ANALYTICAL ANALYSIS OF HIGH-EFFICIENT THIN FILM BASI$_2$/IN$_2$S$_3$ SOLAR CELL WITH SCAPS 1-D SIMULATION

ANALIZA ANALITICĂ A CELULEI SOLARE BASI2/IN2S3 CU FILM SUBȚIRE DE ÎNALTĂ EFICIENȚĂ CU SIMULARE SCAPS 1-D

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Abstract: *The main purpose of this study presented herein is to improve the efficiency of such devices by using low-cost materials and widely available Barium disilicide* ($BaSi_2$) *as absorber layer. In the window layer, the light transmittance* SnO_2 *was much higher than other materials like* (SiO_2) *throughout the whole spectral region. The cell structure consists of* $Al/SnO_2:F/InS_3/BaSi_2:B/Cu$*, resulting in the alternative structure of* $Al/BaSi_2:B/In_2S_3/FTO/Cu$*, with fluorine-doped tin oxide (FTO) as the window layer. Use entirely non-toxic and cost-effective* In_2S_3 *as a buffer layer having a band gap (2.84eV) that helps in avoiding the lower energy photons. The* $BaSi_2:B$ *absorber layer's thickness varies from 0.6 to 2 μm to optimize the device. 31.71% efficiency has accomplished along with 1.0735V open circuit voltage* (V_{oc})*, 34.43 mA/cm*^{2} *short circuit current density* (J_{sc}) *and 85.79% Fill Factor (FF). Used commercial software SCAPS-1D to analysis those layers.*

Keywords: $BaSi_2:B$; In_2S_3; $SnO_2:F$; Fill-Factor; SCAPS 1-D; Simulation; Efficiency; Thin-film Solar cell.

Rezumat: *Scopul principal al acestui studiu prezentat aici este de a îmbunătăți eficiența unor astfel de dispozitive prin utilizarea materialelor cu costuri reduse și a disilicidului de bariu (BaSi2) disponibil pe scară largă ca strat absorbant. În stratul de fereastră, transmisia luminii SnO2 a fost mult mai*

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mare decât alte materiale precum (SiO2) în întreaga regiune spectrală. Structura celulei constă din Al/SnO2:F/InS3/BaSi2:B/Cu, rezultând o structură alternativă de Al/BaSi2:B/In2S3/FTO/Cu, cu oxid de staniu dopat cu fluor (FTO) ca strat de fereastră. Se utilizează In2S3 complet netoxic și rentabil ca strat tampon având o bandă interzisă (2,84eV) care ajută la evitarea fotonilor cu energie mai mică. Grosimea stratului absorbant BaSi2:B variază de la 0,6 la 2 µm pentru a optimiza dispozitivul. S-a atins o eficiență de 31,71% împreună cu o tensiune în circuit deschis de 1,0735V (Voc), o densitate de curent de scurtcircuit de 34,43 mA/cm2 (Jsc) și 85,79% factor de umplere (FF). Am folosit software-ul comercial SCAPS-1D pentru a analiza acele straturi.

Cuvinte cheie: BaSi2:B; In2S3; SnO2:F; factor de umplere; SCAPS 1-D; Simulare; Eficienţă; Celulă solară cu peliculă subțire.

1. Introduction

High efficiency, resourceful and cost-effective solar cells are must have to convert light energy into electrical energy proficiently. In this case, barium silicide absorber and indium sulfide buffer layer based ($BaSi_2/In_2S_3$) thin film solar cell (TFSC) might be an upbeat solution for its low-cost manufacturing and high efficiency.

The main purpose of our study is to reduce fabrication cost and find out first-rate performance of buffer layer for a better substitute of toxic cadmium sulfide buffer layer and obtain high performance. Numerical simulations carried out by 'SCAPS-Solar Cell Capacitance Simulator' to measure the effect of thickness, impurity density, bulk defect density, temperature and voltage on device photo – voltaic performance.

