

High Efficiency CdTe Thin Film Solar Cells with CdSe as a Prospective Window Layer from Numerical Optimization

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Abstract

In this simulation, cadmium selenide (CdSe) has been utilized as a replacement for conventional cadmium sulfide (CdS) window layer by numerical simulation using Solar Cell Capacitance Simulator (SCAPS-1D). CdSe layer thickness, carrier concentration and band gap have been varied to investigate the optimum simulation parameters. An efficiency of 16.53% (J_{sc} of 24.89 mA/cm², V_{oc} of 0.87 V and fill factor (FF) of 76.22%) has been obtained with CdS window layer as the reference case. The proposed structure of SnO₂/CdSe/CdTe/Al showed the highest conversion efficiency of 16.13% (J_{sc} of 24.32 mA/cm², V_{oc} of 0.87 V and FF of 76.19%). Furthermore, CdSe window layer exhibited almost similar results as the conventional CdS. All these simulation results specify that CdSe have the ideal prospects to be utilized as window layer for CdTe thin film solar cells.

Keywords: Numerical optimization, SCAPS-1D, CdSe window layer, CdTe thin film.

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1. Introduction

CdTe thin film technology is considered as one of the most efficient and competitive thin film photovoltaic (PV) technologies. It has high efficiency of 22.1% and costs per kWh are the lowest around \$0.0387 kWh [1]. CdS is well known material that shows high performance as

window layer in CdTe thin film solar cells. CdTe solar cells without CdS has shown very low fill factors (FF) and open circuit voltage (V_{oc}) [2]. The advantage of combining CdS with CdTe allows the configuration of CdTe_{1-y}S_y and CdS_{1-x}Te_x phases where it simplifies lattice incompatibility on the interface [3].

Strong parasite absorption around 300-525 nm range causes CdS to eventually have a limit for performance (photocurrent is not contributed by absorption in CdS) [4]. The focus now refers to the use of the CdSe layer combined with CdTe, which is a substitute for CdS or as an additional element [5].

Although CdSe has narrow band distances (~1.7 eV) from CdS (2.4 eV), improvements in current accumulation in short wavelengths regions can still be accomplished by optimizing the thickness and band gap of CdSe layer [6]. Due to the strong interdiffusion between the CdSe/CdTe interface, improvement of J_{sc} in long wavelengths occurs. This directs to the creation of $CdTe_{1-x}Se_x$. The $CdTe_{1-x}Se_x$ exhibits narrower band gap than CdTe which helps to improve the J_{sc} in the CdTe thin film solar cells for long wavelengths [2]. Numerical simulation has become a very useful tool for the design of any kind of efficient solar cell. Numerical simulation is a basic method to foresee and measure cell performance and certify the possible structural proposition. Cadmium sulfide (CdS) has been the most suitable and extensively studied window material for CdTe thin film solar cells to date. Therefore, simulation validation is needed to solve the bottleneck in photon absorption by applying CdSe as window in CdTe solar cells. The main reason for this simulation is to analyze and validate CdSe as a prospective window layer for CdTe film solar cells.

2. Numerical Simulation

SCAPS-1D is used to simulate DC and AC electrical properties for solar cells. It is developed primarily for CIGS and CdTe solar cells. The main purpose of SCAPS-1D is to investigate all layers of solar cells using the existing database. Outputs such as voltage and currents on illumination and dark characteristics

can be analysed from solutions obtained from SCAPS-1D simulation. This simulation can also produce analysis based on operating temperature. Additionally, key content such as recombination profiles, current density of individual carriers as a positioning function and electrical physical distribution can be obtained from SCAPS-1D simulation. However, CdTe-based solar cells are examined using this simulator. The main intention is to replicate solar cells to obtain high efficiency before starting the actual experimental fabrication using different parameters. The effects of different parameters on V_{oc} , J_{sc} , FF, efficiency and operating temperature can be examined via SCAPS-1D simulation.

Figure 1 indicates the conventional CdS/CdTe structured cell (Glass substrate/n-SnO₂/n-CdS/p-CdTe/Al) and the altered structure (Glass substrate/n-SnO₂/n-CdSe/p-CdTe/Al) as proposed to replace CdS as window layer. Previously, conventional CdS/CdTe structured cell reported an efficiency of 16-17% [7]. Initially, n-CdSe thickness has been altered from 10 nm to 100 nm while other related parameters are unchanged. Later, by using reliable thickness of window layer (50 nm), CdSe window layer carrier concentration, band gap and operating temperatures were varied. Normally, the thickness of the finest window layer should be between 50 nm and 60 nm [8]. It is quite complex to control the thickness below 50 nm during the actual experimental fabrication. Therefore, 50 nm thickness has been chosen for the simulation results compatibility with the actual experimental fabrication. Carrier concentration from 1.0×10^{14} to 1.0×10^{18} and band gap from 1.75 until 2.15 have been differed. It has been reported that there is a common trend of a band gap shift to higher energy for the onset of absorption with different ambient [9]. Based on

practical temperature, variations in operating temperature from 300K to 400K are studied. When one parameter is altered for investigation, other parameters and related are kept persistent. The complete information of the entire parameters exploited in this simulation can be obtained in Table 1.

