

A Simulation Study on the Effect of the Thickness and Carrier Concentration of the Active Layers in the n-CdSe/p-CdSe Solar Cell

Maha Kh. Abdul Ameer

Laith M. Al Taan

Department of Physics/ College of Science/ University of Mosul

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corresponding author:

Maha Kh. Abdul Ameer

Maha.20scp11@student.uomosul.edu.iq

Laith M. Al Taan

laithaltaan@uomosul.edu.iq

ABSTRACT

In this work, thin-film solar cells based on Cadmium Selenide (CdSe) film were used, due to the low manufacturing cost and superior electronic properties, and this type of cell also achieves appropriate efficiency. The current work will focus on investigating the effect of the thickness and carrier concentration of the active layers in the cell, and the thickness of the window on the performance of the proposed solar cell, using the one-dimension solar cells capacitance simulation SCAPS-1D computer program. The proposed structure of this cell consists of ITO/n-CdSe/p-CdSe/Pt, where ITO was used as a window layer, n-CdSe as a buffer layer, p-CdSe as an absorber layer, and platinum Pt as a back conductive electrode. The results revealed that the cell performed best at thicknesses of 5000 and 100nm for the absorber and buffer layers, respectively, and with carrier concentrations of 10^{16} and 10^{17} cm⁻³ for the same layers. The optimal window layer thickness is 100nm. These variables yield open circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF) of 1.0845 V, 20.87 mA/cm², 88.02% respectively, while the conversion efficiency of cell (Eff.) was obtained, which is 19.92%.

Keywords: CdSe, thickness impact, carrier concentration impact. SCAPS

INTRODUCTION

The need for renewable energy has emerged to avoid the use of traditional energy sources based on fossil fuels such as coal, petroleum, and others. Whose use results in environmental pollution such as the emission of carbon dioxide CO₂ (Ranabhat *et al.*, 2016), as well as an increase in the temperature of the Earth's atmosphere, resulting in so-called global warming (Banerjee *et al.*, 2016). In order to reduce this pollution and global warming, solar energy has been used as an alternative source of fossil fuels, because the sun is our greatest source of energy (Banerjee *et al.*, 2016). Where the generation of clean and environmentally friendly renewable energy is an important issue for technological and scientific progress (Bragagnolo *et al.*, 1980), and thus solar cells become an important technology and sustainable energy source for human civilization, represented by different types of solar cells, such as; silicon solar cells, organic, perovskite solar cells (Rai *et al.*, 2020) and thin film solar cells (Ranabhat *et al.*, 2016). Thin-film solar cell materials have undergone much research to reach the highest efficiency and lowest cost (Heriche *et al.*, 2017). Thin film solar cells simply consist of a pn-junction, where p represents the bottom layer, which is the absorber layer, and the top layer is n, which is called the window layer (Ranabhat *et al.*, 2016). This type of solar cells can be obtained by different deposition techniques on cheap substrates such as glass, polymer, metal and others (Ranabhat *et al.*, 2016). Cadmium Selenide (CdSe) material is the subject of this study as a thin film solar cell, it has a high absorption coefficient of $(10^5) \text{ cm}^{-1}$ and a direct band gap energy of approximately (1.74eV) close to the ideal energy bands for AM1.5 solar radiation, it can be used as a window layer as well as an absorber layer in solar cells (Patel *et al.*, 2019). Yasin *et al.* used CdSe as a buffer layer using SCAPS, they found that the efficiency was 28.32%, which is close to the efficiency gained utilizing other buffer layers (Yasin *et al.*, 2020). Rosly *et al.*, used CdSe as a window layer, according to the results, the greatest efficiency attained was 16.13 %, which is close to the efficiency obtained when employing the traditional window layer CdS (Rosly *et al.*, 2019), while Dey *et al.* used CdSe as an absorber layer and they study its effect on cell performance using the AMPS-1D computer program, the researchers obtained a high conversion efficiency of about 17.35% (Dey *et al.*, 2017). Cadmium Selenide (CdSe) is one of the metal chalcogenides compounds (Chaudhari *et al.*, 2016) which is a semiconductor. It is distinguished by its electrical and optical characteristics in the visible region of the spectrum (Abdulkaleq and Al Taan, 2021) (Abdulkaleq and Al Taan, 2022). Where it can be used in a lot of optoelectronic applications such as photoelectrochemical cells, solid-state solar cells and photoconductors (Chaudari *et al.*, 2016) etc. In this work, the SCAPS computer program was used to study the performance of the proposed solar cell, which consists of (ITO/n-CdSe/p-CdSe/Pt). The buffer layer was n-CdSe, the absorber layer was an impure p-CdSe material, the window layer was ITO, and Pt was a back conductive electrode. An investigation of this work was the influence of the thickness and concentration of each layer on the performance of the suggested solar cell.

