

A Comparative Performance Evaluation of Ternary $Zn_xCd_{1-x}S$ and Binary CdS Window Layer in CIGS Solar Cell

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Abstract- In this research work, a thin film CIGS cell is numerically studied with a ternary compound $Zn_xCd_{1-x}S$ as window layer in lieu of binary compound CdS by SCAPS 1D simulator. In this work a comparison between two window layers (CdS and $Zn_xCd_{1-x}S$) is shown to accumulate the better efficiency of the CIGS cell. To observe the cell performance a numerical analysis is done by changing the function of x from 0.05 to 0.3 in ternary compound $Zn_xCd_{1-x}S$ using SCAPS 1D solar cell simulator. Along with it other parameters such as thickness, band gap variation of different layers and temperature are also numerically studied using the simulation software to acquire the optimum cell efficiency. The rising amount of Zn content in $Zn_xCd_{1-x}S$ leads to a fine absorption in the absorber layer in the blue region (400-500nm). It also exhibits the increment of the window layer band gap between 2.42eV to 3.7eV. The proposed cell structure $Zn_xCd_{1-x}S/CIGS$ has shown the highest efficiency of 29.00%, open circuit voltage of 0.9672V, short circuit current density of 37.852mA/cm² and FF of 79.21%.

Keywords- Thin-film solar cell; Absorber layer; $Zn_xCd_{1-x}S$; SCAPS.

Table 1. Nomenclature table

Subscripts	E_g (eV)	Band gap	Latin/Greek symbols	V_{MPP} (V)	Voltage maximum power point
	J_{sc} (mA/cm ²)	Short circuit current density		η (%)	Efficiency
	J_{MPP} (mA/cm ²)	Current maximum power point		σ_p (cm ²)	Capture cross section of holes
	N_A (cm ⁻³)	Acceptor density		σ_m [eV]	Metal work function
	N_c (cm ⁻³)	Conduction band effective density		σ_n (cm ²)	Capture cross section of electrons
	N_D (cm ⁻³)	Donor density		μ_e (cm ² /Vs)	Electron mobility
	N_v (cm ⁻³)	Valance band effective density		μ_h (cm ² /Vs)	Hole mobility
	S_e [cm/s]	Surface recombination velocity (electron)		ϵ_r	Dielectric relative permittivity
	S_h [cm/s]	Surface recombination velocity (hole)		FF (%)	Fill factor
	V_{oc} (V)	Open circuit voltage		W (nm/ μ m)	Thickness
Abbreviations					

	X (eV)	Electron affinity
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1 Introduction

Owing to escalating demand for energy, renewable sources have been one of the utmost ways to meet the world crisis furthermore solar power gained the most acceptances over other renewable sources. Moreover renewable sources can be integrated into smart grid system to reduce the energy crisis[1]. Photovoltaic system has been very popular in industrial application such as for Electric Vehicle to minimize the expense of charging electrical energy [2]. In solar cell technology, the thin-film solar cell (TFSC) technique has become most popular due to its manufacturing cost, high efficiency, reliability and market share [3, 4]. Among thin-film solar cell technology, copper indium gallium selenide (CIGS) provides a high absorption coefficient, good performance of Photovoltaic characteristics comparing with other thin-film solar cells such as CdTe or Si solar cell[4] along with it assures long term stability and maximum conversion efficiencies out of all thin films[5]. Moreover, the bandgap and electron affinity of CIGS cell can be adjusted by the Ga/(In+Ga) ratio, which results in numerical analysis to achieve higher efficiency[6]. The Fraunhofer Institute for Solar Energy Systems (ISE) has disclosed 22.3% efficiency of CIGS solar cell using KF post-deposition treatment also exhibited a way of Cd free CIGS solar cell for environmental well being [7].

CdS has been used in many CIGS and CdTe solar cell as buffer layer [8, 9] and window layer [10] respectively. Toxic Cd free Cu(In,Ga)(Se,S)₂ thin-film solar cell has been proved with a record efficiency of 23.35% by the National Institute of Advanced Industrial Science and Technology[11]. Moreover, CdS have a very low bandgap (E_g=2.42eV) which creates a hindrance of light absorption in the absorber layer in the blue region (400-500) nm wavelength [12]. ZnCdS is an alternative heterojunction partner for CIGS/CIGS₂ solar cell[13]. Alloying CdS (E_g=2.42eV) with ZnS (E_g=3.7eV) turned into ternary compound Zn_xCd_{1-x}S which gives a tunable bandgap between 2.42 to 3.7eV varying the function x from 0 to 1 and allows a good amount of light absorption in the blue region in the absorber layer [13, 14] and improves the overall cell efficiency, V_{oc}, J_{sc} and fill factor than CdS/CIGS cell. For building an ultra-thin CIGS solar cell needed a wide band n-type layer to form pn junction [5] which can be done by n-type ZnCdS ternary compound varying x at the desired level.

