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The SCAPS-1D modeling of ZnO/CdS/CdTe thin film: analysis of thickness and stoichiometric fraction of absorber layer on solar cell performance

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Abstract. Modeling of ZnO/CdS/CdTe solar cells with various thickness and stochiometric fractions has been carried out using SCAPS-1D. The variation in the thickness of the CdTe used was 0.6 μm - 6.0 μm and the variation of the stoichiometric fraction used was 0.6 - 7.0. The SCAPS-1D modeling data were characterized using I-V characteristics to determine the value of V_{oc}, J_{sc}, FF and their efficiency. The I-V characteristic values increased with the increase in the thickness of CdTe. The optimum thickness was 6.0 μm with V_{oc}, J_{sc}, FF values, respectively 0.894 volts; 31,990 mA / cm²; and 84.720%, with a large efficiency of 24.228%. In the variation of the optimum stoichiometric fraction, the stoichiometric fraction was 0.6 with an energy gap of 1.486 eV and an efficiency value of 22.900% for the Voc, Jsc, and FF values, respectively, 0.872 volts; 31,345 mA / cm²; 83,806%.

1. Introduction

A solar cell is an electronic device that uses photovoltaic phenomena to convert sunlight into electrical energy. This photovoltaic system operates without emitting pollutants to the environment. In addition, photovoltaic cells have a lifetime of more than 30 years. So, it can be said that photovoltaic is a semiconductor technology that is environmentally friendly (green technology) and has good prospects [1]. Semiconductor type II-VI alloys are in great demand and research, because their band gap shows excellent physical properties for solar cells. The direct band gap of this semiconductor material covers the spectral wavelengths from ultravioet to infrared.

The energy gap in a material greatly affects the efficiency of solar cells. When the energy of photons in the sun is greater than the band gap, this energy will be absorbed, resulting in electron and hole pairs in the depletion area or the space charge region. CdTe material is usually used as an absorber layer in solar cells because it is a material with a relatively small direct band gap of 1.45 eV at room temperature [2,3]. CdTe has a good ability to absorb many parts of the wavelength spectrum of light radiation.

Swanson [4] states that for CdTe-CdS-based solar cells, the optimum thickness of CdS thin films ranges from 100-200 nm, while the optimum thickness of CdTe is around 1 μm. The good performance of CdTe as an absorber was also shown by Plotnikov [5] with a thickness of 500 nm and Paudel [6] with a thickness of 2.1 μm. The efficiency of CdTe solar cells has reached 20.4% [7], or in other studies it has reached 22.1% [8].

The production of solar cells is not cheap and takes a long time, so there is a need for more efficient steps in making solar cells. The methods commonly used in solar cell research are the experimental

method and the simulation method (modeling). The simulation (modeling) method is used in the early stages of research. This is because the initial research aims to find the optimum preparation parameters such as material, layer thickness, doping, energy gap, and so on. SCAPS-1D is a solar cell modeling software that has a complete variety of characteristic features. Based on this analysis, the performance modeling of ZnO/CdS/CdTe solar cells using SCAPS-1D has been studied in terms of the thickness and stochiometric fraction of the CdTe absorber.

2. Methods

In this modeling, the solar cell consists of ZnO as TCO (transparent conducting oxide), CdS as an n-type semiconductor and as a buffer layer, and CdTe as a p-type semiconductor and as an absorber layer with variations in thickness and energy gap. Figure 1 shows the arrangement of the ZnO/CdS/CdTe thin film solar cells to be modeled.
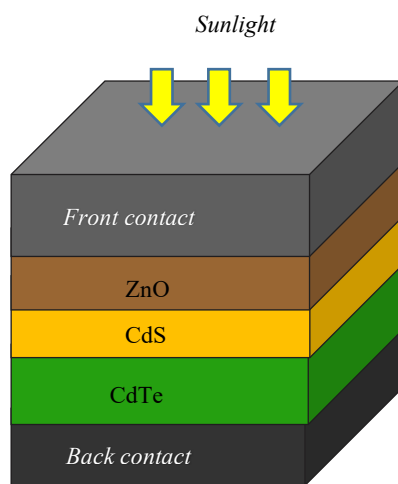