This study is also focused to analyze the effect of thickness, band gap and concentration of both barium disilicide ($BaSi_2$) absorber layer [1] and indium sulfide (In_2S_3) buffer layer [2]. The buffer layer serves as intermediate layers that can prevent shunting between the absorber layer and window layer that is highly resistive. Buffer layer has many tasks to improve cell efficiency.

Among different buffer layers, indium sulfide (In_2S_3) is a very auspicious one. To obtain an environmentally amiable Photovoltaic system, β – In_2S_3 buffer layer has been applied which can be a replacement of CdS [2]. Here fluorine doped tin oxide (SnO_2: F) used as a window layer [3]. A window layer of large band gap is utilized to prevent front surface recombination. This layer is transparent to the incident radiation. Our proposed $BaSi_2/In_2S_3$ based solar cell offers higher efficiency (33.02%) with greater fill factor and open circuit voltage using only 0.835µm thickness.

The simulation and calculations were carried out in the SCAPS – 1D software which raised at the ELTS department of the University of Gent, Belgium. SCAPS was actually developed only for the $CuInSe_2$ and CdTe families cell structures [4]. But recent developments have improved its capabilities to make it now also applicable to others such as Si and GaAs family and a – Si and micro-amorphous Si. SCAPS (version 3.3.10) is used to measure solar cell parameters, for example, conversion efficiency, open circuit voltage, short circuit current density, Fill factor, current at maximum power point, voltage at maximum power point, quantum efficiency etc.

2. Methodology and Structure

Our proposed cell $BaSi_{2/}$ In_2S_3 has a structure of Al/SnO_2: F/In_2S_3/$BaSi_2$: B/Cu as shown in Figure 1. Here boron doped barium disilicide ($BaSi_2$) is used as active p-type absorber, where In_2S_3 as a buffer layer (n-type) and as a window layer SnO_2: F is used which is n+ - type and it's highly transparent and conductive oxide layer.

This solar cell structure is very simple which containing three layers only, Fluorine-doped tin oxide (SnO_2:F) as window layer, Indium(III) sulfide (In_2S_3) as buffer layer and Boron doped Barium Silicide ($BaSi_2$:B) as absorber layer. Here, the window layer thickness is 0.020 μm (20 nm), buffer layer is 0.015 μm (15 nm) and the absorber layer thickness is 0.80 μm (800 nm) only. As front contact (metal) Aluminum is used which metal work-function is 4.06 eV and as back metal-contact we use Copper (Cu) (metal work-function: 4.94 eV). Here SnO_2:F is n+ type, In_2S_3 is n type and $BaSi_2$:B is p+ type.

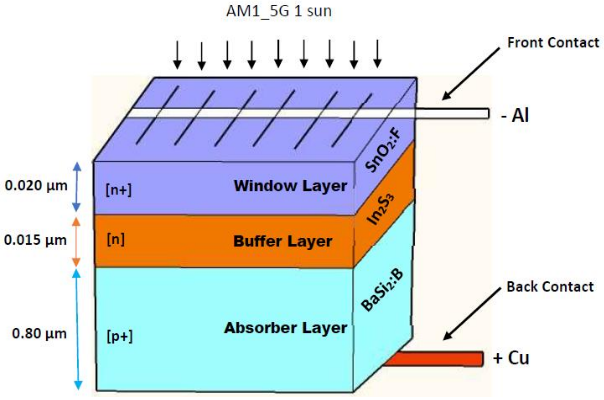
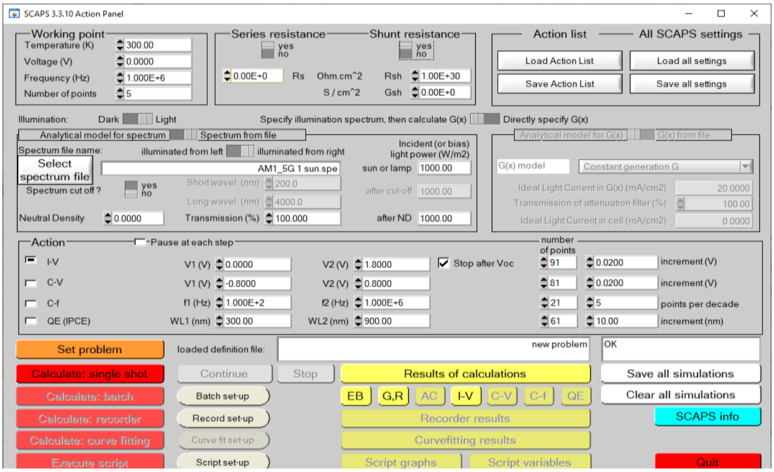