It is noteworthy that there have been very rare published papers with the application of Zn_xCd_{1-x}S as a window layer in CIGS solar cells. In this paper, a numerical analysis of Zn_xCd_{1-x}S has been done and compared the results with toxic CdS by SCAPS 1D simulator for the purpose of rising cell efficiency.

2 Methodology

The proposed design of the cell Zn_xCd_{1-x}S/In₂S₃/CIGS/BaSi₂ is presented in fig.01.

In the layout of the cell, an n-type Zn_xCd_{1-x}S used as a window layer with a p-type CIGS absorber layer coated with

Aluminum (Al) and Molybdenum (Mo) as front contact and back contact respectively. Another two layers are added for the purpose of boosting cell efficiency. In₂S₃ buffer layer is an ideal replacement of CdS because of its toxic impact on the environment along with configuring a pn junction [15]. Also the best efficiency of In₂S₃/CIGS has been found 24.41% [15]. A BSF layer BaSi₂ is inserted between of absorber layer and the back contact to reduce back surface recombination loss. Also, BaSi₂ is a low priced as well as an easily obtainable material [16]. Table 2 & 3 shows the device and layer parameter which was taken based on previous research work. In this work three parameter are examined layer thickness, bandgap and temperature to observe the cell performance. Aiming to perform analysis of the cell the function x in Zn_xCd_{1-x}S is varied from 0.05 to 0.3 as well as the thickness of different layers. In the simulation process, the window layer thickness is varied from 10 to 300nm and for absorber layer 1000 to 2000nm. For window and absorber layer thickness variation, the photovoltaic characteristics (V_{oc}, J_{sc}, FF, η) are compared for proposed Zn_xCd_{1-x}S/CIGS and conventional CdS/CIGS Furthermore, the effect of varying the thickness of the ternary Zn_xCd_{1-x}S window layer on cell Quantum efficiency (QE) is examined. The thickness of the In₂S₃ buffer layer is varied from 50 to 200nm, and the band gap is changed from 2.1 to 2.5eV. The thickness of BaSi₂ is varied from 100 to 1000nm. And to see the cell performance temperature is varied from 300 to 400K and corresponding simulation data is numerically studied. SCAPS 1D is used to measure the cell photovoltaic characteristics fill factor (FF), power conversion efficiency, open circuit voltage (V_{oc}) and short circuit current (J_{sc}) at AM 1.5G and T=300K. Fig 2 depicts the energy band diagram of the proposed solar cell. The energy band diagram is drawn using SCAPS simulation data of energy band panel. It visualizes the layer thickness and bandgap of each layer material used in the proposed cell. This band diagram ensures that the proposed cell will be capable to attain the expected cell performance.

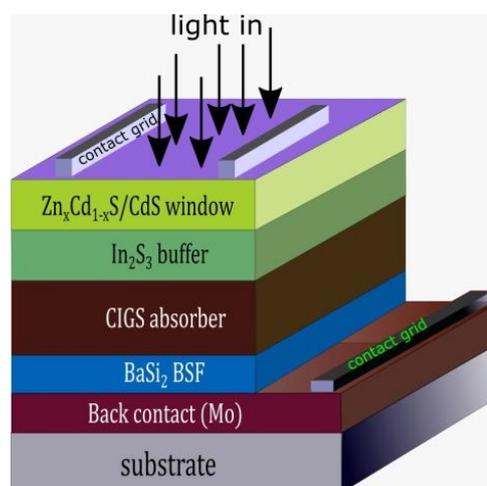


Fig. 1. Proposed Zn_xCd_{1-x}S/CIGS cell structure (layer thickness are not scaled and the color of different layers are arbitrarily chosen)