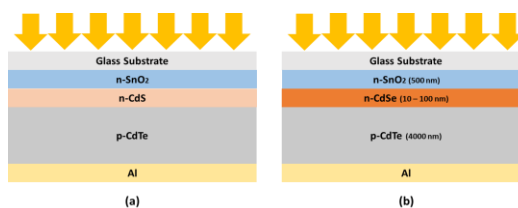


Figure 1: (a) Conventional CdS/CdTe cell structure and (b) proposed CdSe/CdTe cell structure.

Table 1: Material parameters used in simulation

Parameters	Layer			
	n-SnO ₂	n-CdS	n-CdSe	p-CdTe
Thickness, W (nm)	500	10 – 100	10 – 100	4000
Band gap, E _g (eV)	3.6	2.4	1.75 – 2.15	1.5
Dielectric permittivity (ϵ/ϵ_0)	9	10	10.6	9.4
CB effective density of states (cm ⁻³)	2.20x10 ¹⁸	2.20x10 ¹⁸	2.20x10 ¹⁸	8.000x10 ¹⁷
VB effective density of states (cm ⁻³)	1.80x10 ¹⁹	1.80x10 ¹⁹	1.80x10 ¹⁹	1.80x10 ¹⁹
Electron thermal velocity (cm/s)	1.00x10 ⁷	1.00x10 ⁷	1.00x10 ⁷	1.00x10 ⁷
Hole thermal velocity (cm/s)	1.00x10 ⁷	1.00x10 ⁷	1.00x10 ⁷	1.00x10 ⁷
Electron mobility, μ_N (cm ² /Vs)	1.00x10 ²	1.00x10 ²	1.00x10 ²	3.20x10 ²
Hole mobility, μ_P (cm ² /Vs)	2.50x10 ¹	2.50x10 ¹	2.50x10 ¹	4.00x10 ¹
Hole mobility, μ_P (cm ² /Vs)				
Shallow uniform donor density N _D (cm ⁻³)	1.00x10 ¹⁷	1.10x10 ¹⁸	1.10x10 ⁽¹⁴⁻¹⁸⁾	-
Shallow uniform Acceptor density N _A (cm ⁻³)	-	-	-	2.00x10 ¹⁴

3. Results and Discussion

Effect of CdSe window layer thickness on cell performance

Solar cell output results are presented in Figure 2 with the variations in thickness of the CdSe window layer from 10 nm to 100 nm. Thickness variation in the window layer by 10 nm interval is considered to obtain short circuit current (Jsc), open circuit voltage (Voc), fill factor (FF) and efficiency by using SCAPS-1D simulator. It is clearly visible from Figure 2 that there is a slight decrease in the Voc value with the thickness variation in CdSe layer. In addition, the value of Jsc significantly reduced by increasing thickness of CdSe layer. This is caused by photon impression where thicker window layer causes more loss of photons. With the increase in the window layer thickness, the photon carrying energy will be

absorbed more by this layer. Thus, high photon absorption in the window layer will cause only a few photons absorbed in the absorber layer. The efficiency of 16.13% has been achieved with performance parameters of Jsc = 24.32 mA/cm², Voc = 0.87 V and FF = 76.19% by using 10 nm of CdSe.

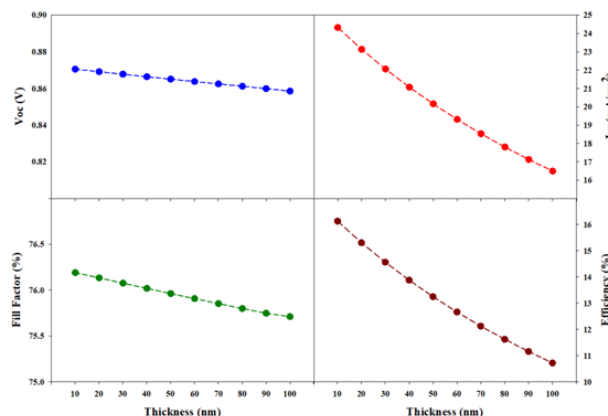


Figure 2: Cell performance with variable thickness of CdSe window layer

Effect of CdSe window layer band gap on cell performance

In this section, the impact of window layer band gap on the cell performance has been analysed. As shown in Figure 3, the variation in Voc and fill factor (FF) resulting from the change in the window layer band gap are very small. Thus, Voc and FF can be considered almost persistent. Both Jsc and efficiency increased due to the rise in the window layer band gap. Cell output efficiency mostly improved due to increased Jsc. The effect of changing window layer band gap in Jsc is significant which relates to lower series resistance in cells with higher band gap [12]. Therefore, it can be stated that the increments of the window layer band gap can improve cell performance. 2.15 eV is selected as the optimum band gap for CdSe window layer that can produce higher efficiency.

