefficient for the Cu_2CdSnS_4 thin film is large enough the layer of micron thickness is able to absorb sunlight sufficiently, Is used of it as an absorber does not have any damaging effects on photocurrents[2]. The Probably of radiative recombination in the thin film is able to exceed that of non-radiative recombination if both absorption and emission of light are caused by an allowed direct transition of carriers between valence and conduction bands without any intermediaries such as crystal defects and phonons. It is therefore possible for cell efficiency to approach the theoretical limit if Shockley–Read–Hall-type recombination centers, which play a role in bypassing the direct recombination, are diminished and at the same time a device structure to confine excited electrons in the Cu2CdSnS4 base layer is implemented [3].

structured experimental reference cell [5].CCTS was simulated using the SCAPS - 1D program, One method enhancing the efficiency and improving the performance of the CCTS-based photovoltaic device is :

- ❖ Validation of the CCTS experimental cell.
- ❖Proposing novel structure of CCTS/CdS/ZnO/AZO for solar cells.
- ❖ Optimization of absorber layer thickness.
- ❖ Optimization of doping concentration.
- ❖Adding aback reflection layer to improve cell efficiency.
- ❖Adding defects to the interface and defects of the absorption layer.
- ❖ Comparison of results.

2. Device structure

The photoelectric device used in this work is CCTS / CdS / ZnO/AZO as in Fig. 1, which contains a CdS buffer layer, ZnO,AZO window layer, CCTS absorption layer , front and back contact(ohmic). In this work, the effect of physical factors such as thickness and carrier concentration on the performance of the device is studied

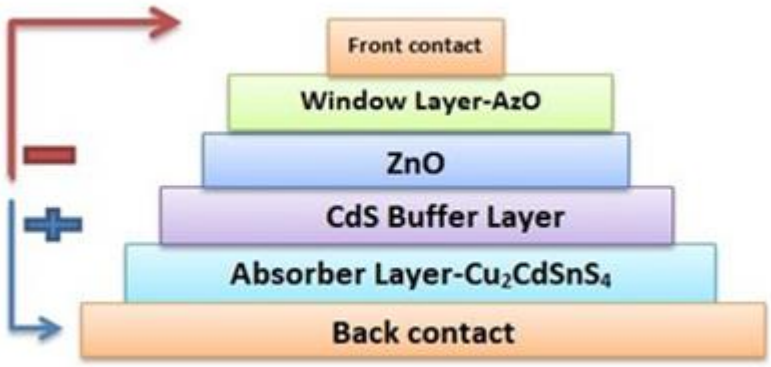

Figure (1) the structure of the device

Simulation of the device was performed in SCAPS software which is a one-dimensional solar cell capacitance simulation program developed in the Department of Electronics and Information Systems (ELIS) at the University of Ghent, Belgium where it is able to calculate the properties of J-V and its photoelectric parameters, the most important of which is the voltage Open circuit (Voc), short circuit current density (Jsc), fill factor (FF), efficiency (η), C-V properties, as well as the QE curve under standard illumination AM 1.5 solar radiation with a power density of 100 mW / cm2 as the light source. [6] by solving basic semiconductor equations

Modeling can be done using the SCAPS program. The program depends on the solution of semiconductor equ. start by writing the Poisson equation: (8)

$$\nabla(E) = \frac{q}{\varepsilon}(p - n + N_D^+ - N_A^-) - - - -1$$

the E is the electrical field ,(q is electron charge) ε is the permittivity of the absorber , np is density electrons (holes) and N_D (N_A) is donor and acceptorconcentration[6]. .

Then the continuity given by equation that is the following relationship(9)

$$\frac{dn}{dt} = \frac{1}{q}(\nabla (J_n) + G_n - R_n - - - - - - - - 2$$

$$\frac{dp}{dt} = - \frac{1}{q}(\nabla (J_p) + G_p - R_p - - - - - - -3$$

Where J_n (J_p) is electron density(hole) current density, Dn (D_p)is electron (hole) generation and R_n (R_p) is electron (hole) recombination rate.