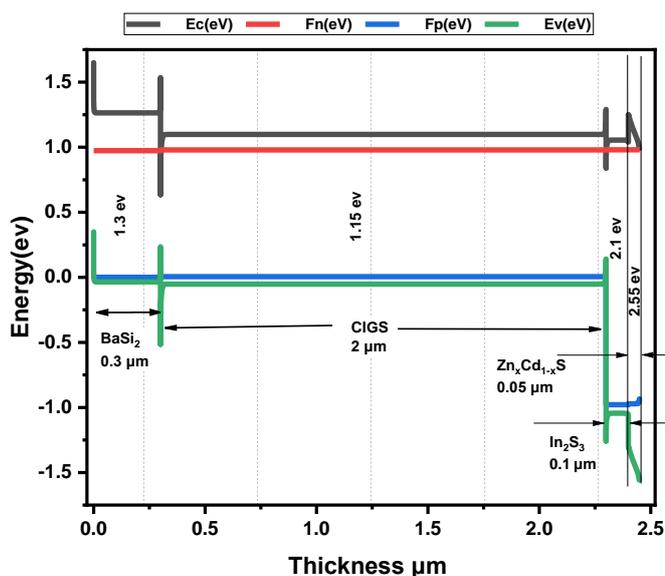


Fig. 2. The energy band diagram of proposed Zn_{0.1}Cd_{0.9}S/CIGS cell

3 Results & Discussion

3.1 Composition Function X Optimization in Ternary Compound Zn_xCd_{1-x}S Window Layer

Fig 3 illustrates the effect of adding Zn content in ternary compound Zn_xCd_{1-x}S as a function of x on photovoltaic

characteristics (V_{oc} , J_{sc} , FF & η). Here x is varied from 0.05 to 0.3 and corresponding numerical simulation is observed. Fig 3 shows a smooth upwarding change of all photovoltaic characteristics with the increasing amount of Zn component in ternary compound Zn_xCd_{1-x}S. Analyzing Zn content in Zn_xCd_{1-x}S, the best cell performance is found at x=0.1 (V_{oc} =0.9672volt, J_{sc} =38.852mA/cm², FF=79.21%, η =29.0%). Increasing Zn content improves the band gap of window layer in between 2.42 to 3.7 eV that signifies more light can pass through the ternary compound Zn_xCd_{1-x}S window layer and improve blue light (400-500nm) absorption in the absorber layer.

Table 2. Material properties of ternary Zn_xCd_{1-x}S window layer [17]

parameter	X=0.05	X=0.08	X=0.1	X=0.2	X=0.3
E _g (ev)	2.48	2.50	2.55	2.58	2.64
X (ev)	4.47	4.46	4.44	4.38	4.32
μ_e (cm ⁻² /Vs)	100	100	95	85	75
μ_h (cm ⁻² /Vs)	40	40	35	30	25
ND (cm ⁻³)	3.0×10 ¹⁶	2.5×10 ¹⁶	2.5×10 ¹⁶	1.7×10 ¹⁶	1.6×10 ¹⁶

Table 3. Layer properties of CIGS solar cell

LAYER PROPERTIES							
Parameters	Zn _x Cd _{1-x} S [17]	CdS [18]	In ₂ S ₃ [18]	CIGS [18]	BaSi ₂ [16]	Front contact (Al) [12]	Back Contact (Mo) [12]
W(nm)	10-300	10-300	50-200	1000-2000	100-1000	-	-
E _g (ev)	2.550	2.4	2.1	1.150	1.3	-	-
X (ev)	4.44	4.4	4.65	4.2	3.3	-	-
ϵ_r	9.3	10	13.5	13.6	11.170	-	-
N _c (cm ⁻³)	2.1×10 ¹⁸	2.20×10 ¹⁸	1.80×10 ¹⁹	2.20×10 ¹⁸	2.60×10 ¹⁹	-	-
N _v (cm ⁻³)	1.7×10 ¹⁹	1.80×10 ¹⁹	4.00×10 ¹³	1.80×10 ¹⁹	2.0×10 ¹⁹	-	-
μ_e (cm ⁻² /Vs)	95	100	400	100	820	-	-
μ_h (cm ⁻² /Vs)	35	25	210	25	100	-	-
N _D (cm ⁻³)	2.5×10 ¹⁶	5.00×10 ¹⁷	1.00×10 ¹⁸	0	0	-	-
N _A (cm ⁻³)	0	0	0	2.00×10 ¹⁸	5.0×10 ¹⁸	-	-
Defects Energetic distribution	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	-	-
Type	Acceptor	Acceptor	Acceptor	Donor	Donor	-	-
σ_n	1.00×10 ⁻¹⁵	1.00×10 ⁻¹⁵	1.00×10 ⁻¹⁵	5.00×10 ⁻¹⁷	5.00×10 ⁻¹⁷	-	-
σ_p	1.00×10 ⁻¹⁵	1.00×10 ⁻¹⁵	5.00×10 ⁻¹³	1.00×10 ⁻¹³	1.00×10 ⁻¹³	-	-
Contact properties	-	-	-	-	-	4.45	4.95
σ_m [ev]	-	-	-	-	-	-	-
Se [cm/s]	-	-	-	-	-	1.00×10 ⁷	1.00×10 ⁷
Sh[cm/s]	-	-	-	-	-	1.00×10 ⁷	1.00×10 ⁷
R _f	-	-	-	-	-	0.05	0.9