Effect of CdSe window layer carrier concentration on cell performance

The effect of CdSe window layer carrier concentration on CdSe/CdTe solar cell output characteristics is shown in Figure 4. Cell efficiency altered by changing the carrier concentration of the CdSe window layer. It is worth noting that when concentration rises, Jsc and efficiency are decreasing. The key cause for this incident is that semiconductors tend to become metallic when the acceptor carrier concentration exceeds 10^{17} . Because of this finding, the simulation results in the range between 10^{17} and 10^{18} are irrelevant. Experimentally, carrier concentration of CdSe semiconductor should be in the range of 10^{14} or 10^{15} [10]. Therefore, based on Figure 4, the optimum carrier concentration for this CdSe window layer is $1.0 \times 10^{14} \text{ cm}^{-3}$.

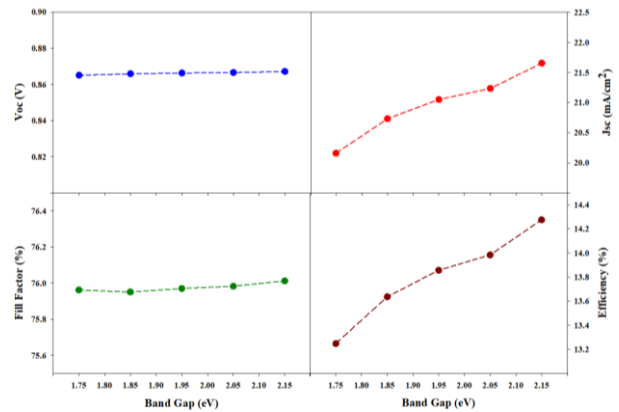


Figure 3: Cell performance with variable band gap of CdSe window layer

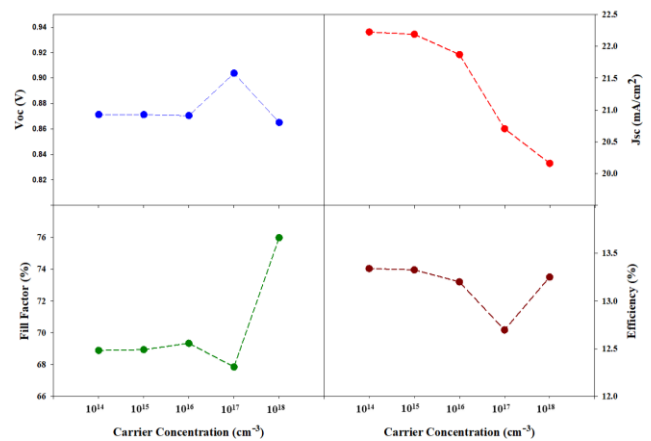


Figure 4: Cell performance with variable carrier concentration of CdSe window layer

Effect of operating temperature on cell performance

Figure 5 shows the effect of operating temperature on the performance of solar cells. In most simulations, the optimum operating temperature used in is 300K or 27°C. The overall efficiency of CdSe/CdTe solar cells is dependent on operating temperature as seen from Figure 5. Parameters such as hole and electron mobility, band gap and carrier concentrations will result in low efficiency solar cells especially at higher temperatures [8]. Efficiency of solar cells decreased by 0.4% with every 10K increase in operating temperature. With the rise in operating temperature,

recombination of the electron-hole pair (EHP) between conduction band and valence band happen. It has been reported that the instability of the band gap energy at high operating temperatures can cause the recombination of the holes and electrons while moving through the whole area even though more free electrons are produced when the operating temperature is high [8]. In this simulation, the utilization of parameters on the same structure has been performed in all temperature changes so that the resulting plot is simplified. Based on the results, 300K is the best operating temperature for CdSe/CdTe solar cell performance.