Figure 1. $Basi_2$:B/In_2S_3 Cell Structure (Designed by SketchUp Pro, PowerPoint & Microsoft Word)

3. Simulation

The simulation of Al/SnO_2:F/In_2S_3/$BaSi_2$:B/Cu. Here, $BaSi_2$:B is a the p-type absorber(active) material for the thin-film solar cell, where In_2S_3 as a buffer layer which is n-type and Fluorine doped Tin Oxide, FTO (SnO_2:F) is TCO n^+type window layer [5].

All the simulation done by SCAPS-1D (Version: 3.3.10) [Figure 2] for measuring cell output parameters (η, J_{sc}, V_{oc}, FF, J_{mpp}, V_{mpp} etc.). SCAPS-1D is a simulation programme for thin film solar.


SCAPS 3.3.10 Action Panel

Working point
Temperature (K) 300.00
Voltage (V) 0.0000
Frequency (Hz) 1.000E+6
Number of points 5

Series resistance: yes / no; 0.00E+0 Rs Ohm.cm^2
Shunt resistance: yes / no; Rsh 1.00E+30; S / cm^2 Gsh 0.00E+0

Illumination: Dark / Light
Specify illumination spectrum, then calculate G(x) / Directly specify G(x)
Analytical model for spectrum / Spectrum from file
Spectrum file name: AM1_5G 1 sun.spe
illuminated from left / illuminated from right
Spectrum cut off ? yes / no
Short wavel. (nm) 200.0
Long wavel. (nm) 4000.0
Neutral Density 0.0000
Transmission (%) 100.000
Incident (or bias) light power (W/m2)
sun or lamp 1000.00
after cut-off 1000.00
after ND 1000.00

Analytical model for G(x) / G(x) from file
G(x) model: Constant generation G
Ideal Light Current in G(x) (mA/cm2) 20.0000
Transmission of attenuation filter (%) 100.00
Ideal Light Current in cell (mA/cm2) 0.0000

Action ☐ Pause at each step

					number of points		
☒ I-V	V1 (V) 0.0000	V2 (V) 1.8000	☑ Stop after Voc	91	0.0200	increment (V)
☐ C-V	V1 (V) -0.8000	V2 (V) 0.8000		81	0.0200	increment (V)
☐ C-f	f1 (Hz) 1.000E+2	f2 (Hz) 1.000E+6		21	5	points per decade
☐ QE (IPCE)	WL1 (nm) 300.00	WL2 (nm) 900.00		61	10.00	increment (nm)

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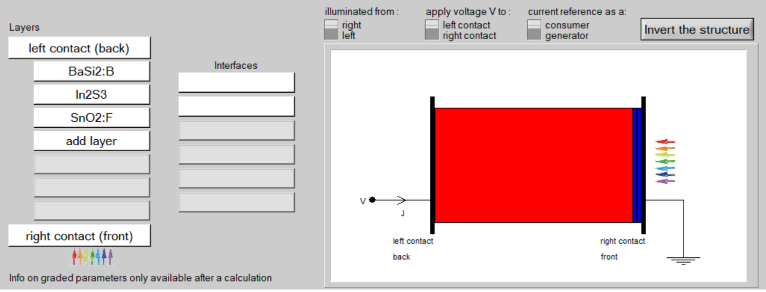
Figure 2. SCAPS-1D Simulator Front Page

100 mW/cm^2 illumination, AM 1.5G spectrum is used for the illumination-spectrum [6]. Absorption-coefficients, α(cm^{-1}) and wavelength, λ(nm) are inserted for the values of $BaSi_2$ from table 1, and also for In_2S_3, and SnO_2:F.


