Numerical optimization of tin sulphide based solar cell for different buffer layers using SCAPS

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Researchers are doing intense research in tin sulfide (SnS)-based solar cells because of their outstanding semiconducting features. In this work, the solar cell capacitance simulator (SCAPS-1D) has been used to do the simulation study of thin films solar cells using SnS absorber layer with different buffer layers (ZnO, ZnSe, CdZnS, TiO2) in comparison to the toxic CdS buffer layer. Photovoltaic parameters (open circuit voltage, fill factor, short-circuit current density and efficiency) is evaluated as a function of absorber layer thickness, different buffer layer and buffer layer thickness. Device stability at different operating temperature is also evaluated. The simulation results reveal the fabrication of high efficiency SnS based solar cells.

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Keywords: Scaps-1D, Solar cell, Buffer layer, SnS, Efficiency, Fill factor

1. Introduction

There has been an intensive research in the field of photovoltaic due to global energy crisis in the last few years. Solar energy is a clean energy that can help us to maintain our lives [1,2]. Currently, the dominated crystalline silicon solar cell is of high production cost due to expensive manufacturing methods and large usage of the material [3, 4]. Therefore, the primary objective of solar energy research is to find environmentally friendly,stable, efficient and low-cost solar cell materials [5,6]. In this respect CdTe ,Cu(In,Ga)Se_2,$Cu_2ZnSn(S,Se)_4$, Sb_2S_3 and Sb_2Se_3 which are metal chalcogenide solar cells have played significant roles [7-11].

In recent years, tin sulphide (SnS) has emerged as a promising absorber material for heterojunction solar cells due to suitable band gap of 1.3 eV and high absorption coefficient $\sim 10^4$ cm^{-1} [12–15]. The intrinsic properties of SnS is conductivity of p-type. Researchers have made attempts to fabricate heterojunction thin film solar cells based on SnS absorber layer [16–20]. 4.35% efficiency of SnS based solar cells is achieved experimentally [21].There are few reports available on the synthesis of n-type [22–24]. Homo-junction SnS solar cells fabrication can result in enhancement of efficiency.

It is needed to optimize SnS absorber layer and used buffer layer in practical implementation to increase the efficiency. In this work, both homo-junction and hetero-junction SnS based thin film solar cells are simulated using the SCAPS-1D software to evaluate the best electrical parameters. Moreover, the impact of various operating temperatures along with various buffer layers have also been investigated.

2. Simulation methodology and device structure

Scientists are involved in increasing thin-film solar cell efficiency by simulation with the help of various available software which are COMSOL [25], SCAPS [26], AMPS [27] and wxAMPS [28]. Solar Cell Capacitance Simulator (SCAPS-1D) is one-dimensional solar cell simulation software developed at the Department of Electronics and Information Systems (EIS), University of Gent, Belgium, and used to numerically predict and analyze solar cells [29]. It solves

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one dimensional semiconductor basic equations to provide results. (Poisson's equation and continuity equations of electrons and holes) [30-33]. SCAPS-1D can generate simulation results which is in good agreement with experimental reports. So this simulation tool outperforms other solar cell simulator software (34). Therefore, SCAPS-1D software version 3.3.09 was used in the research work to simulate the SnS-based solar cells with five different buffer layers, n-type CdS,ZnO, ZnSe, CdZnS and TiO_2 to analyze the solar cell electrical performance such as open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (FF) and efficiency (η). Impact of different operating temperature on SnS based solar cell with different buffer layers are also investigated.

Figure 1 shows the schematic structure of the Mo / SnS / Buffer layer / ITO where the Mo plays the role of back contact, the SnS the p-type absorbent layer, the CdS,ZnO, ZnSe, CdZnS and TiO_2 the different n-type buffer layers used in our simulation and ITO the window layer. The parameters used in our simulations are summarized in Table 1. Here, temperature of 300 K, a global spectrum Air Mass of 1.5 G and an illumination of 1000 W/m^2 have been considered for all simulations.

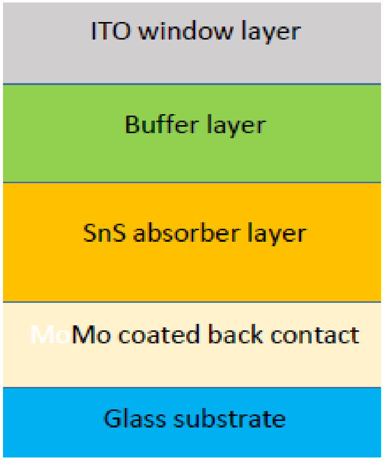

Fig. 1. Schematic diagram of SnS solar cell.

