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Analytical Modelling Study of CZTS Thin Film Solar Cell for High Efficiency Performance

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ABSTRACT

In this paper, ZnO:AL/ZnO/n-ZnS/p-CZTS/MoS_2 solar cell was studied by SCAPS simulation process. We performed enhancement using the influence of changing the energy gap of the window layer ZnO:AL and absorption layer CZTS. Furthermore, the impact of the carrier concentration of the window ZnO:AL and absorption layer CZTS were studied. It was found the efficiency of the solar cell rises with the energy gap value of the window layer. The best efficiency was obtained at (η=29.1%), when the energy gap of the window layer was found to be (3.5eV). Additionally. the best efficiency was found to be (η=28.9%) when the absorption layer was exhibited to be (1.35eV). After doped concentration, the best efficiency of the solar cell of the window layer ZnO:AL and absorption layer CZTS were found to (η=28.0%, 28.7%) when the doping concentration were found to be (ND=1.00E+16 cm^{-3}, 1.0E+19cm^{-3}) respectively. Clearly, the comparison between the experimental and theoretical solar cell was studied. The results illustrate the good matching between the experimental and theoretical results and the interface defect layers of the CZTS/ZnS contributed to this match.

1. INTRODUCTION

Solar cell has been promoted as renewable energy source and considered one of the most important inventions that have emerged in recent decades [1]. The main important properties of solar cell are low-cost and environmental friendly [2]. Polycrystalline thin film technology has developed in recent years and entered into strong competition with polycrystalline silicon, which still dominates the photovoltaic market [3, 4]. Cu_2ZnSnS_4 (CZTS) compound has recently widely abundant and versatile compound instead of CIGS cells and can be formed by many types of deposition processes, such as spin coater, chemical spray process., such as spin coating, chemical spray deposition. Thin film solar-cell (CZTS) exhibited excellent stability and has unique electrical and optical properties as well as provides an excellent conversion efficiency. CZTS is quaternary compound and direct bandgap (1.5eV) with high absorption coefficient ($10^4 cm^{-1}$). In addition, CZTS is one of the best thin films for structural stability [5]. CZTS solar cells were first revealed in 1966 and the efficiency of solar cells was raised to 5.6% [6]. In 1988, Ito and Nakazawa used the chemical spray method to fabricate CZTS solar cell layers. They synthesized the cell (CZTS) by spraying deposition process and obtaining the cell (CZTS) with a band gap (1.45eV) [7]. In 2012, Nagaoka National College used the electronic radiation evaporation technique for solar cell structure at (400mV), current (6.0mA/cm^2), fill factor (0.277%) and conversion efficiency (0.66%) [8]. In 2015, Ito studied and fabricated of (CZTS) thin films using spray method in order to enhance thin film solar cell performance and obtained an efficiency of (3.7%) [9]. In 2020, Kistanov studied the solar cell based on (Cu_2ZnSnS_4) thin film layer by the SCAPS program. Optimal result was obtained of the solar simulation. The optimal value of the absorber layer (CZTS) can be found between (2500-3000nm) and the window layer (AZO) can be found between (20-30nm). Furthermore, the efficiency of solar cell was 19.82% [10]. In 2021 Bouarissa prepared (CZTS/ZnS/ZnO) thin film solar cell layers using the (SCAPS-1D). Buffer Layer (ZnS) was replaced by the layer of MoS_2 for the best enhancement of the device. It obvious that the values of thickness of window layer, storage layer and absorption layer were found to be (0.1, 0.2, 1 μm) respectively. The conversion efficiency was found to be (23.69%) [11]. In 2022 Santu studied CZTS-bilayer solar cell and exhibits an improvement in efficiency value compared to another layer [12]. In 2024 Olcay prepared Binary ZnS–ZnO films and show that the structure of ZnS–ZnO was studied by formation of ZnO phase structure in the ZnS lattice phase [13]. The goal of this paper is to enhance the description of the CZTS thin solar cell layers by Scaps-1D simulation of the high quality and efficient solar cell can be designed by manipulating the layers parameters for improving the device of solar cell. Our main purpose is to effect of changing the energy gap the window and absorption layers CZTS. Furthermore, the influence of the carrier concentration of the window layer and absorption layer CZTS were investigated.