Finally, the carrier charge equations for the density of diffusion current and drifting can be obtained from the following equ:[18]

$$J_n = q(\mu_n nE + D_n \nabla n) - - - - - - - - -4$$

$$J_p = q(\mu_p PE + D_p \nabla p) - - - - - - - - -5$$

Where μ_n (μ_p) is mobility Electron (hole) and Dis the diffusion constant .

There are many basic equations explain the work of solar cells. The following equ gives the total current (the sum of the photo current I_L and the dark current) which are: [8,10]

$$I = I_o \left[\exp\left(\frac{qv}{KT}\right) - 1\right] - I_L - - - - - - - - -6$$

is Boltzmann's constant and T is temperature in(K)Where K,

know the properties of the (I-V) curve of the solar cell under lighting, an open circuit voltage (V_{oc}) is the max voltage when the current is zero and the V_{oc} equation abllty be obtained by making the total current of equation (6) equal to zero so the equation becomes:

$$V_{oc} = \frac{KT}{q} Ln \left(\frac{I_L}{I_o} - 1\right) \approx \frac{KT}{q} Ln \left(\frac{I_L}{I_o}\right) - - - - - 7$$

Where I_o It represents the saturation current of the its equation :

$$I_o = DT^3 \exp\left[\frac{-E_g}{KT}\right] = A \left[\frac{q D_e n_i^2}{L_e N_A} + \frac{q D_h n_i^2}{L_h N_D}\right] - - - - - -8$$

Where Eg is energy gap electrons (holes) and Area cross section. , [11]. L_e(L_h) is diffusion length

From equation (7), we observe the logarithmic increase of the open circuit voltage as the saturation current decreases, The short circuit current I_{sc} is obtained when the circuit open voltage is zero. the ideal case, the short circuit current is equal to the optical current, and relationship between the circuit current and the circuit open voltage, can be written with the following relationship:-

$$I_{sc} = I_o\left[e^{qV_{oc}/KT} - 1\right] - - - -9$$

To measure the quality of the photovoltaic cells, as these variables , factor FF, short current, voltage circuit open and conversion efficiency following equations (10)

$$FF = \frac{P_{max}}{P_{in}} = \frac{V_{max}I_{max}}{Voc\ J_{sc}} - - - - - - - 10$$

$$\eta = \frac{P_m}{P_{in}} = \frac{J_{sc}\ .V_{oc}.FF}{P_{in}} - - - - \ - - - 11$$

Where V_{max} Voltage max, P_{max} is power maximum, I_{max} is current maxand P_{in} is Incoming power[12]. .

It can be determined the lift time minority carriers, which is the average time to recombines minority carriers, and it is associated with the concentration of Traps N_t and recombination with the following relationship (7)

the impurities of the absorption layer and interface. We taken the series resistance 9 Ωcm^2 and the parallel resistance 800Ω cm^2 and the temperature 310 k . Figure (1) shows structure the solar cell.

Table 1: Physical parameters for device modeling in SCAPS-1D[14].

Parameters	Cu_2CdSnS_4	CdS	ZnO	AzO
thickness (μm)	5	0.2	0.2	0.2
bandgap (ev)[4]	1.35-1.42	2.4	3.3	3.4
electron affinity (eV)[5]	4.5	4.4	4.5	4.5
dielectric permittivity [6]	9	9	9	9
CB effective density of states($1/cm^3$)	1.7×10^{16}	1.8×10^{19}	1×10^{19}	4×10^{18}
VB effective density of states$1/cm^3$) [7]	2.2×10^{16}	2.4×10^{18}	1.8×10^{19}	9×10^{18}
electron thermal velocity (cm/s)(cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
hole thermal velocity (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
electron mobility (cm^2/Vs)[7]	20	20	100	100
hole mobility (cm^2/Vs)[7]	20	20	25	30
shallow uniform acceptor density NA (1/cm3)	1×10^{15}	0	0	0
shallow uniform donor density ND (1/cm3)	0	1×10^{9}	1×10^{9}	1×10^{20}
absorption constant A (1/cm)	2×10^{4}	1×10^{5}	1×10^{5}	1×10^{5}

2. Results and discussion

3-1 Effect Add back surfers reflection layers

To perform the optimization process on the previously simulated cell (CCTS/CdS/ZnO/AzO), the simulation results showed that this cell has a quantitative efficiency with the presence of interface defects and absorption layer defects of 6.94%. .(BSL/CCTS/CdS/ZnO/AzO)

The back reflection layer helps the electrons to return and improve the performance of the solar cell [15]. Five back-contact layers were selected, namely Cu2Te,SnS,MoSe2,ZnTe,Cu2O), and the best layers are the ones that have an electronic affinity less than the electronic affinity of the absorption layer.the table 4 parameters of the back reflection layer used in the optimization process. And the thickness of the layers was fixed at (80nm) and the midwives were impregnated at (10^{20}cm-3) and the table 3 shows the results of the cell parameters after adding the back-reflection layers to the cell.