Table 1. Physical parameters of different layers used for the simulation.

Parameter	SnS	CdS	ZnSe	ZnO	CdZnS	TiO_2	SnS	ITO
Thickness(µm)	0.5-3	0.05-0.1	0.06	0.09	0.05	0.09	0.07	0.1
Band gap (eV)	1.31	2.4	2.9	3.3	3.18	3.2	1.31	3.6
Electron affinity (eV)	4.2	4.4	4.1	4	3.71	4	4.2	4.5
Dielectric permittivity	13	10	10	9	10	9	13	8.9
CB effective density of states (cm^{-3})	1.18×10^{18}	2.2×10^{18}	1.5×10^{18}	3.7×10^{18}	2.5×10^{18}	2×10^{18}	1.18×10^{18}	2.2×10^{18}
VB effective density of states (cm^{-3})	4.76×10^{18}	1.8×10^{19}	1.8×10^{18}	1.8×10^{19}	2.5×10^{19}	1.8×10^{19}	4.76×10^{18}	1.8×10^{19}
Electron thermal velocity (cms^{-1})	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Hole thermal velocity (cm^{-1})	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Electron mobility(cm^2/Vs)	130	100	50	100	340	20	130	10
Hole mobility(cm^2/Vs)	4.3	25	20	25	50	10	4.3	10
Shallow uniform donor density, N_D (cm^{-3})	0	1×10^{17}	1×10^{17}	1×10^{17}	1×10^{18}	1×10^{17}	1×10^{17}	1×10^{19}
Shallow uniform acceptor density, N_A (cm^{-3})	1×10^{15}	0	0	0	0	0	0	0

3. Results and discussion

3.1. Effect of SnS Absorber Layer's Thickness

The impact of SnS layer thickness on solar cell performance was evaluated through simulation in CdS/SnS solar cell structure. For simulation, the thickness of SnS was varied from 0.5 to 3 μm with a step size of 0.5 μm with a fixed CdS buffer layer thickness of 50 nm at a temperature of 300 K. Photovoltaic parameters (V_{oc}, J_{sc}, FF and efficiency) of SnS solar cells with various absorber thicknesses are shown in Fig. 2.

It is observed that when the thickness of the active layer increases to 1 μm, the short circuit current increases from 32.3 mA/cm^2 to 34.5 mA/cm^2, Voc increases from 0.76 V to O.78 V which results in enhancement of the efficiency at high rate. The efficiency achieved is 22.1%. But fill factor decreases. When the thickness of absorber layer is above 1 μm, the increase of efficiency , V_{oc}, fill factor and short circuit current occurs at a slow rate.

If the thickness of absorber layer is decreased below 1 μm . the depletion area becomes close to the back contact which results in high recombination process. As a result quantum efficiency decreases. Due to inadequate absorption of longer wavelength photons, V_{oc} and J_{sc} is also reduced. As thickness is increased to 1 μm , the SnS absorber layer will generate more electron-hole pairs due to absorption of more photons which increases J_{sc} and V_{oc} [35] . If thickness of absorber layer is above 1 μm, electron hole pair has to travel longer distances which causes the efficiency to increase at a slow rate [35,36]. So the optimal value for the thickness of the SnS absorber layer is 1 μm, because it is unnecessary to use more material which reduce deposition time and production cost for large scale industrial production [37,38].

Fig. 3 shows the quantum efficiency(QE) of SnS based solar cells for different SnS absorber layer thicknesses. The mechanism of electron transfer increases due to increase in absorber layer thickness in a solar cell [39,40]. A high QE above 90% is gained with absorber layer thickness greater or equal to 1 μm for long wavelength. These results suggest absorption of large number of photons will be done with the absorber layer thickness increment.