Simulation Model and Device Structure

In the present work, the used solar cell simulation was achieved using SACPS (Solar Cell Capacitance Simulator) (Rai and Dwivedi., 2020). SCAPS is a one-dimensional solar cell modeling application created by Gent University's Department of Electronics and Information System (ELIS) (Qu *et al.*, 2019). It is generally developed to simulate thin film and polycrystalline solar cell measurements (Khoshsirat *et al.*, 2015). The user can add up to seven layer and also can add the individual parameters for each layer that should be well defined. In terms of the thickness(t), electron affinity (χ), energy gap (E_g), dielectric permittivity (ϵ), conduction and valence band density of states (N_C and N_V), donor and acceptor density (N_D and N_A), and electron and hole mobility (μ_n and μ_p), the property of each layer were used as an input to the simulator (Rai and Dwivedi, 2020) (Qu *et al.*, 2019). These parameters were taken from different literature, which is listed in (Table 1).

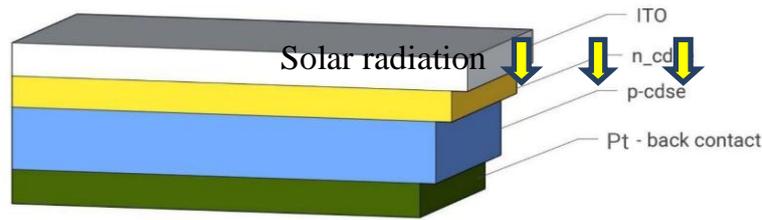


Fig. 1: Structure of CdSe thin film solar cell

As shown in Fig. (1), the current device has a structure of ITO (Indium Tin Oxide), n-CdSe, and p-CdSe as window, buffer and absorber layers respectively, and Pt (platinum) was used as a back contact electrode. The thickness and concentration of each layer were changed to get the best solar cell structure with the best performance. The illumination of light passes through the side of the layer of n-ITO. The structural study was carried out under the standard conditions, using the AM1.5G solar spectrum, 100 mW.cm^{-2} incoming power density, at a temperature of 300°K . The back contact parameters and initial values of thickness and carrier concentration for each layer are given in (Table 2) and (Table 3) respectively.

Table 1: Simulation Parameters for ITO/n-CdSe/p-CdSe solar cell layers.

Parameter	ITO (a [*])	n-CdSe (b [*])	p-CdSe (c [*])
Thickness (nm)	50-250	50-150	500-5000
Band gap E_g (eV)	3.6	2.16	1.74
Electron affinity χ (eV)	4.5	4.3	4.56
Dielectric permittivity (relative)	8.9	10.6	10.6
CB effective density of state N_C ($1/\text{cm}^3$)	2.2×10^{18}	2.2×10^{18}	2.75×10^{18}
VB effective density of state N_V ($1/\text{cm}^3$)	1.8×10^{19}	1.8×10^{19}	2.8×10^{19}
Electron thermal velocity (cm/s)	10^7	10^7	10^7
Hole thermal velocity (cm/s)	10^7	10^7	10^7
Electron Mobility μ_n (cm^2/Vs)	20	100	650
Hole Mobility μ_p (cm^2/Vs)	20	25	50
Shallow uniform donor density N_D ($1/\text{cm}^3$)	10^{18}	$10^{14}-10^{18}$	0
Shallow uniform acceptor density N_A ($1/\text{cm}^3$)	0	0	$10^{14}-10^{18}$

a^{*} (Kuddus *et al.*, 2021) (Anware *et al.*, 2017) (Al-Hattab *et al.*, 2021), b^{*} (Yasin *et al.*, 2020) (Rosly *et al.*, 2019) (Tung *et al.*, 2018), c^{*} (Dey *et al.*, 2017).