Figure 1. Structure of ZnO/CdS/CdTe solar cells

Table 1. ZnO/CdS/CdTe solar cell parameters

Layer	CdTe	CdS	ZnO
Thickness (µm)	varied	0.1	0.5
Bandgap (eV)	varied	2.4	3.3
Electron Affinity (eV)	4.28	4.2	4.4
Dielectric Permitivity (relative)	9.4	10	9
CB effective density of states (1/cm³)	8×10^{17}	2.2×10^{18}	2.2×10^{18}
VB effective density of states (1/cm³)	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Electron thermal velocity (cm/s)	1×10^7	1×10^7	1×10^7
Hole thermal velocity (cm/s)	1×10^7	1×10^7	1×10^7
Electron mobility (cm²/Vs)	3.2×10^2	1×10^2	2.5×10^1
Hole mobility (cm²/Vs)	4×10^1	2.5×10^1	1×10^2
Donor density ND (1/cm³)	0	1×10^{17}	1×10^{18}
Aceptor density NA (1/cm³)	4×10^{14}	0	0

Sources: [7, 8 ,9 ,10 ,11 ,12]

Table 1 shows the parameters to be used for modeling using SCAPS-1D. Furthermore, characterized by using I-V characteristics, QE characteristics and absorption characteristics. The I-V characteristics are carried out to determine the performance of solar cells, QE characteristics to determine the quantum

efficiency of solar cells, and the absorption coefficient is used to determine the absorption coefficient value of the absorber layer. The results obtained from the modeling are a graph of the relationship between voltage (V) and current density (J), a graph of the relationship between wavelength and quantum efficiency (QE), and a graph of the relationship between absorption coefficient (α) and photon energy.

The data that can be seen from the I-V characteristics are the values that can be obtained from the I-V characteristics, including open circuit voltage (V_{oc}), short circuit current (J_{sc}), fill factor (FF), and efficiency (η) [13, 14]. V_{oc} is the voltage when the current is zero, while Jsc is the current density when the voltage is zero. FF is a dimensionless quantity that states the ratio of the maximum power produced by the cell to the multiplication of V_{oc} and J_{sc}. Efficiency is the ratio of the cell's output power to its input power.

3. Result and Discussion

Figure 2 shows the effect of variations in the thickness of the CdTe layer on the increase in current density J, where the increase in the thickness of the CdTe layer, the value of the current density J increases. This increase was due to the increased thickness of the CdTe (p-type semiconductor) which resulted in more electrons in the CdS (n-type semiconductor) layer moving to the CdTe layer. The space carge region widens towards CdTe and causes the acceptor concentration to increase. Increasing the acceptor concentration value can cause the dQ value to increase, causing the current density J to increase as well.
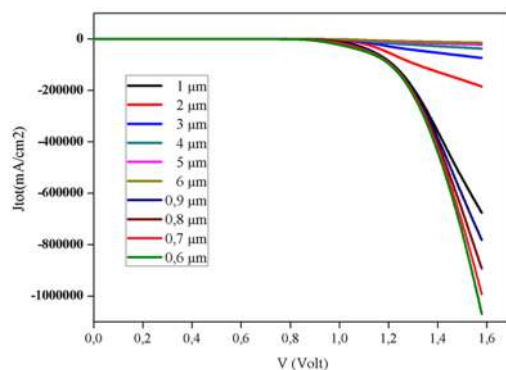
Figure 2. The graph of the relationship between voltage and current density in the thickness variation of solar cells ZnO/CdS/CdTe