2. SIMULATION

2.1 Numerical modeling in SCAPS-1D

The simulation was carried out by the SCAPS -1D program. This program is one of the most important solar cell simulation programs, which was designed at Ghent University in Belgium. Numerical analysis methods contributed effectively to simulate solar cells. This program is free and easy used also give good results additionally, effectively contributed to obtain solar cells with high efficiency and low costs [14]. Furthermore, this program can solve by the equations of the semiconductor like as the equation of the continuity and carrier transport equations. It uses the Newton-Raphson method and the carriers of charge density (carrier concentrations). These equations are as follows [15].

$$Jn = q\mu n\, n\mathcal{E} + qDn\frac{dn}{dx} = q\mu n\left(n\mathcal{E} + \frac{KT}{q}\frac{dn}{dx}\right) = nn\frac{dEFn}{dx} \quad (1)$$

$$Jp = q\mu pP\mathcal{E} + qDp\frac{dp}{dx} = q\mu p\left(P\mathcal{E} + \frac{KT}{q}\frac{dp}{dx}\right) = \mu pP\frac{dEFp}{dx} \quad (2)$$

$\mathcal{E}$ is electric field (V/cm), μn, μp are the mobility of electron's and hole's (cm^2/V-s) respectively, Jn, Jp are the electron's and hole's current density (mA/cm^2), dn, dP are diffusion coefficient for electron's and hole's (cm^2/s) respectively.

Continuity equation can be calculated from the following equations:

$$\frac{\partial n(x)}{\partial t} = Gn(x) - Rn(x) \quad (3)$$

$$\frac{\partial p(x)}{\partial t} = Gp(x) - Rp(x) \quad (4)$$

where, Gn(x), Gp(x) are the generation process of electron and hole respectively, Rn(x) , Rp(x) are the mean recombination of electron and hole.

Poisson's equation can be obtained as the following equation:

$$\frac{d\,ln\big(E(x)\big)}{\partial x}\cdot\frac{d\Phi(x)}{dx} + \frac{d2\Phi}{dx^2} = \frac{\rho(x)}{\mathcal{E}_0(X)} \quad (5)$$

If $\mathcal{E}_0$ is constant, Poisson equation was estimated as:

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho(x)}{\mathcal{E}_0} \quad (6)$$

$\mathcal{E}_0$ is Electron Permittivity (F/cm).

The current of the solar cell can be estimated using:

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

where, I is the load circuit current, I_0 is the reverse current, k and T are the Boltzmann value and the temperature receptively. Also, open voltage current (Voc) can be estimated using the following equation:

$$V_{oc} = \frac{kT}{q}In\frac{I_{SC}}{I_o} + 1 \quad (8)$$

We can calculate the fill factor by the square of the curve (I-V) and the resistance loss of the device from the following equation.

$$FF = \frac{V_m I_m}{V_{oc} I_{sc}} \quad (9)$$

The solar cell efficiency may be measured of the equation:

$$\eta = \frac{OutPut\ Power(P_{out})}{InPut\ Power(P_{in})} \times 100\% \quad (10)$$

On the other word, the solar cell conversion efficiency is given as:

$$\eta = \frac{FF \times I_{sc} \times V_{oc}}{P_{in}} \times 100\% \quad (11)$$

2.2 Solar cell structure

The solar cell was studied in this work, which is consists of five layers (MoS_2/p-CZTS/n-ZnS/i-ZnO/n-ZnO:Al) with thickness (0.1, 1.5, 0.12, 0.1, 0.2 μm) respectively as show in Figure 1.

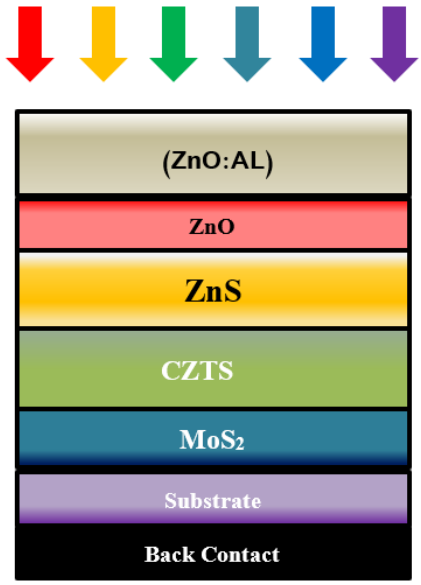

Figure 1. Solar cell structure (MoS_2/p-CZTS/n-ZnS/i-ZnO/n-ZnO:AL)