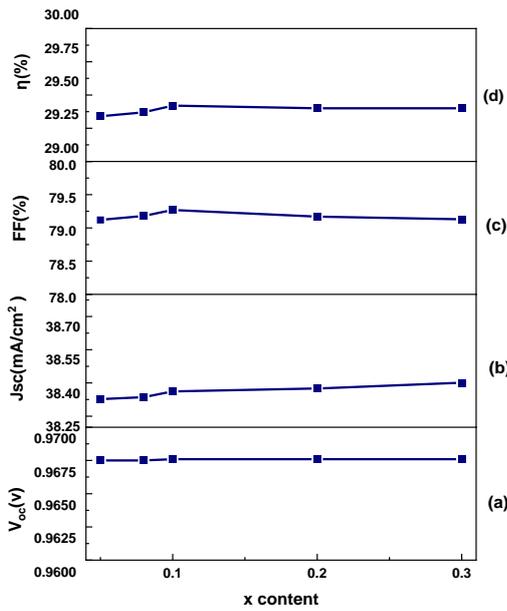


Fig. 3. Effect of composition of Zn_xCd_{1-x}S on cell performance (a) open circuit voltage, (b) short circuit current, (c) fill factor and (d) cell efficiency

3.2 Effect of Window Layer Thickness and Comparing the Results of Proposed and Conventional Cell

Fig 4 shows a comparison of photovoltaic characteristics between conventional CdS and proposed Zn_xCd_{1-x}S cells with the variation of window layer thickness. Window layer thickness is varied from 10 to 300 nm in numerical analysis. Fig 4 describes as the thickness of the window layer decreases, the photovoltaic characteristics V_{oc}, J_{sc} and η increases. At lower thickness of the window layer, it passes more sunlight into the absorber layer which causes to increase V_{oc}, J_{sc} and η. In case of FF, it decreases slightly as window layer thickness rises. This emerges because V_{oc} and J_{sc} both goes up, but V_{MPP} and J_{MPP} fall. As a result, according to Eq. (1) [16] the FF decreases.

$$FF = \frac{V_{MPP} \times J_{MPP}}{V_{oc} \times J_{sc}} \tag{1}$$

The values of V_{MPP} and J_{MPP} for the material of ternary Zn_xCd_{1-x}S and binary CdS at thickness width 10 and 50nm are shown in table 4.

3.3 Effect of Absorber Layer Thickness

The photovoltaic characteristics of Zn_{0.1}Cd_{0.9}S/CIGS and CdS/CIGS are compared in Fig 5 varying the thickness of the CIGS layer from 1000 to 2000nm. Fig 5 depicts the proposed Zn_{0.1}Cd_{0.9}S/CIGS has better photovoltaic characteristics (V_{oc}, J_{sc}, and FF) than CdS/CIGS. Increasing the CIGS absorber layer thickness, J_{sc} slightly increases. And V_{oc} slightly decreases with increasing layer thickness. Fig 5 shows FF and

η remain nearly constant. Analyzing the numerical data of absorber layer thickness for the proposed and conventional cell, Zn_xCd_{1-x}S can be a good alternative hetero-partner of CIGS cell.