By varying the thickness of the CdTe layer from 6μm-0.6μm, which has been calculated using SCAPS-1D in characterization I-V, it is found that there is an increase in the performance of solar cells which can be seen from the value of open circuit voltage (Voc), short circuit current (Jsc), fill factor (FF).), and efficiency (η). In theory, an increase in the value of open circuit voltage (Voc) and short circuit current (Jsc) can increase the efficiency value. Figure 3 shows an increase in the value of efficiency accompanied by an increase in the value of the open circuit voltage (Voc) and the short circuit current (Jsc) which is caused by the greater thickness of the absorber layer, but the thicker the absorber layer is also not good because it will increase in terms of financing. Efficiency is defined as the ratio between the electric voltage generated by solar cells and the amount of light energy received from the sun's rays. In order for solar cells to have high efficiency, the resulting I-V curve must be good, namely with high Voc and and Jsc values, and better fill factors. The increase in the thickness of the intrinsic semiconductor layer shows a symptom of an increase in the performance or performance of the solar cell which will cause the depletion area to become wider so that more electrons and holes are used as donor and acceptor ions.
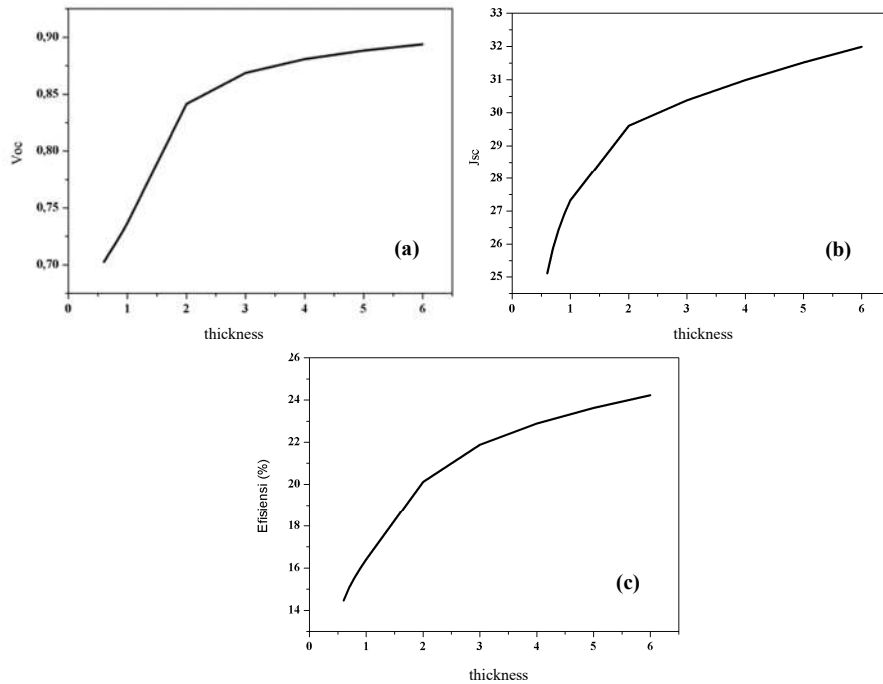
Figure 3. Graph of thickness relationship with (a) open circuit voltage (V_{oc}) (b) short circuit current (J_{sc}) (c) efficiency (η).
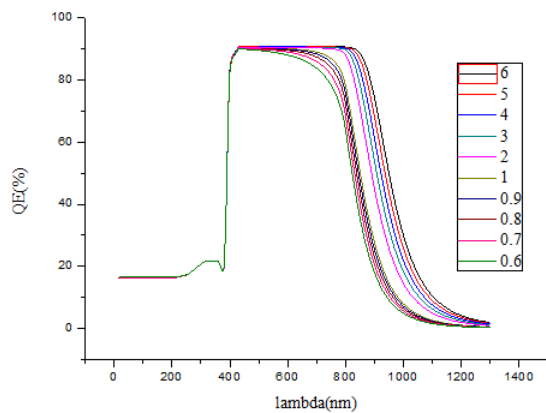

Figure 4. Graph of the Relationship between Wavelength and Quantum Efficiency Value
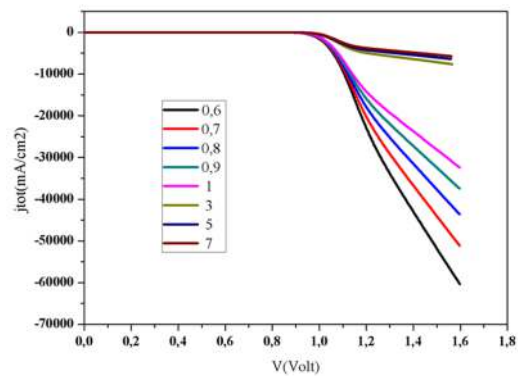
Figure 5. Graph of the relationship between voltage and current density in the variation of the stoichiometric fraction of solar cells ZnO/CdS/CdTe

The quantum efficiency values of the thickness variations of CdTe are quite similar, where the quantum efficiency (QE) is the ratio of the number of charge carriers collected in the solar cell to various wavelength spectra as seen in Figure 4. All quantum efficiency values show the same shift, which is closer to infrared wavelength showing a little alloying of CdTe with CdS. The bent or crest shape on the QE curve shows the alloy between CdS and CdTe. The bent form is in the wavelength range from 450 nm to 810 nm, or the energy range from 2.42 eV to 1.46 eV. When compared with the parameters used in this modeling, the values obtained are not much different, namely 2.4 eV for the CdS layer and 1.5

for the CdTe layer. This refers to the value of the wavelength transmitted by CdS and the wavelength absorbed by CdTe.

Figure 5 shows the magnitude of the voltage in proportion to the current density for the variation of the stoichiometric fraction of the CdTe layer, stoichiometry is the basis for chemical calculations which states the quantitative relation of the chemical formula of a compound. The variation of the stoichiometric fraction of the CdTe layer ranges from 0.6 to 7 using equations

$$Eg = 0{,}05x + 1{,}4555$$

x is the stoichiometric fraction of the CdTe layer, then the energy gap value (band gap) is obtained for each fraction.