Table 3 shows the parameters used in the optimization of the back reflection layers[17].

Type of back reflection layer	Cu_2O	ZnTe	SnS	$MoSe_2$	Cu_2Te
bandgap (ev)	2.17	2.19	1.1	1.06	1.18
electron affinity (eV)	3.2	3.73	4.2	4.3	4.2
dielectric permittivity	7.11	10.3	12.5	13.6	10
CB effective density of states(1/cm3)	2.0×10^{17}	1.17×10^{18}	2.8×10^{19}	2.2×10^{18}	7.5×10^{17}
VB effective density of states1/cm3)	1.1×10^{19}	1.16×10^{19}	1.8×10^{19}	1.8×10^{19}	1.5×10^{19}
electron thermal velocity (cm/s)	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}
hole thermal velocity (cm/s)	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}
electron mobility (cm^2/Vs)	200	330	25	100	500
hole mobility (cm^2/Vs)	80	80	100	25	210

2-3 Effect of absorption layer CCTS defects

The reason for adding impurities to the absorption layer is to control the cell performance or to increase the conductivity. When adding defects, these defects are often a loss factor. Therefore, the increase in the concentration of defects leads to a decrease in the efficiency of cell conversion. In this research, we added the defects to reach an ideal simulation of the cell[20].. The experimental process where we studied the defects of the absorption layer, the type of defect is fixed at the interface (Neutral) where the density of the defect concentration was changed from 10^{13}) to 10^{18} $1/cm^2$) The best concentration was observed at 10^{17} and the cross-sectional area of the defect was changed from 10^{13} to 10^{18} cm2 and better Area at 10^{15} and the energy of the defect level from (0.1eV to 0.6eV) and the best energy of the defect level is at 0.6eV and the closest results for the experimental cell at the defects of the absorption layer (Accepter),we notice from Table 5 the increase in the efficiency of the cell at low concentrations and the scientific explanation is that the increase in defect states can add centers to recombine the photogenerated carriers, which leads to an increase in the density of the reverse current Io and a decrease in both Voc and Isc[19]..

Table: 5 CCTS absorption layer defects at the interface Defect type constant at the interface (Neutral) Effect of changing the Capture cross section

Defect type	Total density(1/cm^2)	Energetic distribution	Energy with respect to reference(ev)	Capture cross section (electrons/hole) (cm2)	Voc(v)	Jsc(mA/cm^2)	F.F(%)	eta(%)
Neutral	10^{15}	Single	0.6	$10^{13}/10^{13}$	0.5717	14.4812	48.10	3.98
				$10^{14}/10^{14}$	0.5866	18.9659	52.00	5.79
				$10^{15}/10^{15}$	0.5952	22.3642	52.34	6.97
				$10^{16}/10^{16}$	0.5975	23.4828	52.53	7.37
				$10^{17}/10^{17}$	0.5975	23.6290	52.51	7.42
				$10^{18}/10^{18}$	0.5978	23.6440	52.51	7.42
Donor	10^{15}	Single	0.6	$10^{13}/10^{13}$	0.5305	11.6522	28.41	1.74
				$10^{14}/10^{14}$	0.5546	19.0491	31.81	3.36
				$10^{15}/10^{15}$	0.5473	23.0809	34.44	4.35
				$10^{16}/10^{16}$	0.5450	23.4862	34.93	4.57
				$10^{17}/10^{17}$	0.5447	24.0917	34.97	4.59
				$10^{18}/10^{18}$	0.5447	24.1025	34.98	4.59
Accepter	10^{15}	Single	0.6	$10^{13}/10^{13}$	0.5711	14.1848	48.85	3.96
				$10^{14}/10^{14}$	0.5858	18.7328	52.23	5.73
				$10^{15}/10^{15}$	0.5945	22.2908	52.38	6.97
				$10^{16}/10^{16}$	0.5968	23.4791	52.01	7.29
				$10^{17}/10^{17}$	0.5970	23.6352	52.34	7.39
				$10^{18}/10^{18}$	0.5970	23.6527	52.34	7.39