Table 2: Contact electrical properties

Parameters	Right contact*	Back contact
Work function (eV)	Flat band	$5.7(d^*)$
Surface Recombination Velocity of electron (cm/s)	10^7	10^5^*
Surface Recombination Velocity of hole (cm/s)	10^5	10^7^*

* SCAPS Library, d^{*} (Derry *et al.*, 2015)

Table 3: Initial values of thickness and carriers concentration of the proposed cell layers

Layer	Thickness (nm)	Concentration (cm^{-3})
Absorber (p-CdSe)	1200	10^{17}
Buffer (n-CdSe)	50	10^{14}
Window (ITO)	100	10^{18}

RESULTS AND DISCUSSION

Impact of layers thickness

In order to obtain an optimum structure for the current solar cell, which has the best performance. In this section, the effect of the thickness of the absorber layer and the buffer layer on cell performance was studied. A suitable thickness was chosen for each layer to provide the best cell performance.

Impact of absorber layer thickness

The thickness of the absorber layer is one of the critical factors that clearly impact the performance of the solar cell, as it varied from 500 to 5000 nm using the SCAPS software to acquire the optimum absorption of solar radiation and therefore increase the cell's performance. Figure 2 shows how the parameters of a solar cell vary as the absorber layer thickness increases, the figure illustrates that when the thickness of the absorber layer rises, the V_{OC} , J_{SC} , FF and Eff. are all increase. Figure 2 shows a slight increase in V_{OC} from 1.1514V to 1.183V for the thickness range under examination, And the J_{SC} increases sharply from (14.44 to 20.5) mA/cm^2 . A sharp rise in the fill factor and efficiency was notice, as the fill factor increases from 61.27% to 72.28% the efficiency increases from 10.19% to 17.53%. In reality, the back contact in a cell with a thin absorber layer is near the depletion area. In this instance, a portion of the incoming photons, particularly low-energy photons, are absorbed deep inside the absorber layer towards the back contact and away from the depletion area. As a result, at the rear contact, the photo-generated carriers recombined. The absorber layer's thickness rises, which minimizes recombination of photo-generated carriers at the back contact and so improves solar cell performance, and this agrees with the (Khoshsirat *et al.*, 2015). From Fig. (2), one can conclude that the absorber layer thickness cannot be raised excessively and is still requires tuning. The thickness over 5000nm, increases the V_{OC} , J_{SC} , FF and Eff. just marginally and can be considered almost saturated. If the thickness of this layer is increased further, a portion of the incoming photons will be absorbed deeply far from the space-charge area, and the produced carriers will be unable to reach the depletion zone during their lifetime and will be recombined. This indicates that raising the thickness of the absorber layer increases the probability of bulk recombination (Khoshsirat *et al.*, 2015). As a result, the optimal absorber layer thickness is 5000nm, resulting in an efficiency of 17.53 %, the reason for selecting this thickness as the optimal thickness is to achieve a high efficiency thin film solar cell. The effect of absorber layer thickness on open circuit voltage, short circuit current density, fill factor, and cell efficiency is depicted in Fig. (2).