The performance of solar cells increases with the reduction in the value of the energy gap, this is due to the influence of the distribution of more photons from sunlight. The performance of ZnO/CdS/CdTe solar cells has good characteristics, namely the energy gap of 1.4855 eV with an efficiency value of 22.900%.

Figure 6 shows the graph of the relationship between the stoichiometric fraction of the CdTe layer to the value of open circuit voltage (V_{oc}), short circuit current (J_{sc}), fill factor (FF), and efficiency, by varying the energy gap in the parameters using the stoichiometric fraction equation, an increase was obtained. which is significant in the fraction 0.6 to 1, this is in accordance with the value of the energy gap in the CdTe parameter used, which is ranging from 1.45 eV to 1.5 eV, in fractions 3 to 7 an increase in the energy gap is obtained that approaches the value of 2 eV where part of the photon will be absorbed and partially reflected. In contrast to the value of the short circuit current (J_{sc}) which has decreased with the increase in the stoichiometric fraction of the CdTe layer. Where photons with a gap energy of 1.4 eV - 1.5 eV will be absorbed optimally and produce electron-hole pairs.

The efficiency value of the ZnO/CdS/CdTe solar cell shows two different states where the stoichiometric fraction is 0.6; 0.7; 0.8; 0.9; and 1 with a gap energy of 1.4855 eV, respectively; 1,4905 eV; 1.4955 eV; and 1,5005 eV, the fill factor (FF) value and efficiency increase because in this range all the photons are absorbed by the layer so that there will be more electron pairs and holes. The highest FF value is 83.834% and the highest efficiency value is 22.883% with a fraction of 0.6. Whereas in the next situation, namely when the stoichiometric fractions of CdTe 3, 5, and 7, with the energy gap respectively 1.6055 eV; 1.7055 eV; and 1.8055 eV, the fill factor value and efficiency decreased significantly, for the lowest FF value was 83.417% and the lowest efficiency was 15.871% with a fraction of 7.

Figure 7 shows a graph of the relationship between wavelength and quantum efficiency values, the peak on the QE curve shows the alloy between CdS and CdTe, this peak is in the range 442 nm to 830 nm, or in the energy range of 2.8 eV to 1.49 eV. At wavelength 830 shows a fraction less than 1, while for fractions more than 1 the QE curve shifts away from the visible energy. This is because fewer photons are absorbed by the CdTe layer so that the charge carriers of the electrons and the charge carriers of the holes experience a decrease and result in reduced electron-hole pairs.

The graph in Figure 8 shows the relationship between wavelength and absorption coefficient ($\alpha[1/cm]$) with variations in the stoichiometric fraction, from the graph it can be seen that the greater the stoichiometric fraction value, the smaller the absorption coefficient value. The highest absorption coefficient is when the energy gap is 1.4855 eV. At this energy gap, the absorption of photons is increasing so that the better the CdTe layer becomes an absorption layer with an absorption coefficient of $13{,}18\times10^4$ cm^{-1}. The smallest absorption coefficient value is at the energy gap of 1.8055 eV, which is $11{,}18\times10^4$ cm^{-1}. The shift in the absorption coefficient value shows that the smaller the energy gap in the absorber layer, the longer the wavelength spectrum is absorbed.
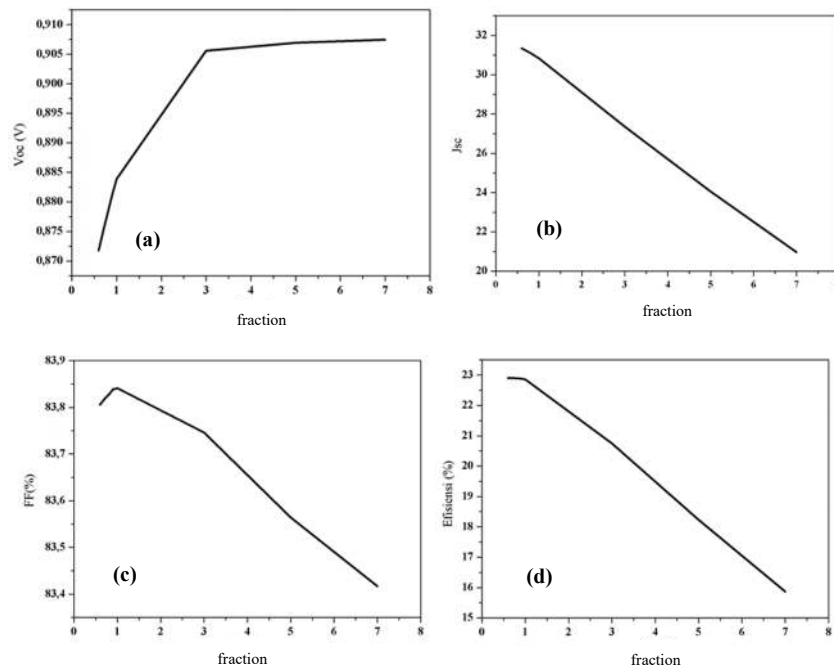
Figure 6. Graph of the relationship of the stoichiometric fraction of the CdTe layer to (a) open circuit voltage (V_{oc}) (b) short circuit current (J_{sc}) (c) fill factor (FF) (d) efficiency (η)
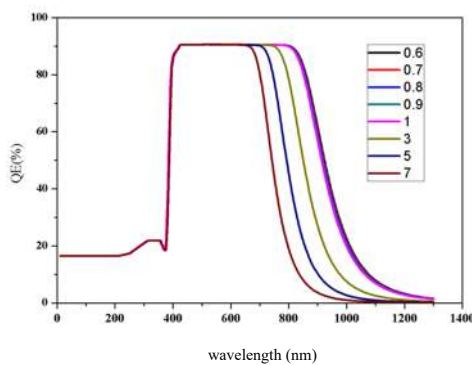