Table: 6 CCTS absorption layer defects at the interface Defect type Constant at the interface (Neutral) Effect of Nt

Defect type	Capture cross section (electrons/hole) (cm2)	Energetic distribution	Energy with respect to reference(ev)	Total density(1/cm^2)	Voc(v)	Jsc(mA/cm^2)	F.F(%)	eta(%)
Neutral	$10^{15}/10^{15}$	Single	0.6	10^{13}	0.5978	23.6290	52.51	7.42
				10^{14}	0.5975	23.4828	52.53	7.37
				10^{15}	0.5952	22.3642	52.34	6.97
				10^{16}	0.5866	18.9659	52.00	5.79
				10^{17}	0.5717	14..4812	48.00	3.98
				10^{18}	0.5422	8.2533	41.16	1.84
Donor	$10^{15}/10^{15}$	Single	0.6	10^{13}	0.5978	23.6306	52.50	7.42
				10^{14}	0.5988	23.5366	52.41	7.39
				10^{15}	0.5473	23.0809	34.44	4.35
				10^{16}	0.1565	1.2003	39.47	0.07
				10^{17}	/	/	/	/
				10^{18}	/	/	/	/
Accepter	$10^{15}/10^{15}$	Single	0.6	10^{13}	0.5978	23.6292	52.51	7.42
				10^{14}	0.5974	23.4835	52.51	7.37
				10^{15}	0.1801	22.2945	52.38	6.94
				10^{16}	0.1673	17.7872	54.10	5.59
				10^{17}	0.2098	10.9588	57.92	3.50
				10^{18}	0.3034	4.9654	59.16	1.50

Table: 7 CCTS absorption layer defects at the interface Defect type Constant at the interface (Neutral) Effect of defect energy

Defect type	Capture cross section (electrons/hole) (cm2)	Energetic distribution	Total density(1/cm^2)	Energy with respect to reference(ev)	Voc(v)	Jsc(mA/cm^2)	F.F(%)	eta(%)
Neutral	$10^{15}/10^{15}$	Single	10^{15}	0.1	0.5960	22.7273	52.27	7.08
				0.2	0.5953	22.3882	52.32	6.97
				0.3	0.5952	22.3663	52.34	6.97
				0.4	0.5952	22.3643	52.34	6.97
				0.5	0.5952	22.3643	52.34	6.97
				0.6	0.5952	22.3642	52.34	6.97
Donor	$10^{15}/10^{15}$	Single	10^{15}	0.1	0.5986	23.0249	51.70	7.12
				0.2	0.6108	23.3533	48.14	6.87
				0.3	0.6185	23.8571	43.16	6.37
				0.4	0.6096	23.6700	40.34	5.82
				0.5	0.5867	23.4080	37.18	5.11
				0.6	0.5473	23.0809	34.44	4.35
Accepter	$10^{15}/10^{15}$	Single	10^{15}	0.1	0.5875	22.1806	53.04	6.91
				0.2	0.5916	22.1656	52.63	6.90
				0.3	0.5943	22.2789	52.40	6.94
				0.4	0.5945	22.2906	52.38	6.94
				0.5	0.5945	22.2909	52.38	6.94
				0.6	0.5945	22.2908	52.38	6.94

Table: 8 shows the values of interface defects. Defect type is constant at Neutral

Defect properties	Unit	Interface defect p-CCTS/n-CdS
Energy Level with respect to reference	eV	0.6
Total density	cm^{-2}	1.0×10^{13}
Capture cross section area of electrons	cm^2	1.0×10^{15}
Capture cross section area of holes	cm^2	1.0×10^{15}

3-3 Comparison of CCTS/CdS/ZnO/AZO cell outputs before defect addition and after defect addition

The best thickness of the CCTS absorbing layer was 5µm)) and the best concentration for this layer was 1015cm^{-3}, while the best thickness of the alignment layer was 0.2µm) and the best concentration of the donors was 10^{19}cm^{-3}. As for the first window layer ZnO, the best thickness was 0.2µm and the best concentration It is 10^{19}cm^{-3} and the second window layer AZO was the best thickness of 0.2µm and its best concentration was 10^{20}cm^{-3}.