Layers
left contact (back)
BaSi2:B
In2S3
SnO2:F
add layer
right contact (front)

Interfaces

illuminated from : right / left
apply voltage V to : left contact / right contact
current reference as a: consumer / generator

Info on graded parameters only available after a calculation

Figure 3. Simulation Structure of p+-$BaSi_2$:B/n-In_2S_3/n+-SnO_2:F solar cell.

All the necessary values and parameters that are required for all layers, listed in listed in Table 1.

Table 1. **Material properties (input-data) which is required for simulation and analysis. [7][8][9][10]**

Properties	Absorber ($BaSi_2$:B)	Buffer (In_2S_3)	Window (SnO_2:F)
W (Thickness-nm)	800	15	20
E_g (Bandgap-eV)	1.3	2.1	3.6
$\varkappa$ (Electron affinity-eV)	3.300	4.1	4
Dielectric-permittivity, Ɛ	11.170	13.5	9
CB, N_c (cm^{-3})	2.6×10^{19}	1.8×10^{19}	2.2×10^{18}
VB, N_r (cm^{-3})	2.00×10^{19}	4.00×10^{13}	1.80×10^{19}
Electron-Velocity, S_n (cm/s)	1.00×10^{7}	1.00×10^{7}	1.00×10^{7}
Hole-Velocity, S_p (cm/s)	1.00×10^{7}	1.00×10^{7}	1.00×10^{7}
Electron-mobility, μ_n $(cm^2V^{-1}s^{-1})$	820	4.00×10^{2}	100
Hole-mobility, μ_p $(cm^2V^{-1}s^{-1})$	100	2.00×10^{2}	25
Donor-density, N_D $(\text{Shallow uniform} - cm^{-3})$	0	1.00×10^{18}	1.00×10^{18}
Acceptor density, N_A $(\text{Shallow uniform} - cm^{-3})$	$5.00\times 10^{19*}$	0	0
Defect-type	Single Acceptor (0/+)	Single Donor (0/+)	-
Energetic-distribution	Uniform	Uniform	-
N(t) total $(\text{Bulk defect density} - cm^{-3})$	$1.00\times 10^{14*}$	$1.00\times 10^{14*}$	-
N(t) peck $(\text{Bulk defect density}, -eV^{-1}cm^{-3})$	$1.00\times 10^{16*}$	$1.00\times 10^{16*}$	-

4. Results & Findings

The purpose of the study and analysis to find out $BaSi_2$ absorber based thin-film solar cell that can be able to absorb high sun-light for higher efficiency, also thermal-stability. For the thin film technology, it can reduce making time and the cost as well. The band-diagram of p+-$BaSi_2$:B/n-In_2S_3/n+-SnO_2:F hetero-structure solar-cell is shown in Figure 1, pictorial using SKETCHUP PRO 3D design, Power Point and MS Word. For analyzing the performance of the designed cell, we were tested a wide range of parameters and values with SCAPS, it's investigated with thickness cell as well as the layers, as our primary root to find a cost-effective (low thickness) solar cell with high performance. At Figure 4, there a clear vision of the overall performance of the cell with efficiency, open circuit voltage (V_{oc}), short circuit current density (J_{sc}) and Fill Factor (FF). There's a noticeable point that it could achieve the highest efficiency at 0.82µm (overall thickness) and with increasing the range, it's drop slightly which can be solved by some minor modifications. Other parameters were much stable as they are in that figure and for all input parameters for the simulation, all are listed in Table 1.

This structure can be able to gain higher efficiency with the increment of the absorber layer ($BaSi_2$:B) thickness. At 1.2µm (N_D=0, N_A=1.00× $10^{14*}cm^{-3}$) at 300°K, it can achieve more than 32% efficiency though there are some changes in V_{oc}, J_{sc} and FF, it's clearly spectacle at Figure 5.