Figure 7. A graph of the relationship between wavelength and quantum efficiency

Mohamed [15] conducted experiments varying the thickness of the 3 μm CdTe layer; 2.1 μm; 1.1 μm; 0.75 μm; and 0.5 μm. Figure 10 shows the comparison of the experimental results with the SCAPS-1D simulation which shows that the greater the thickness of the CdTe layer, the more the efficiency value will be. The difference in efficiency values obtained from experiments and simulations is due to the fact that the film conditions are considered ideal in the simulation, but the experimental results do not occur. From this comparison, we can see that SCAPS-1D can be used in solar cell modeling because the simulation results show the same trend or pattern as the experimental results and the results obtained in the simulation are not much different from the experimental data.
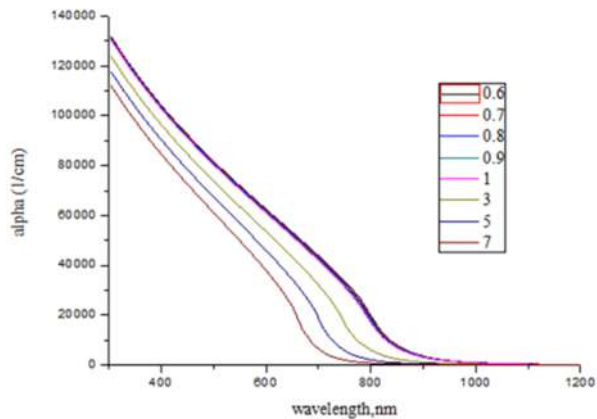
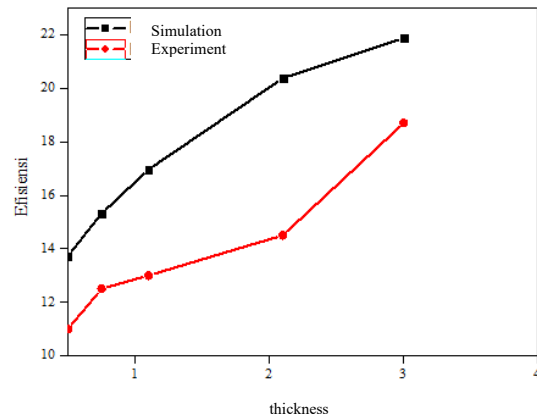**Figure 8**. Graph of the relationship between the wavelength spectrum and the absorption coefficient

Figure 9. Graph of comparison of simulation results with experimental results

4. Conclusion

Modeling of ZnO/CdS/CdTe thin film solar cells using SCAPS-1D has been carried out on the effect of thickness and energy gap, with several characteristics contained in the modeling, it can be seen that the greater the thickness of the absorber layer the greater the efficiency obtained, but the thicker the solar cell layer. it can also reduce the economic value of fabrication. The optimum value of 6 μm CdTe thickness was obtained with an efficiency of 24.228% and a low energy gap of 1.4855 eV with an efficiency value of 22.900%.

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