Table 1 shows the parameters used in the numerical modeling in SCAPS-1D, which includes the Back Layer (MoS_2), Absorption Layer (CZTS), Buffer Layer (ZnS), as well as the oxide of the transparent layer (i-ZnO) and window Layer (ZnO-Al). Furthermore, the parameters of this paper are Forbidden band gap (Eg), thickness, Affinity of the Electron (χ), permittivity of the Dielectric (ε), Electron Mobility (μn), mobility of the Hole (μp), donor density (NA), acceptor density (ND), concentration of the states (NC) in conducting band, donor or acceptor defects and concentration density in valance band (NV).

Table1. Parameters of solar cell layers

Parameter	MoS_2	CZTS	ZnS	i-ZnO	ZnO:Al
Thickness (nm)	0.1	1.5	0.12	0.1	0.2
Band gap (eV)	1.65	1.45	3.5	3.3	3.3
Affinity of Electron (eV)	4.2	4.5	4.5	4.4	4.6
Permittivity of the Dielectric	13.6	10	10	8	8
Density of states CB (cm^{-3})	2.3E+17	2.3E+17	1.8E+17	2.3E+17	2.3E+17
Density of states VB (cm^{-3})	1.7E+18	1.7E+18	1.7E+18	1.7E+18	1.7E+18
Hole thermal velocity (cms^{-1})	1.0E+7	1.0E+7	1.0E+7	1.0E+7	1.0E+7
Mobility of Electron (cm^2/V_s)	100	100	100	100	100
Mobility of Hole (cm^2/V_s)	25	25	25	25	25
Donor density, N_D (cm^{-3})	0	0	5.0E+14	1.0E+16	1.0E+14
Acceptor density, N_A (cm^{-3})	1.0E+13	1.0E+17	0	1.0E+16	0
Defect type	_	Donor	Acceptor	Acceptor	Acceptor

3. RESULTS AND DISCUSSIONS

The solar cell layers were designed in this work order to enhance the performance the efficiency of the cell (MoS2/p-CZTS/n-ZnS/i-ZnO/n-ZnO:AL) with thickness (0.1, 1.5, 1.2, 0.1, 0.2 µm) respectively. The results of output were as following [16]:

η=26.43%, FF=79.90%, Jsc=29.93 mA/cm^2, Voc=1.10 V

The results can be obtained when the energy gap values of the ZnO:AL layer and the CZTS layer were constant at 3.3eV and 1.45eV respectively. Besides, the donor concentration of ZnO:AL was found to be ND=1.00E+14 cm^{-3} and acceptor concentration of CZTS was found to be NA=1.00E+17 cm^{-3}.

3.1 Comparison between the experimental and theoretical solar cell

We can compare and simulate between the experimental part by Guo et al. [17] and theoretical part in order to know the performance of the device and the good matching quality using the SCAPS program. Table 2 shows the parameters of the experimental and theoretical design.

The results illustrate a good matching between the experimental and theoretical part and the interface defect layers of the CZTS/ZnS have a good role to this match. The difference between experimental and theoretical part is due to that the fill factor of the experimental cell decreases, this is attributed to the formation of the defects, this leads to reduce the lifetime of carriers due to increase the recombination and thus the efficiency value decreases of the experimental cell as Figure 2.

3.2 Study the effect of changing energy gap of window layer of I-V characteristic

To simulate the best performance of the window layer, energy gap values were changed from 3 to 3.5eV. It can be seen the open voltage circuit (Voc) was constant and is not affect of the change of the energy gap value, while the short circuit current density Jsc decreases at 3.1eV, then, it begins to increase with increasing energy gap. The results of I-V measurements were obtained as Figure 3.

Furthermore, the fill factor value (FF) remains constant at Eg=3.3eV and then, it also begins to increase, the efficiency value η was constant at Eg=3.3eV and it comes back to increase due to the window layer absorbs the incident phonons and does not allow to reach the absorption layer. When the energy gap value increases at Eg=3.3eV, the number of photons allow to reach of absorption layer, this leads to improve the output of cell structure [18]. The best efficiency was obtained when the energy gap value at Eg=3.5eV and the efficiency was found to be η=29.1%. We can conclude that the solar cell efficiency improves with doping concentration.