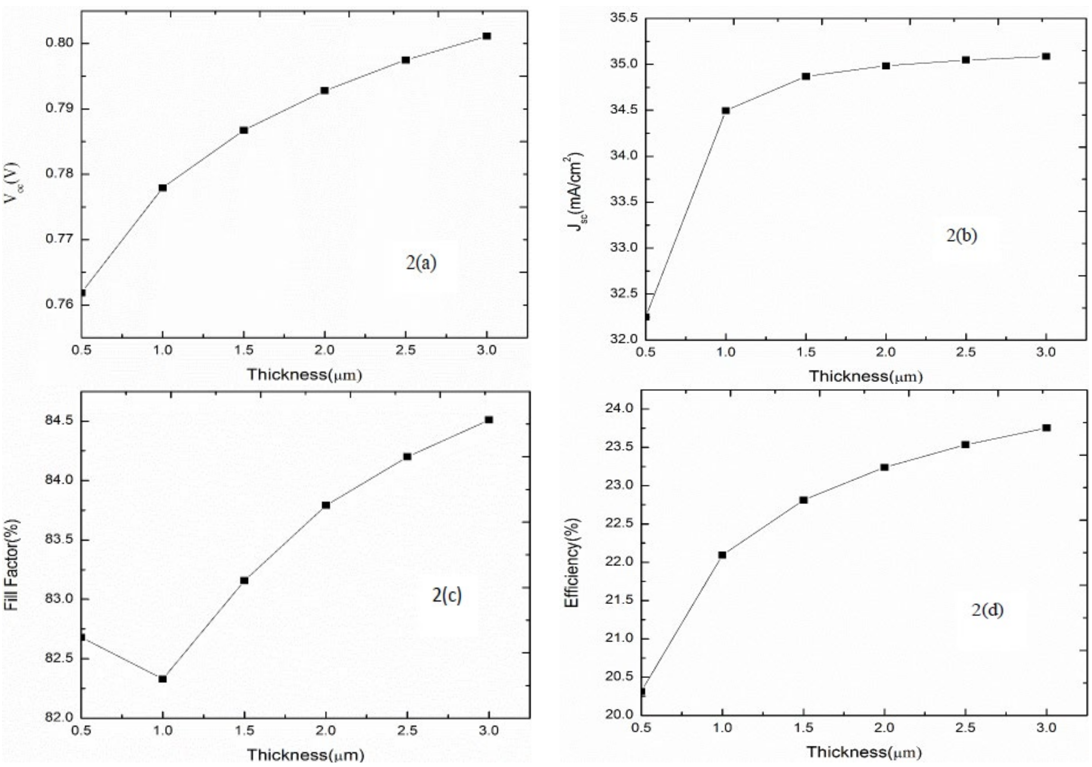

Fig. 2. a V_{oc} vs. absorber layer thickness. b J_{sc} vs. absorber layer thickness. c Fill factor vs. absorber layer thickness. d Efficiency vs. absorber layer thickness.

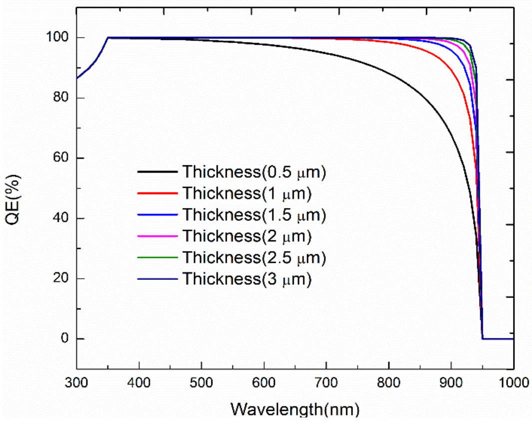

Fig. 3. Quantum efficiency for different SnS absorber layer thicknesses

3.2. Effect of CdS buffer layer thickness

The thickness of CdS layer was varied from 0.05 to 0.1 µm with a step size of 0.01 µm with a fixed SnS absorber layer thickness of 1 µm at a temperature of 300 K in this simulation. Fig. 4 shows the impact of varying thickness of CdS buffer layer. It is found that none of the parameters V_{oc}, J_{sc}, fill factor and efficiency is heavily impacted by the variation of buffer layer thickness. Fig. 5 shows quantum efficiency of SnS based solar cells with variable thickness of CdS buffer layer. The SnS based solar cell has high absorption that achieves above 90% quantum efficiency which creates a strong electron–hole pair for the range of 350-900 nm wavelength. Thickness of CdS buffer layer has no significant impact on QE in this simulation.

With increase in thickness of buffer layer, a large number of photons are absorbed into buffer layer[35]. The quantum efficiency of the solar cell is decreased due to lower number of photons at the absorber layer. The optimal thickness of CdS buffer layers is 0.05 µm in this simulation.