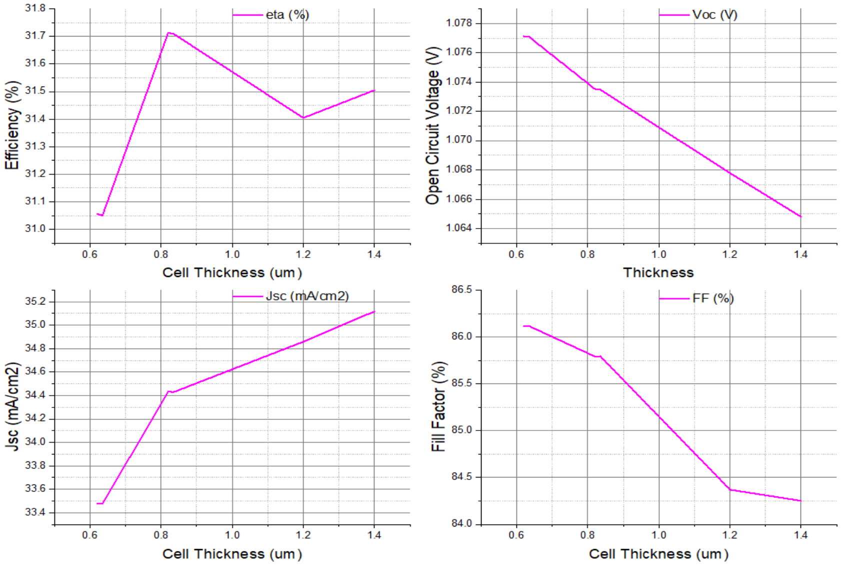


Figure 4. Cell Performance with thickness (Efficiency, FF, V_{oc}, J_{sc})

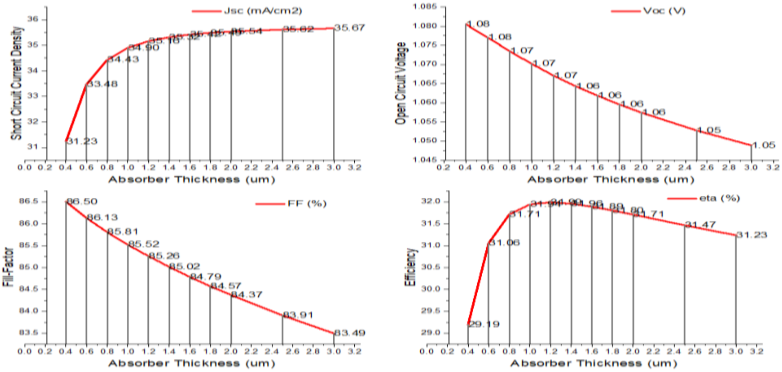


Figure 5. Cell performances with absorber layer thickness.

With 800 nm thickness $BaSi_2$ absorber (N_A =5.00× 10^{19} cm^{-3}, Defect= $1\times10^{14*}$ cm^{-3}) and 20 nm for SnO_2:F(window, N_D =5× $10^{18}cm^{-3}$) and In_2S_3 buffer (N_D =1× $10^{18}cm^{-3}$, Defect= 1× $10^{14}cm^{-3}$), there was a variation in layer thickness and that was 10-200nm. At Figure 6, there's a view of $\mathrm{V_{oc}}$, $\mathrm{J_{sc}}$, *FF*, and η with rising thickness of In_2S_3. From the analyzing simulation, it's clear that $\mathrm{V_{oc}}$ is dropping from 1.0735 V to 1.0687 V, and the drop rate is very low that is 0.001 V. J_{sc} is also decrease by the increasing thickness. The J_{sc} decreasing rapidly in small value from 10 nm to 200 nm J_{sc} 34.4296 mA/cm^2 to 34.1203 mA/cm^2. *FF* increasing until 15nm, and that is the maximum value 85.8093%, then it is decreasing slowly.