Table 2. Parameters of solar cell CZTS/ZnS/i-ZnO/n-ZnO:AL)

	Structure	V(V)	J(mA/cm^2)	FF%	η%
1	CZTS/ZnS/i-ZnO/n-ZnO:AL) Experimental	1.03	29.12	75.3	25.1
2	CZTS/ZnS/i-ZnO/n-ZnO:AL) Theoretical	1.10	29.93	79.9	26.43

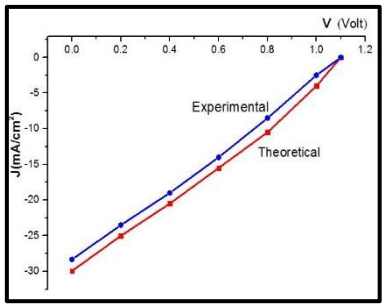

Figure 2. Experimental and theoretical of I-V characteristic

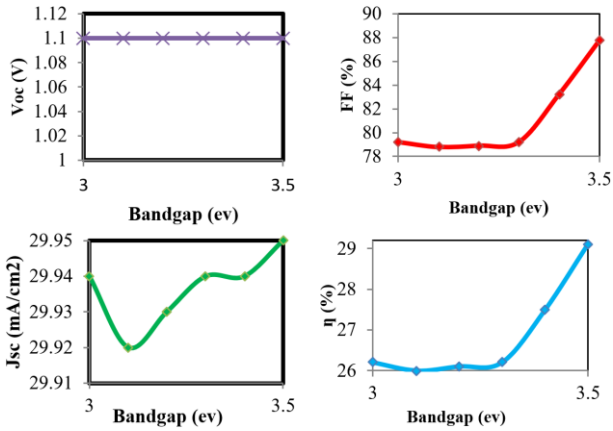

Figure 3. Effect of changing energy gap of the window layer of I-V characteristic

3.3 Study the effect of changing energy gap of absorption layer of I-V characteristic

The changing of the energy gap values was studied from 1.35eV to 1.55eV. The results of I-V measurements were obtained as Figure 4.

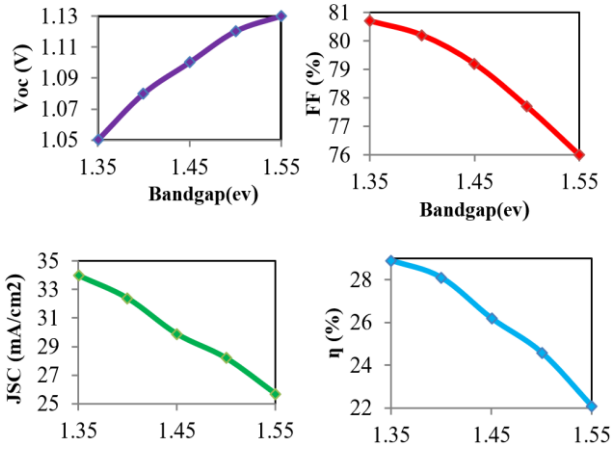

Figure 4. Effect the changing energy gap of absorption layer of I-V characteristic

Figure 4 illustrates that the open voltage circuit (Voc) increases with the energy gap while the current short circuit density Jsc reduces with raising the energy gap. The fill factor FF reduces with raising the energy gap of absorption layer. Similarity, the efficiency value η reduces with raising the energy gap Eg due to that the absorption process does not occur until the condition (hu < Eg). The electron moves from valance band to band conduction which is increased the potential energy (Eg=qV). We can conclude that the Voc value is proportional with the energy gap value. Conversely, the density of the short current and the efficiency value η are inversely proportional with energy gap because the increasing of energy gap reduces of the number of electrons which have the energy greater than energy gap [19].

3.4 Study of effect of doping concentration of window layer of I-V characteristic

The ratio of doping concentration influences on two important factors, the first one is diffusion length and the second one is minority carriers' life time. the operating of the solar cell requires that the carriers can be able to move from absorber layer to the junction. Furthermore, the charge carriers combine before the reach the junction [20]. The doping concentration (ND) of window layer ZnO:AL was changed from 1.00E + 13 cm^{-3} to 1.00E + 16cm^{-3}. The result of I-V measurements as illustrated in Figure 5.