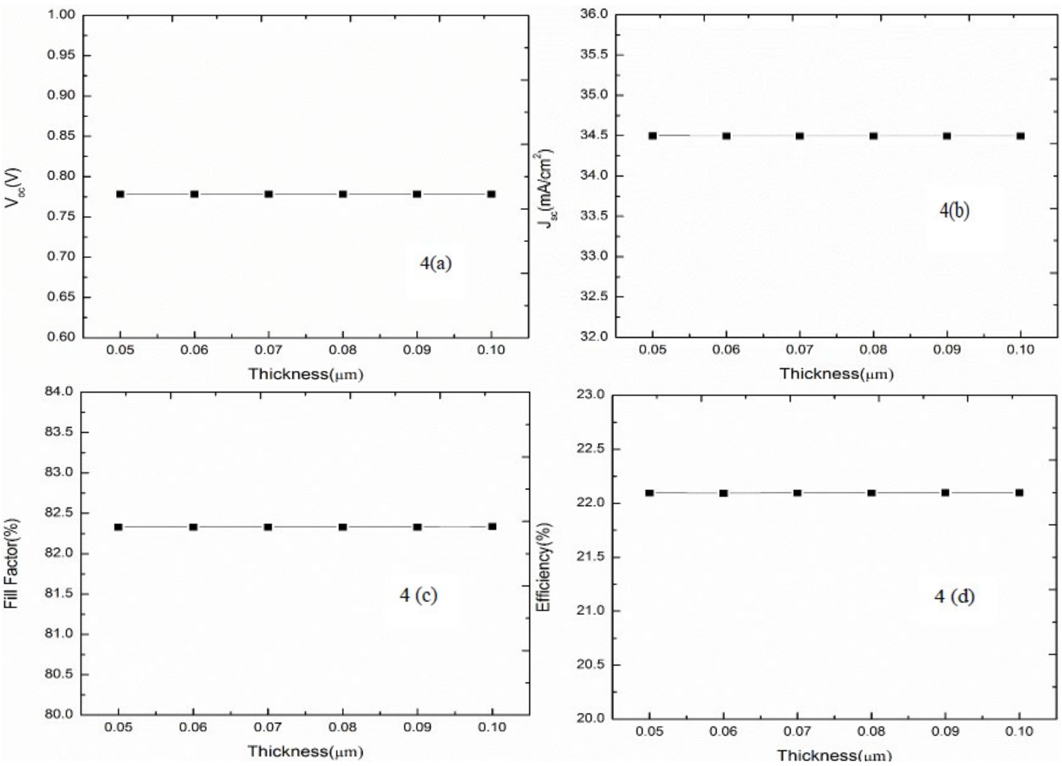

Fig. 4. a V_{oc} vs. buffer layer thickness. b J_{sc} vs. buffer layer thickness. c Fill factor vs. buffer layer thickness. d Efficiency vs. buffer layer thickness.

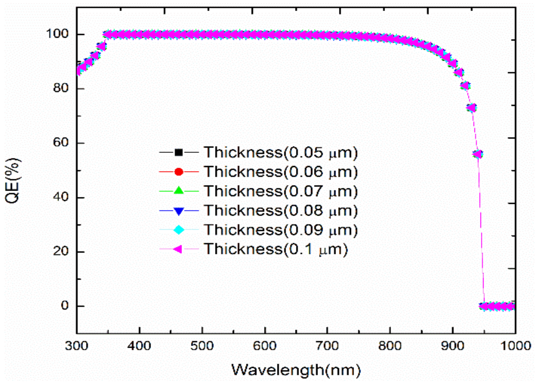

Fig. 5. Quantum efficiency of SnS based solar cell with variable thickness of CdS buffer layer.

3.3. Effect of different buffer layers on cell performance

Due to toxicity of CdS, other promising buffer layers such as ZnO, ZnSe, CdZnS and TiO_2 have also been investigated with optimal thickness of 0.09 µm, 0.06 µm,0.05 µm and 0.09 µm respectively while keeping thickness of SnS absorber layer fixed at 1 µm. Fig. 6 shows the comparative study of electrical parameters (V_{oc}, J_{sc}, FF and η) for different buffer layers. The current density–voltage (J–V) and quantum efficiency (QE) for different buffer layers are shown in Fig. 7 and Fig. 8 respectively. Different buffer layer has very small impact on J_{SC}. The V_{OC} with CdS, ZnO, ZnSe, CdZnS and TiO_2 as buffer layers is respectively 0.778 V, 0.772 V, 0.773 V, 0.896 V and 0.771 V respectively. SnS based solar cell with CdZnS buffer layer has low QE compared to other buffer layers. SnS based solar cell with ZnO, ZnSe, CdZnS and TiO_2 as buffer layers results in efficiency of 21.9%, 22.3%, 14.4% and 21.5 %, respectively. Hence, ZnSe is highly potential candidate to replace CdS buffer layer in SnS based solar cell as it achieves efficiency above 22.1% which is gained by using CdS buffer layer.