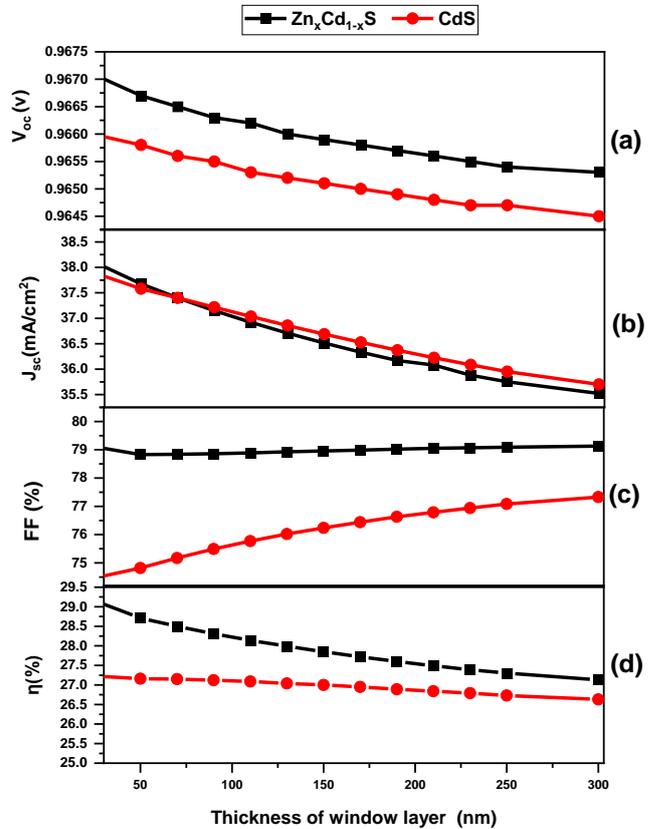


Fig. 4. Effect of window layer thickness variation performance (a) open circuit voltage, (b) short circuit current, (c) fill factor and (d) cell efficiency

Table 4. Data of voltage and current maximum power point

Material	Thickness (nm)	V _{MPP} (v)	J _{MPP} (mA/cm ²)
Zn _x Cd _{1-x} S	10	0.828	35.540
Zn _x Cd _{1-x} S	50	0.827	35.050
CdS	10	0.828	32.392
CdS	50	0.824	32.947

3.4 Effect of Buffer Layer Thickness Variation on Solar Cell

The buffer layer is a film that sits between the absorber and window layers and has two functions: structural stability and electrostatic correction within the absorber layer. The In₂S₃ material not only removes hazardous cadmium but it also increases light transmission having a wider band gap than CdS, which serves to increase light absorption in the absorber layer and increase cell efficiency.

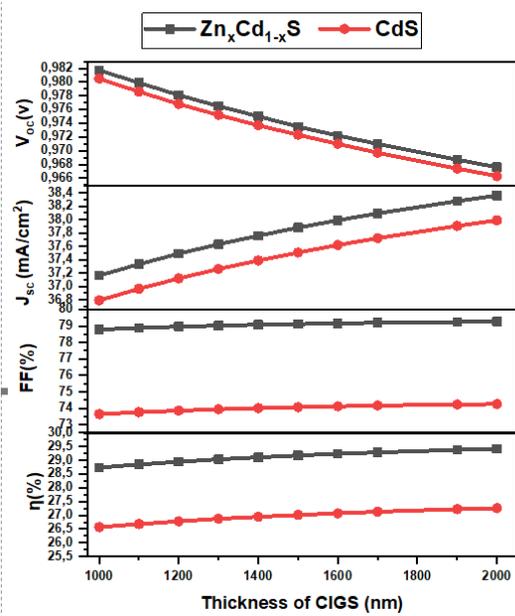


Fig. 5. Effect of absorber layer thickness variation on photovoltaic characteristics (open circuit voltage, short circuit current, fill factor and cell efficiency)

Fig 6 shows the impact of varying the thickness of the In_2S_3 buffer layer on photovoltaic characteristics of the cell. Buffer layer thickness is varied from 50 to 200nm. The proposed cell's photovoltaic characteristics (FF and η) rises smoothly as the buffer layer thickness falls. This occurs as the thickness of the buffer layer rises, more sunlight are absorbed in the buffer layer. As a result, the number of photons reaching in the absorber layer is reduced. In other words, when the buffer layer is thinner, more light can be absorbed in the absorber layer. The V_{oc} and J_{sc} of the cell remains almost flat. Buffer layer forms a barrier for sunlight to be absorbed in the absorber layer at higher thicknesses which is an indication that a thinner buffer layer allows the cell to absorb more light. The use of buffer layer thickness variation in this numerical analysis cell shows a significant favorable impact on the proposed solar cell performance.

3.5 Effect of Buffer Layer Bandgap Variation on Solar Cell

The band gap of the In_2S_3 buffer layer is increased from 2.1 to 2.5 eV to visualize the changes of photovoltaic characteristics of proposed $\text{Zn}_x\text{Cd}_{1-x}\text{S}/\text{CIGS}$ solar cell. The bandgap in the n-type area is widened more by the n-type In_2S_3 buffer layer, which boosts light absorption in the absorber layer. In Fig 7 FF, and η decreases till 2.3eV, after which begin to increase. For the variation of buffer layer bandgap, V_{oc} and J_{sc} remain almost constant. Analyzing the numerical data, FF and η it shows a good impact on overall cell performance at higher bandgap of buffer layer.