This figure illustrates that the open voltage circuit keeps c-onstant and is not influence of the concentration ratio of window layer due to the carrier's recombination does not occur. This is attributed the doped concentration of window layer in this paper was greater than doped concentration of absorption layer. The current short circuit Jsc keeps fixed and then decreases slightly after doping ratio at 1.00E + 15 cm^{-3}. It can be seen the fill factor FF and the values efficiency η increase with raising ratio of concentration due to reduce of charge carriers' recombination process. The best efficiency can be obtained at η=28%), when the concentration ratio of the window layer was found to be ND=1.00E + 16 cm^{-3}).

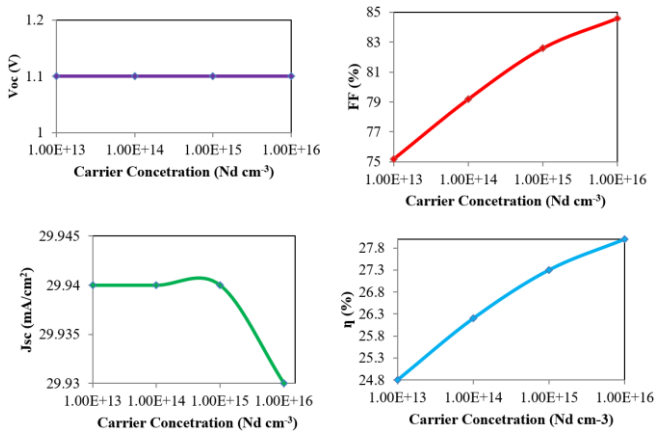

Figure 5. Effect of doping density (ND) of window layer of I-V characteristic

3.5 Study of effect of doping concentration of absorption layer of I-V characteristic

The doped of the acceptor density (NA) of the absorber layer CZTS was changed from 1.00E + 16- 1.00E + 19cm^{-3}. The curves of electrical parameters as shown in Figure 6.

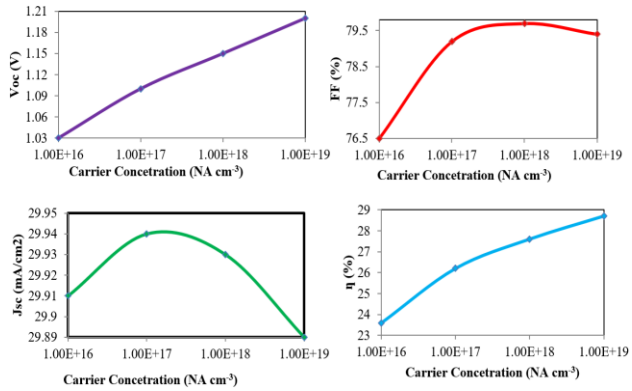

Figure 6. Effect of Doping Concentration(N_D) of absorption layer of I-V characteristic

This figure illustrates that the open voltage circuit rises with doped concentration NA of absorption layer due to reduce in the recombination process in quasi natural region, whereas the short current circuit keeps fixed with increasing doping ratio of absorption layer due to the short current circuit which is depended on thickness of absorption layer, while we notice that the value decreases at NA=1,00E + 17 cm^{-3} due to reduce of carriers time and also the high recombination process [21]. It can be seen that the values of the efficiency and the fill factor increase with increasing of doping ratio NA of absorption layer due to reduce of recombination process in this layer .The best efficiency η can be obtained was η=28.7% at NA=1.00E + 19 cm^{-3}.

3.6 Influence of the window layer thickness ZnO:AL of the electrical properties

ZnO:AL is one of the most important parts of the window layer that can be utilized in numerous applications. This layer has been extensively studied recently due to potential applications in electronics and photonics devices [22]. This layers usually designed thinner than the absorption layer to raises the absorption of the solar radiation (photons) in P-

CZTS layer. The thickness of the ZnO:AL layer was changed from 0.1 to 0.5µm in order to obtain the best thickness. Furthermore, when the window layer ZnO:AL thickness was increased, the open voltage and the short- current reduced due to increase of the carrier's recombination at the surface as Figure 7(a)-(b). Besides, we can disuse the results that the fill factor FF raises with the thickness due to the low resistivity and doping of ZnO:AL layer as shown in Figure 7(c). Whereas the efficiency reduces with raising thickness due to reduce in the incident photons which is absorbed by CZTS layer. Therefore, the pair generation rate (electron-hole) reduces whereas the recombination process increases as in Figure 7(d).