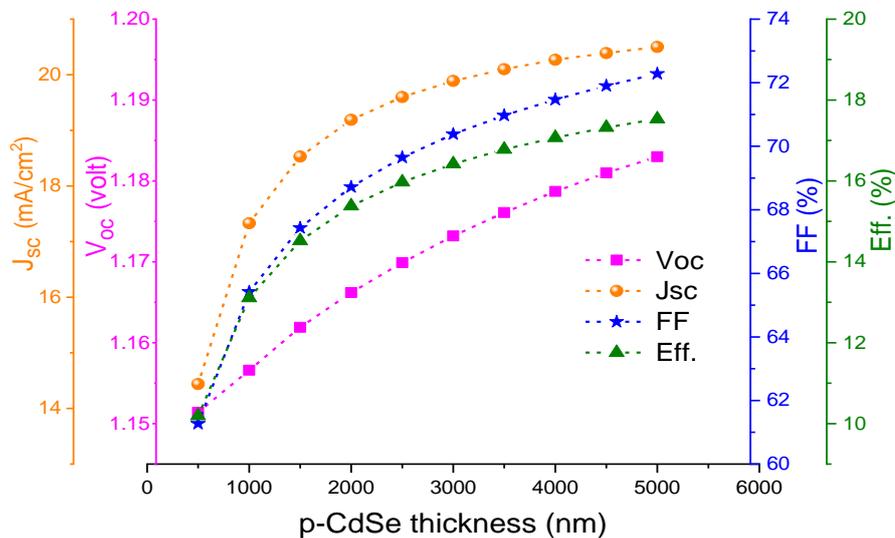


Fig. 2: Impact of p-CdSe absorber layer thickness on solar cell parameters

Impact of buffer layer thickness

This section of the simulation depicts the effect of buffer layer thickness on solar cell performance, as the thickness of this layer varies from 50 to 150nm by 10 steps each time after the p-CdSe absorber layer thickness is fixed at the optimal thickness (5000nm). Fig. (3) illustrates that increasing the thickness of the buffer layer decreases the cell's performance. Where there is a significant decrease in efficiency and fill factor, the efficiency value drops from 17.53% to 5.74%, the fill factor drops from 72.28% to 22.3 %, and the short circuit current density (J_{SC}) drops slightly compared with FF and Eff. from (20.5 to 20.11) mA/cm^2 , while the open circuit voltage increases slightly from 1.183V to 1.2791V. This rise in open circuit voltage is because n-CdSe has a high energy gap, which reduces the diode's saturation current. As the thickness of this layer rises, the absorbed photons increase outside the hole diffusion length area, resulting in a drop-in recombination rate and an increase in open circuit voltage V_{OC} (Green, 1982). Short-circuit current density decreases with increased buffer layer thickness due to a drop in electron-hole pair creation, as very few electron-hole pairs reach the absorber layer and are absorbed by the buffer layer. The decrease in the fill factor is due to the series resistance which increases with increasing thickness and thus reduces the maximum achievable power output. Finally, the drop in efficiency is due to the combined effect of V_{OC} , J_{SC} , and FF (Jhuma *et al.*, 2019). Although thinner buffer layers result in improved cell performance, too thin buffer layers might result in leakage current, and Controlling the thin thickness during the actual experimental production is difficult (Rosly *et al.*, 2019). Hence the optimal and recommended buffer layer thickness in this cell is 100nm.

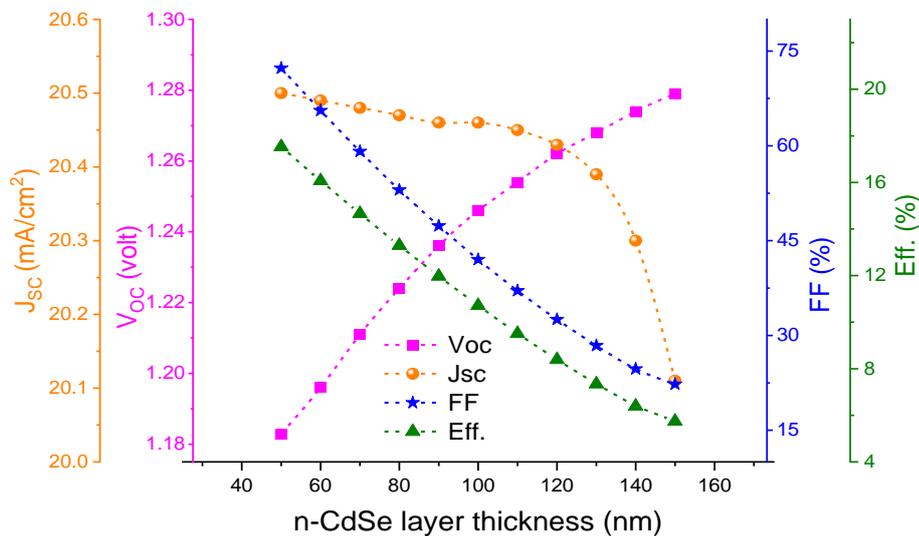


Fig. 3: Impact of n-CdSe buffer layer thickness on solar cell parameters

Impact of layers carriers' concentration

To get the best power conversion efficiency, each layer of the cell must have a specific carrier density. The parametric study begins by holding the thicknesses of the absorber and buffer layers constant at the optimum values and then begins varying the doping density in a single layer independently while holding the doping of the other layers constant at the initial values to study the effect on cell performance.