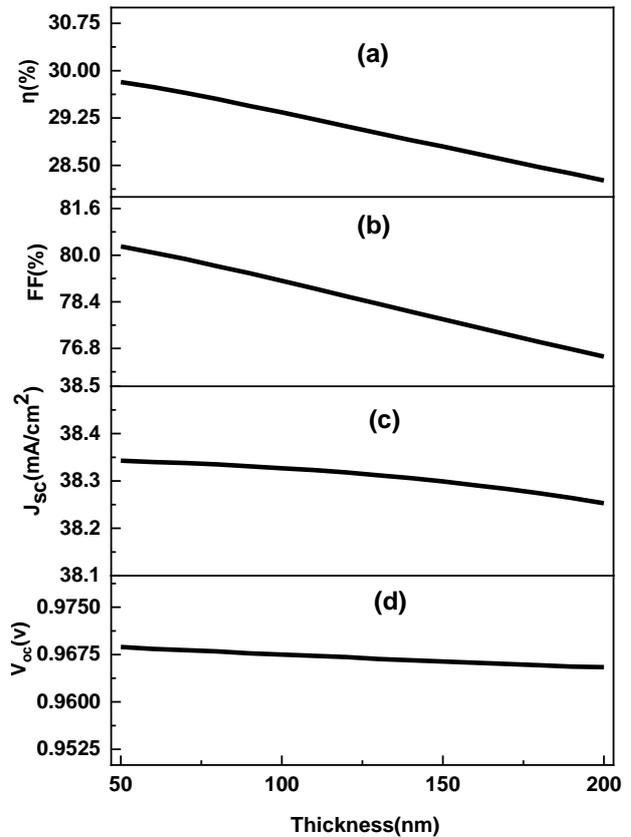


Fig. 6. Effect of buffer layer thickness variation (a) cell efficiency, (b) fill factor, (c) short circuit current (d) open circuit voltage

3.6 Effect of BSF Layer Thickness Variation on Solar Cell

A high impurity doping concentration on the back side of the solar cell can prevent high recombination of minority ion carriers (electrons) at the metallic back contact layer. Inserting a back-surface field (BSF) layer with a higher doping concentration than the active absorber layer can accomplish this. In many past research paper it is shown after adding BSF layer in cell reduces the recombination of minority carriers and increases cell efficiency[19, 20]. A thin BaSi_2 layer is kept next to the CIGS absorber layer (with doping of $2.00 \times 10^{18} \text{ cm}^{-3}$) to act as a BSF layer (with doping of $5.00 \times 10^{18} \text{ cm}^{-3}$) in this study. In this work the width/thickness of the BaSi_2 layer is changed from 0.1 to 1 μm or 100 to 1000nm. And the corresponding photovoltaic characteristics (V_{oc} , J_{sc} , FF and efficiency) are evaluated for the recommended $\text{Zn}_x\text{Cd}_{1-x}\text{S}/\text{CIGS}$ cell. Varying the BSF layer thickness, the cells photovoltaic characteristics (V_{oc} , J_{sc} , FF and η) changes in upwarding direction very slightly as shown in Fig 8. Cell efficiency increases from 29.23 to 29.53% in a slightly linear manner. The interface between p+ -type BaSi_2 and p-type CIGS serves as a p-n junction, providing an electric field that acts as a shield to minority carrier movement to the rear surface. As a result, bouncing back the minority carriers, the BaSi_2 BSF layer will increase short-circuit current while

decreasing dark current. As a result of the BSF layer's inclusion, the solar cell's surface recombination rate is reduced, and the solar cell's performance is improved.