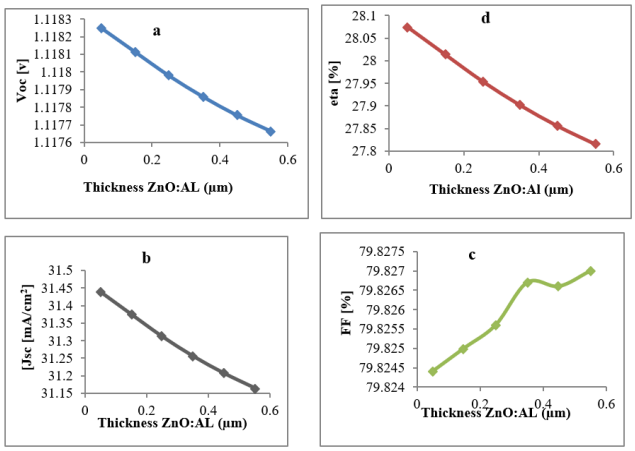

Figure 7. Influence of the window layer thickness ZnO:AL of I-V characteristic

3.7 Influence of the absorber layer thickness CZTS of the I-V properties

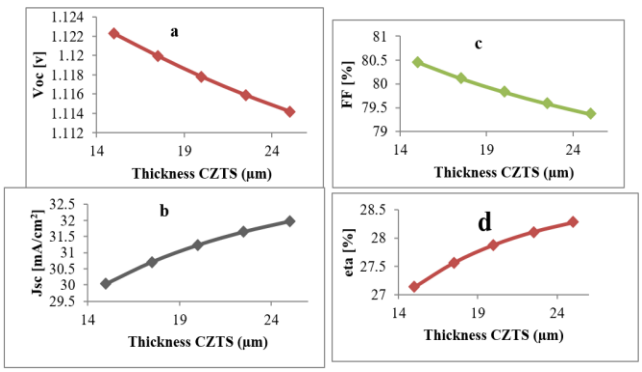

Figure 8. Effect of the absorption layer thickness CZTS of the electrical properties

The absorption layer (CZTS) has a high absorption coefficient up to 10^4 cm^{-1} so the high efficiency can be achieved at a low cost. The absorption layer was changed from 2.5 to 25µm in order to get the best efficiency. It can be seen, the open voltage circuit (Voc) value decreases with increasing thickness due to increase in the possibility of recombination which in turn leads to increase in the reverse saturation current generated in the depletion region as Figure 8(a). Whereas the values of the short current increases dramatically because of the increase of the recombination and incomplete photons absorption at the thicknesses below 2.5 µm. The values of Jsc increases clearly at the thickness more than 2.5 µm, due to the absorption of larger number of the incident photons as Figure 8(b). The fill factor decreases with increasing thicknesses due to increase of recombination process as Figure 8(c). In Contrast, the efficiency slightly increases with increasing thickness due to increase the generation rate. Thus, the incident photons are absorbed at different depths as Figure 8(d).

4. CONCLUSION

The performance and efficiency of MoS2/p-CZTS/n-ZnS/i-ZnO/n-ZnO:AL cell was improved using the SCAPS program. The results show the best efficiency of the window layer ZnO:AL was found to be 29.1% when the energy gap was found 3.5eV. Comparable, the best efficiency of the absorption layer was found to be 28.9% when the energy gap was found 1.35eV. On the other side, the best efficiency of the window layer was found to be η=28% at doping concentration ND=1.00E + 16 cm^{-3} and efficiency of the absorption layer were found to be η=2 8.7% at doping concentration ND=1.00E + 19 cm^{-3}. We have completed the comparison between the experimental and theoretical solar cell. The good matching between the experimental and theoretical part was observed. Solar cell was designed to enhance the cell efficiency in order to increase energy production with good conversion efficiency at low operating costs of experimental results. Finally, the high quality and efficient solar cell can be designed by manipulating the layers parameters for improving the performance of solar cell.

Future Suggestion: Doping concentration on reflection layers in order to improve the device of the cell efficiency.

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