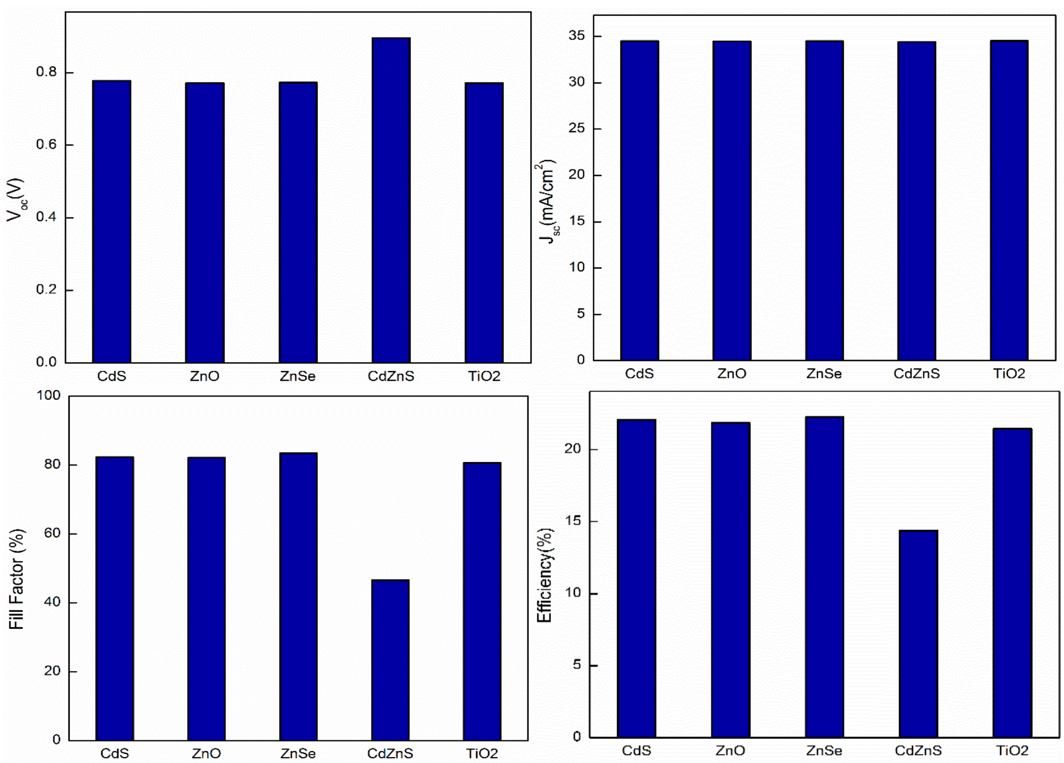

Fig. 6. SnS based solar cell performance with different buffer layer.

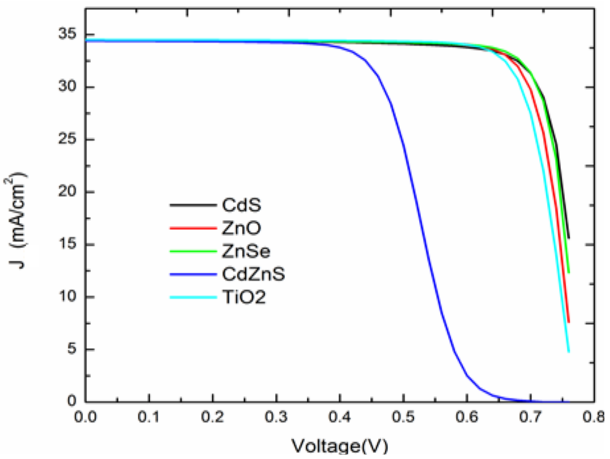

Fig. 7. J–V characteristics of SnS based solar cell with different buffer layer.