Impact of absorber layer carriers' concentration

In this part of the research, the influence of absorber layer carrier concentration on cell performance studied by varying the acceptor carrier's concentration in this layer from 10^{14}cm^{-3} to 10^{18}cm^{-3} . Fig. (4), shows the change in cell parameters with carrier concentration when the absorber layer and buffer layer were both fixed at the optimum thickness. The primary purpose of this study is to acquire a carrier concentration (N_a) of the p-CdSe absorber layer with minimizing cell performance losses. As a result, reduced costs can be achieved by lowering the number of costly materials utilized (Zyoud *et al.*, 2021) From figure 4, one can note that J_{SC} drops as carrier concentration increases, but V_{OC} increases. The decrease in J_{SC} with increasing carrier concentration occurs primarily because the process of carrier recombination increases with increasing carrier concentration, and thus the probability of photo-generated carriers gathering decreases, and this is due to increased carrier recombination in the deep region, where high-wavelength and low-energy photons are absorbed in this layer. Fig. (4), further shows that the greatest efficiency value is 18.78% when acceptors concentration is 10^{16}cm^{-3} . Also, the results show that increasing the concentration of carriers from 10^{14}cm^{-3} to 10^{16}cm^{-3} enhances efficiency, whereas efficiency falls dramatically when the carrier concentration rises over the optimum value. The drop in efficiency at high concentrations is caused by an increase in the process of carrier recombination and carrier scattering, which reduces the chance of photo-generated carriers being collected, resulting in a fall in J_{SC} and cell efficiency (Rana *et al.*, 2021). With increasing carrier concentration, the saturation current drops, resulting in a rise in V_{OC} as well as the fill factor FF. This is because the highest shunt resistance and lowest series resistance result in a rise in V_{OC} and FF (Noman *et al.*, 2016). Finally, the current results reveal that the absorber layer's carrier density is 10^{16}cm^{-3} , whereby the cell has the maximum efficiency.

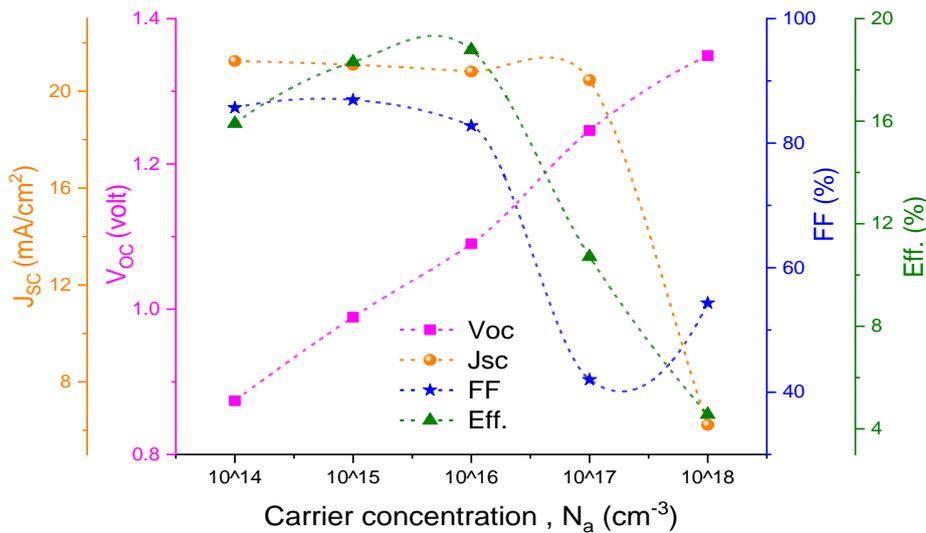


Fig. 4: Impact of absorber layer carrier concentration on solar cell parameters

Impact of buffer layer carriers' concentration

In this section, the influence of the buffer layer (n-CdSe) carrier concentration on the performance of the proposed cell parameters was investigated. The goal of this study is to decrease optical and electrical losses in this layer (Zyoud *et al.*, 2021). Where the donor concentration in this layer was changed from 10^{14} to 10^{18}cm^{-3} , while the carrier density in the other layers kept at the previous optimum values. Figure 5 depicts the effect of changing the concentration of carriers in the

buffer layer on cell performance in the range 10^{14} to 10^{18} cm^{-3} , where we see that J_{SC} , FF, and Eff., rise with increasing carrier concentration, but V_{OC} drops. The rise in J_{SC} may be explained by the fact that as carrier concentration increases, the electric field in the heterojunction becomes stronger. As a result, the collection of photo-generated electron-hole pairs rise, and thus J_{SC} increases. And when the carrier density in the buffer layer rises, more traps of charge carriers are generated, which enhances the interaction possibility, increasing the chance of recombination, and thus the V_{OC} drops. An increase in J_{SC} and a slight drop in V_{OC} result in an increase in the solar cell maximum power, and as a result, an improvement in efficiency and fill factor (Khaissa *et al.*, 2021). The optimal concentration of n-CdSe buffer layer carrier is 10^{17} cm^{-3} . In summary, the donor carrier concentration of 10^{17} – 10^{18} cm^{-3} can significantly enhance efficiency.