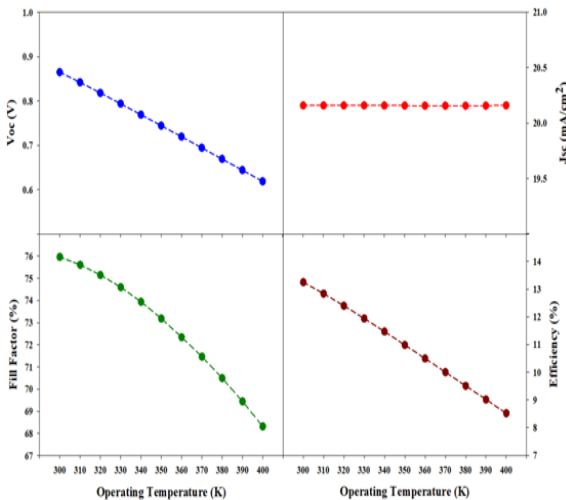


Figure 5: Operating temperature effect on CdSe/CdTe solar cell performance

J-V characteristics

Figure 6 shows the J-V curves for conventional CdS/CdTe structure and the proposed CdSe/CdTe structure. The comparison shows that the solar cell output characteristics of the proposed CdSe/CdTe solar cells are almost identical to the conventional CdTe cell outputs in terms of Jsc, Voc and FF. From Figure 6, it is apparent that the proposed CdSe/CdTe solar cell have shown almost same performance in terms of efficiency compared to the conventional CdTe. The difference in efficiency for both

solar cells is only 0.4%. However, there is a slight reduction in Jsc in the proposed CdSe/CdTe solar cells.

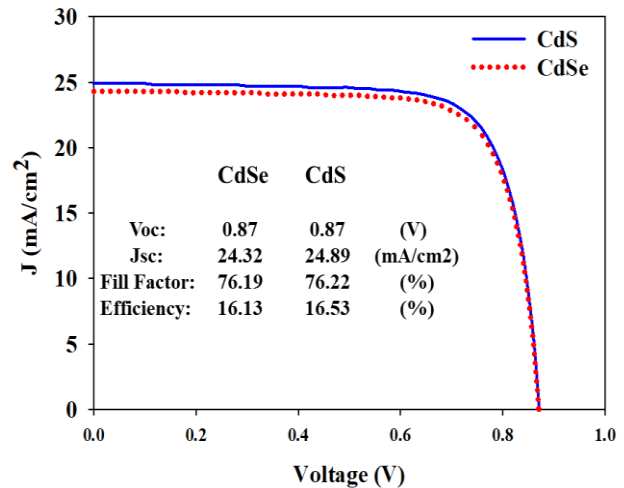


Figure 6: J-V characteristics for conventional CdS/CdTe cell and proposed CdSe/CdTe cell

External Quantum Efficiency (EQE) characteristics

Quantum efficiency (QE) indicates the wavelength that being transformed into electron-hole pairs and gathered as currents [11, 12]. Figure 7 shows QE graph that illustrates the absorption of light for conventional CdTe and proposed CdTe structure with CdSe window layer. Both structures show almost similar absorption for short and long wavelengths. This situation will lead to the accumulation and generation of electron-hole pairs [12]. The results can be viewed precisely from Figure 7 for both solar cells. Based on the entire wavelength range, conventional CdTe absorption is slightly higher than that of the proposed CdTe with CdSe window layer solar cell structure.

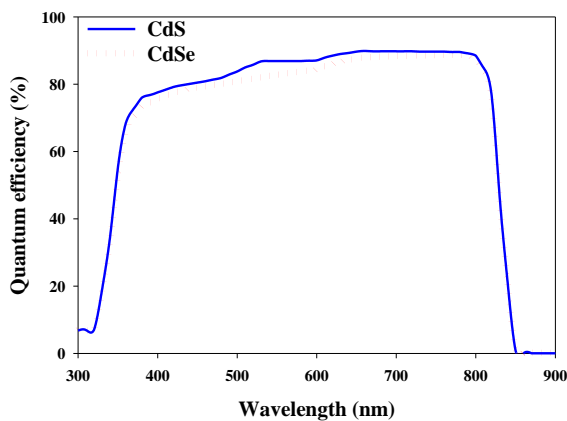


Figure 7: EQE characteristics for conventional CdS/CdTe cell and proposed CdSe/CdTe cell

4. Conclusion

To investigate the prospects of CdSe as window layer, numerical analysis is executed using SCAPS-1D simulator. From this simulation, the new parameters of the optimal solar cells have been found based on the thickness of the CdSe window layer. The simulation results have shown that the proposed CdTe with CdSe window layer structure depicted almost similar efficiency as conventional CdTe solar cells. The optimum CdSe/CdTe solar cell output parameters such as $J_{sc} = 24.32 \text{ mA / cm}^2$, $V_{oc} = 0.87 \text{ V}$ and $FF = 76.19\%$ with efficiency of 16.13% are attained compared to the conventional CdTe cell efficiency of 16.53%. Furthermore, the operating temperature plays an important role in determining the efficiency of the proposed CdTe cells with CdSe window layer. With the increase in operating temperature, solar cell efficiency decreased. Therefore, considering the results of SCAPS-1D simulation, it can be concluded that CdSe is a good candidate as an alternative window layer in CdTe solar cells.

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