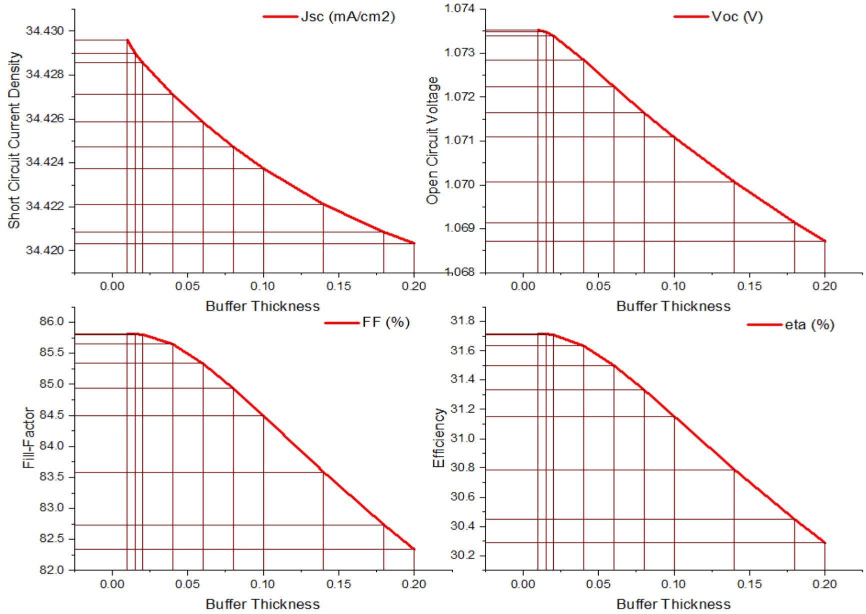


Figure 6. Cell performances with buffer layer thickness.

The 200 nm thickness FF value is 34.4203%. η decrease in increasing the thickness value, the decreasing rate is very low. The value of efficiency is varied from 31.71% to 30.28%. And for the overall buffer layer effect on the cell, have an eye on Figure 6, all details are calculated and suitable range is chosen for the actual simulation, for In_2S_3 it's 15nm.

For the designed cell, we choose (FTO) SnO_2:F (Fluorine doped) for the window layer, as it should be high conductive with low loss as much as possible at the time of it's sunlight-absorption [11]. When increasing the thickness of this layer, V_{oc}, J_{sc}, η and FF all parameters decreases as it able to transmit less energy to absorber (BaSi₂:B). As per the analysis and simulation, 20nm is preferred for window layer and the outputs are remain almost same (J_{sc} = 34.43mA/cm^2, V_{oc} = 1.073 V, FF = 85.81%, η = 31.71%).

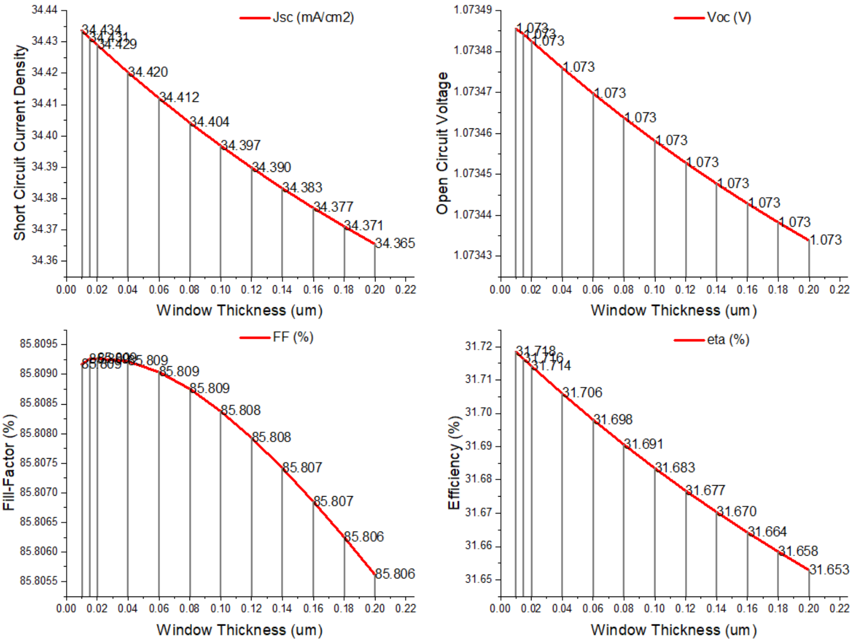


Figure 7. Cell performances with window layer increment

There are some basic differences (PV parameters) compared in Table 2 with FTO and AZO-Aluminum doped Zinc Oxide, and from that it's clear that FTO can better perform than AZO.