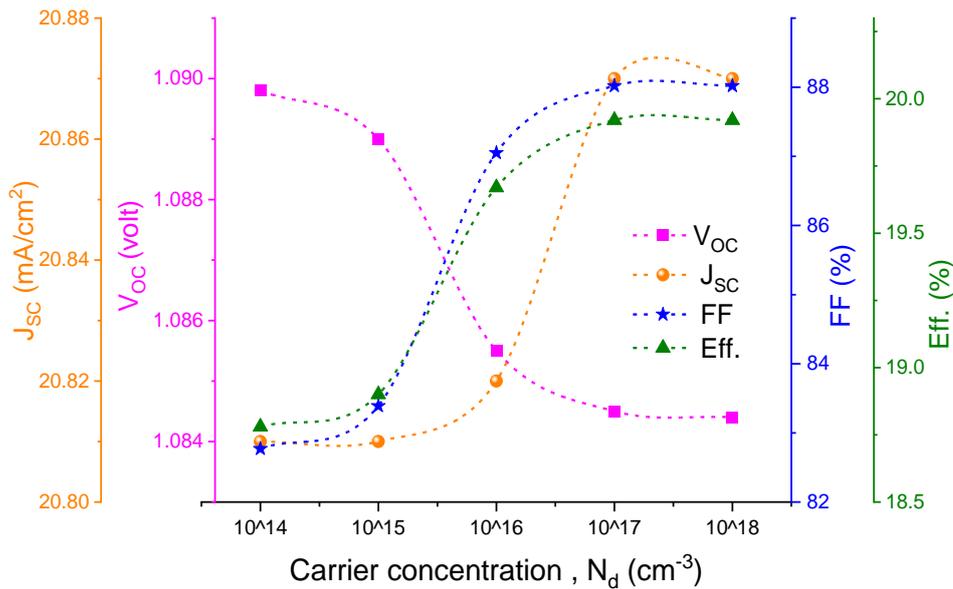


Fig. 5: Impact of buffer layer carrier concentration on solar cell parameters

Impact of window layer thickness:

The effect of the thickness of the ITO (Transparent Conductive Oxide TCO) window layer on the performance of the solar cell was studied in this part of the research after fixing the thickness and carrier concentration of each of the absorber layer and the buffer layer at the optimum thickness and carrier concentration for each layer, where the thickness of the ITO layer was changed from 50-250 nm. Figure 6 demonstrates that the open circuit voltage and the fill factor are both constant at the values 1.0845V and 88.02%, respectively, but J_{SC} and Eff. decrease by such a little percent that they appear nearly constant. Increasing the thickness of the TCO layer increases optical absorption in this layer due to the rising length of light propagation, and therefore the loss in this layer due to absorption, lowers the number of photons that pass through the TCO layer to the active layers of the cell. As the current density participating in the photovoltaic process falls, so does the cell's conversion efficiency and this agrees with the (Chadel *et al.*, 2017).