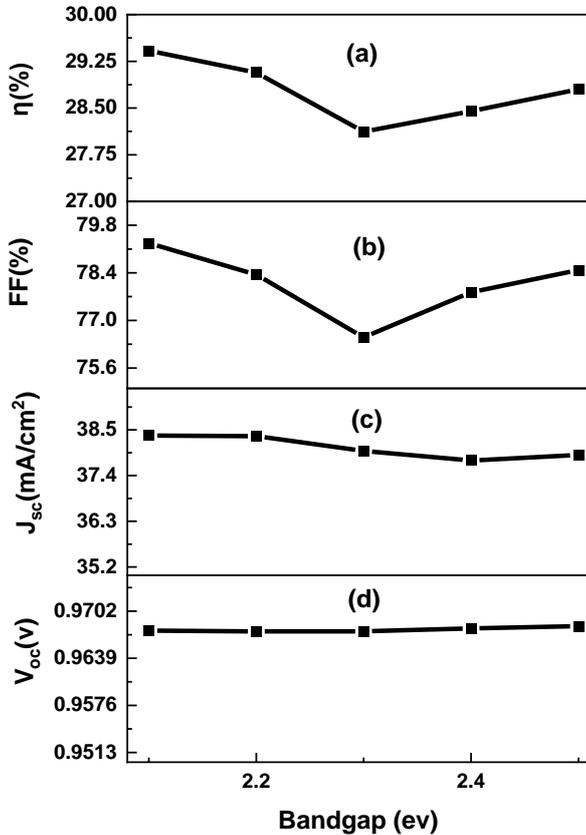


Fig. 7. Effect of buffer layer bandgap variation (a) cell efficiency, (b) fill factor, (c) short circuit current (d) open circuit voltage

3.7 Effect of Temperature on Photovoltaic Characteristics

Fig 9 depicts the impact of changing temperature on photovoltaic characteristics. Temperature or solar illumination plays a vital role on changing cell efficiency[21]. The temperature is varied from 300 to 400k keeping other layer parameters constant. As shown in Fig 9 all photovoltaic characteristics (V_{oc} , J_{sc} , FF and η) falls with rising temperature. The best cell efficiency is found at 300k. The lower cell performance is due to high recombination rate at higher temperature. At higher temperature the energy band gap is unstable which causes to accelerate the recombination rate of electrons and holes [22]. Thus high in temperature affects the overall cell performances.

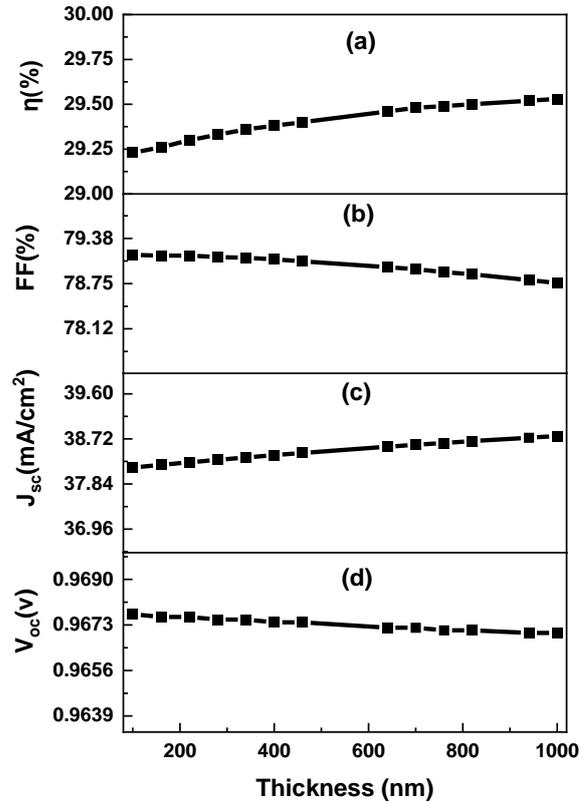


Fig. 8. Effect of BSF layer thickness variation (a) cell efficiency, (b) fill factor, (c) short circuit current (d) open circuit voltage

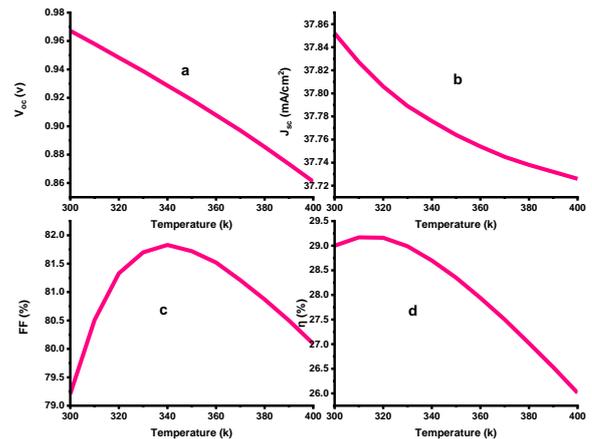


Fig. 9. Effect of temperature on cell (a) open circuit voltage, (b) short circuit current, (c) fill factor and (d) cell efficiency