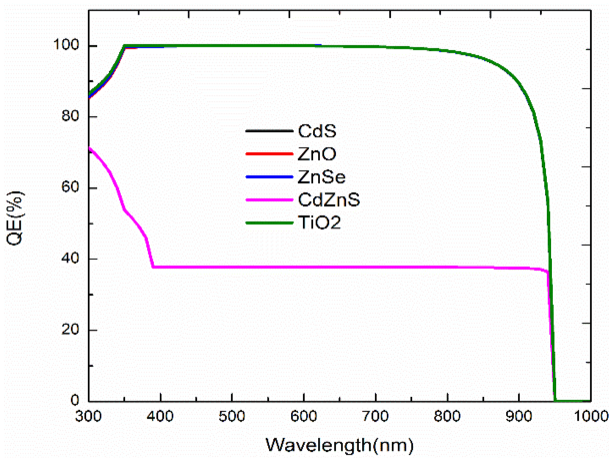

Fig. 8. Quantum efficiency of SnS based solar cell with different buffer layers.

3.4. Effects of operating temperature with various buffer layer

The impact of temperature was investigated for SnS based solar cell with various buffer layers by varying it from 300 K to 375 K. For all structure the SnS absorber layer's thickness was kept fixed at 1 µm, while the buffer layer's thickness was fixed at optimum value as discussed in previous section for every structure. Effect of temperature on SnS solar cell with different buffer layers is shown in Fig. 9.

With increase in temperature, due to reduction of bond energy, implemented by increase in charge carriers' velocity, the semiconductor band gap decreases. The increased recombination rate of electrons with holes results in decrease in V_{OC}[41]. The reverse saturation current also increases with increase in temperature, which also results in decrease in V_{OC} and fill factor[42]. J_{sc} is almost constant with increase in temperature. The combined effect of J_{sc}, fill factor and V_{oc} decrease efficiency. The efficiency of SnS based solar cell with CdS,ZnO, ZnSe, CdZnS and TiO_2 as buffer layer decreases with the increase of temperature at a gradient of 0.338%/K, 0.329%/K, 0.347%/K , 0.093%/K, 0.316%/K, respectively.

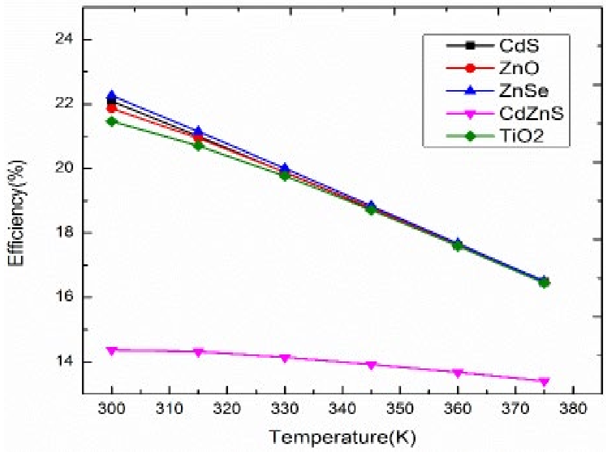

Fig. 9. Effect of temperature on efficiency of SnS based solar cell with different buffer layers.

3.5. Effects of SnS based homo-junction solar cell structure

In this work, homo-junction Mo / p-SnS / n-SnS / ITO device structure is also investigated with 0.07 µm buffer layer and 1 µm absorber layer. A promising result has been achieved by simulation. The, homo-junction device structure shows an efficiency of 22.6% with V_{oc} = 0.771 V, J_{sc} = 34.6 mA/cm^2 and a fill factor of 84.5%.

4. Conclusions

In this work, numerical simulations were done for SnS based solar cell using five different buffer layers such as CdS,ZnO, ZnSe, CdZnS and TiO_2.The electrical parameters were determined by varying absorber layer thickness, buffer layer thickness and temperature. The main objective was to optimize the thickness of absorber and buffer layer as well as to find a suitable material in place of toxic CdS buffer layer. After optimization, the highest efficiency achieved for hetero-junction SnS based solar cells is 22.3% (Jsc = 34.5 mA/cm^2, Voc = 0.773 V and FF = 83.5%) with 0.06 µm thick ZnSe buffer layer and homo-junction is about 22.6%(Jsc = 34.6 mA/cm^2 , Voc = 0.771 V and FF = 84.5%) with 0.07 µm thick SnS buffer layer. The optimized absorber layer thickness is 1 µm. From simulation results, it is revealed that the solar cell parameters are degraded for different type of buffer layers at various rate of temperature coefficient with increase in temperature. Based on the study, SnS and ZnSe show very impressive result to be a potential choice in SnS based solar cells instead of toxic CdS layer and the investigation can lead to fabrication of high-efficiency SnS based solar cell.

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