Table 2. **Comparing parameters with FTO and AZO [12][13][14]**

Parameter	FTO	AZO
V_{oc} (V)	1.07348	1.0654
J_{sc} (mA/cm2)	34.429	33.9921
FF%	85.81	72.149
η%	31.71	26.131
V_{mpp} (V)	0.9648	0.8303
J_{mpp} (mA/cm2)	32.87	31.47

This designed structure has some effect on defects (donor and acceptor). P-type absorber $BaSi_2$:B is basically donor and N-type buffer In_2S_3 is acceptor. Bulk defects density values for absorber and buffer are listed in Table 1. And there also an overview on the simulation outcomes with and without defects at the Table 3.

Table 3. **Performances comparison of modelled cell including and excluding defects at 300°K.**

Cell type	**Absorber Thickness (μm)**	**Open Circuit Voltage, V_{oc} (V)**	**Maximum Power Point Voltage, V_{mpp} (V)**	**Short circuit current density, J_{sc} (mA/cm^2)**	**Maximum Power Point Current Density, J_{mpp} (mA/cm^2)**	**Fill Factor, FF (%)**	**Efficiency, η (%)**
With Defect	0.8	1.0735	0.9648	34.429	32.8708	85.809	31.7142
Without Defect	0.8	1.0983	0.99585	34.431	34.4307	87.307	33.0165
With Defect	2	1.0574	0.9419	35.541	33.6638	84.373	31.7087
Without Defect	2	1.0992	0.99655	35.546	35.5464	87.293	34.1039

5. Discussion and Conclusion

In some experimental work, 9% and 9.9% efficiency had confirmed by Si and heterojunction cell, respectively, both by the molecular beam epitaxy (MBE) method [15][16]. Theoretically 22.5% efficiency is achieved by n + -$BaSi_2$ / p-$BaSi_2$ and homogenization solar cell by 5×10^{19} metal thickness absorbent material [17]. CdTe/CdS cell can achieve 15% efficiency with 5800nm thickness [18]. There's an overview on some solar structure in Table 4. Our proposed cell with only 3 major layer, simple structure and low thickness (absorber 800nm, buffer 15nm and window 20nm) can be able to higher efficiency (up to 32%). This should be low-cost design and eco-friendly as it can be able to replace Cd based solar cell.

Overall, this solar cell mainly designed for high efficiency with a basic simple structure (having only 3 basic layers) & thin film which thickness varied within 0.6μm to 1.3μm only and with this thickness, it can provide 29% to 34% efficiency. It's not only a high-efficient thin film solar cell, also a cost effectiveness & toxic free (less than CdTe/CdS based solar cell & others) structure.

Table 4. **Comparison between different types of solar cells (all the data are collected from various literature with reference in the last)**

Name	**Parameters**	**Thickness (nm)**	**FF (%)**	**V_{oc} (mV)**	**J_{sc} (mA/cm^2)**	**Efficiency (%)**
Organic Solar cell [19]	LA9 ternary	7250	74.58	0.864	24.42	15.75
Hybrid Solar cell [20]	a-Si:H(i) & nc-SiOx(n)	6830	75.9	724	38.95	21.4
CIGS Solar Cell [21]	$CuIn_{(1-x)}Ga_xSe_2$	2500	44	686	10.32	**7.89**
Heterojunction-Si Solar Cell [22]	CNT/n-Si	CNT:50-200uL PSS:100mL SiO_2:500nm	75	550	34.5	14.1
Cadmium telluride solar cell [23]	CdTe/CdS	5800	88.85	0.808	20.9	15%
Thin-film solar cell	$BaSi_2$**:**B	835	85.809	1.0735	34.43	31.72

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