Where the cell outputs were as follows: Voc=0.597V, Jsc=23.645ma/cm2, FF=52.51%, eta=7.42%

But when defects are added to the interface and the absorption layer, the output of the cell is reduced to Voc=0.594V, Jsc=22.290ma/cm2, FF=52.28%, eta=6.94%

The table:9 below shows the difference between cell output before and after adding defects

CCTS solar cell	Voc(V)	Jsc(mA/cm^2)	FF(%)	eta(%)
Before adding defects	0.597	23.645	52.51	7.47
After adding defects	0.594	22.290	52.28	6.94

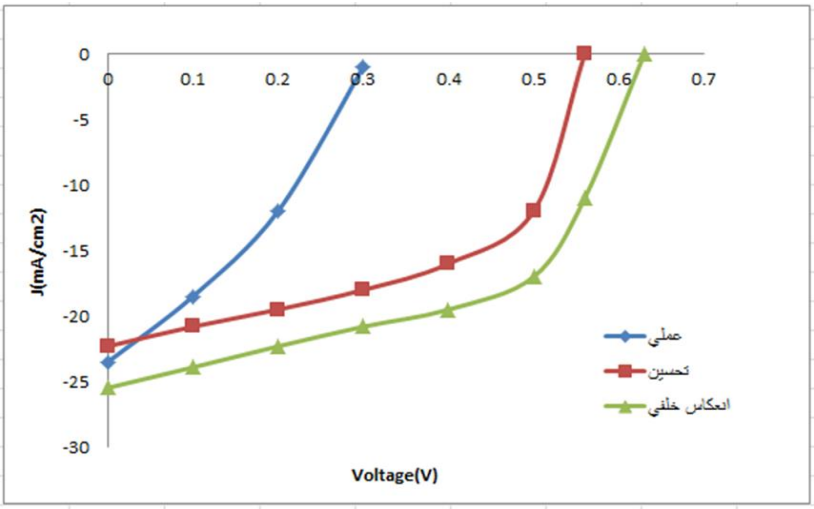

Figure :2 illustrates the comparison of the voltage and current curve of the process cell and the cell after optimization and after adding Cu2O back reflection layer.

3. Conclusions

In this research, the solar cell (CCTS/CdS/ZnO/AZO) was simulated using the simulation program (SCAPS 1-D), which is a virtual simulation program that simulates the experimental reality of solar cells using previously defined mathematical equations to suggest results for the cells to be simulated. The results are close to the experimental reality and save a lot of time and effort for the researchers. During the simulation, it was found that:

A - When comparing the results of the practical cell outputs with the theoretical cell, we found a great convergence between the results and that these results proved that this program has great credibility.

B- When simulating the first two-layered CCTS/CdS cell with the process cell, it was found that the conversion efficiency of the process cell was 7.7%, while the simulation results were 7.96%

C- When simulating the second cell with four layers CCTS/CdS/ZnO/AZO, it was found that the efficiency of the practical cell conversion was 1.14%, while the simulation results were 1.80%.

D- The two-layer cell was relied on as a base cell, then a first window layer was added, which is ZnO, and then another window layer was added, which is AZO, to become a cell of four layers similar to the practical cell in terms of the absorption layer, the alignment layer and the two penetration layers.

E- Then he took the best readings of thickness and concentrations for the absorption layer and the alignment layer the first and second permeability layer, where it was found that the best conversion efficiency of the cell is 7.42%

To get more realistic, defects were added to the interface. The defect type at the interface was fixed at Neutral, and defects were added to the absorption layer. For the best results, the defect type was fixed at Accepter, and the conversion efficiency results were 6.94%.

F- To improve the cell, a BSL back reflection layer was added and five layers were identified, the best of which was Cu2O, and the conversion efficiency was 7.69%, which is the best efficiency reached in this research.

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