3.8 Quantum Efficiency of the Proposed Cell

In Fig 10 Quantum Efficiency (QE) for different window layer $Zn_xCd_{1-x}S$ thickness is delineated. Quantum efficiency (QE) is defined as the ratio of electricity flowing into an external load to the number of incident photons. The $Zn_xCd_{1-x}S$ window layer thickness is varied from 10-100nm and corresponding cell quantum efficiency is observed. As seen in Fig 10 the cell's quantum efficiency is diminishing as its thickness increases. In other words the quantum efficiency improves as the window layer thickness gets lower. At lower thickness of $Zn_xCd_{1-x}S$ window layer allows more photon to be absorbed in the absorber layer which increases cell's quantum efficiency (QE). Table 5 showing the comparison of cell performance between $Zn_xCd_{1-x}S/CIGS$ and $CdS/CIGS$. It proclaims a remarkable improvement in the application of solar cell due to using $Zn_xCd_{1-x}S$ as window layer instead of toxic CdS . A comparison data between the proposed cell and previous relevant work is summarized in Table 6.

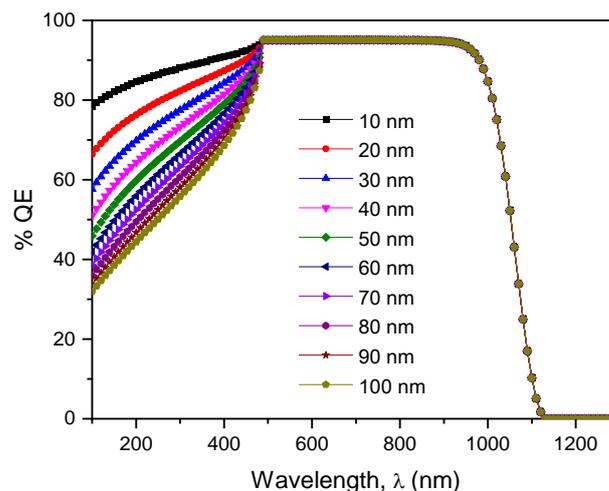


Fig. 10. Data of quantum Efficiency (QE) with proposed $Zn_xCd_{1-x}S$ window layer thickness variation.

Table 5. overview of simulation result

Material	Thickne ss (nm)	Voc (volt)	Jsc (mA/cm ²)	FF (%)	η (%)
$Zn_xCd_{1-x}S$ (proposed)	50	0.967 2	37.852	79.2 1	29.0 0
CdS (convention al)	50	0.966 0	37.575	74.7 9	27.1 5

Table 6. The photovoltaic characteristics of proposed cell in comparison with previous relevant work

No	Type of research	Absorber layer	Window layer	V _{oc} (v)	J _{sc} (mA/cm ²)	FF (%)	η (%)	Ref
1	Experimental	CIGS	CdZnS	0.5458	36.71	68.38	13.7	[23]
2	Experimental	CIGS	ZnO	0.678	35.22	78.65	18.8	[24]
3	Experimental	CIGS	ZnO/CdS	0.689	35.72	78.12	19.2	[25]
4	Experimental	CIGS	ZnO/CdS	0.693	35.34	79.4	19.5	[26]
5	Theoretical	CdTe	$Zn_xCd_{1-x}S$	1.1	27.18	66.65	19.93	[27]
6	Theoretical	CdTe	$Zn_xCd_{1-x}S$	0.98	29.35	0.85	22.42	[28]
7	Theoretical	CIGS	ZnO	0.843	40.56	76.80	26.24	[29]
8	Theoretical	CIGS	$Zn_xCd_{1-x}S$	0.9672	37.852	79.21	29.00	[^a]

[^a] The proposed cell herein

4 Conclusion

A numerical investigation has been carried out between ternary compound $Zn_{0.1}Cd_{0.9}S$ and binary CdS window layer to perceive the best cell performance of CIGS cell. The finest cell efficiency of 29.00% ($V_{oc}=0.9672v$, $J_{sc}=37.852 \text{ mA/cm}^2$ and $FF=79.21\%$) is found at $x=0.1$, 50nm $Zn_xCd_{1-x}S$ layer width and 2000nm CIGS layer width. Our proposed $Zn_{0.1}Cd_{0.9}S/CIGS$ cell efficiency is increased 6.81% with 5.37% increment of window layer band gap than the conventional CdS/CIGS cell. Analyzing all the data, it shows that the proposed ternary window $Zn_xCd_{1-x}S$ layer can be an ideal replacement than the toxic CdS to make an ultra thin-film CIGS solar cell for practical uses.

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