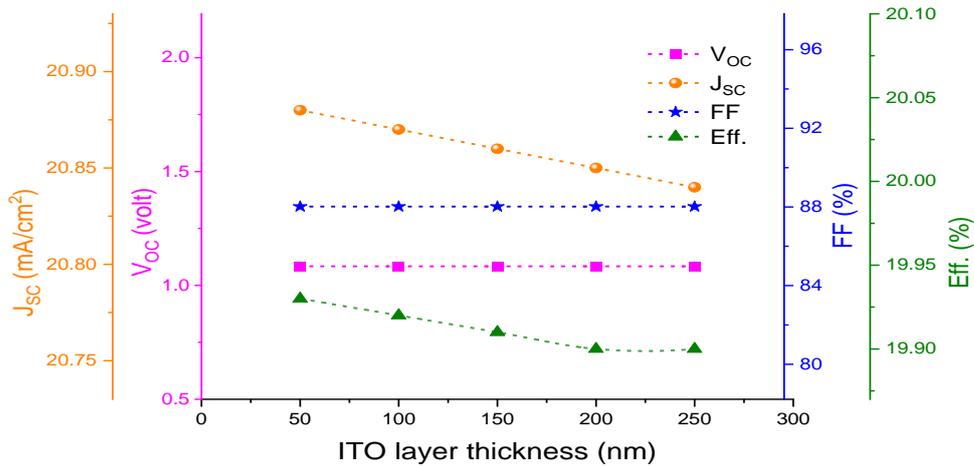


Fig. 6: Impact of ITO window layer thickness on solar cell parameters

CONCLUSIONS

The influence of absorber and buffer layer thickness and carrier concentration on solar cell performance, as well as the effect of window layer thickness on the performance of the proposed cell, were investigated in this work using the SCAPS-1D simulation software. The optimal thickness values for each layer were found to be 5000nm, 100nm, and 100nm for p-CdSe, n-CdSe, and ITO layers, respectively, providing the best efficiency of 19.92%. The current study showed that increasing the thickness of the p-CdSe layer enhances the performance of the proposed cell because photo-generated carriers collect before recombining and that increasing the thickness of this layer above the optimum value causes the cell parameters to increase slowly and appear nearly constant. While the cell performance degradation as the thickness of the n-CdSe layer rises. This is due to increased photon absorption in this layer and the lowest number of electron-hole pairs reaching the absorber layer, thus lowering cell performance. Also, it was found that the increase of the carrier concentration of the p-CdSe layer ($>10^{16}\text{cm}^{-3}$) is not suitable for obtaining the best cell performance due to efficiency fall, whereas increasing the carrier concentration of the n-CdSe layer ($>10^{16}\text{cm}^{-3}$) improves the cell performance. When increasing the thickness of the window layer (ITO), the V_{OC} and FF remain completely constant, while J_{SC} and Eff. decrease by a very small percentage it appears constant, this decrease is due to an increase in absorption in this layer as well as a decrease in the quantity of photons reaching the active layers in this cell. Although these results can assist in the production of a CdSe thin-film solar cell, certain other effects influence cell performance that needs to be investigated in future studies.

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دراسة محاكاة لتأثير السمك وتركيز الحاملات للطبقات الفعالة في الخلية الشمسية n-CdSe/p-CdSe باستخدام SCAPS

الملخص

في هذا العمل تم استخدام الخلايا الشمسية ذات الاغشية الرقيقة القائمة على اساس سيلينيد الكاديوم (CdSe)، نظرا لتكلفة التصنيع المنخفضة والخصائص الالكترونية الفاتحة، بالإضافة الى ذلك فان هذا النوع من الخلايا يمكن ان يحقق كفاءة مناسبة. تركزت الدراسة في هذا العمل على تأثير كل من السمك وتركيز الحاملات للطبقات الفعالة في الخلية، وسمك الطبقة النافذة على اداء الخلية الشمسية المقترحة، وذلك باستخدام البرنامج الحاسوبي (SCAPS-1D) (محاكاة سعة الخلايا الشمسية احادية البعد). يتكون الهيكل المقترح لهذه الخلية من (ITO/n-CdSe/p-CdSe/Pt) حيث تم استخدام ITO كطبقة نافذة، و n-CdSe كطبقة عازلة، و p-CdSe كطبقة امتصاص، بينما تم استخدام البلاتين Pt كقطب موصل خلفي. اظهرت النتائج ان افضل اداء للخلية كان عند السمك 5000nm و 100nm لطبقة الامتصاص و الطبقة العازلة على التوالي و بتركيز الحاملات 10^{16}cm^{-3} و 10^{17}cm^{-3} للطبقات نفسها. بينما يكون سمك الطبقة النافذة الامثل هو 100nm. تنتج هذه المتغيرات فولتية الدائرة المفتوحة (V_{oc}) و تيار الدائرة القصيرة (J_{sc}) و عامل الملء (FF) و البالغة (V) (1.0845) و (20.87 mA/cm^2) و (88.02%) على التوالي فيما تم الحصول على كفاءة التحويل للخلية (Eff.) تساوي (19.92%).

الكلمات الدالة: CdSe، تأثير السمك، تأثير تركيز الحاملات، SCAPS.