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Numerical Simulation of an Improved CZTS/WS_2 PV Cell by SCAPS 1-D

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Abstract—CZTS solar cells are promising among the third-generation solar cell. Because of its earth abundant materials and less toxicity CZTS solar cell can perform a sustainable role as an absorber layer. The optimization of a buffer layer is still a challenge and efficiency are still low than other thin film solar cells. In this study, WS_2 buffer layer have been used to simulate the PV cell structure in SCAPS-1D simulation software. No research has been found where CZTS and WS_2 is used together. We have achieved a maximum efficiency of η = 18.90 % at 300 K working temperature and other factors i.e., Voc, Jsc and FF are also promising. The highest certified efficiency of CZTS solar cell is nearly 12%. The simulation profile can be a guideline for fabricating the improved PV cell.

Index Terms— Solar cell, CZTS, WS_2, SCAPS-1D, Buffer layer.

I. Introduction

The renewable energy sources are proving to be more potential and convenient method of generating electrical power. Solar, wind, geothermal, wave energy are the examples of renewable energy sources. Among these energy sources solar energy is easy to use as it converts light into electrical energy. But the conversion efficiency is less than 30% [1]. Typically, solar cell is classified into three generations. Silicon wafer solar cells are the first-generation solar cell [2-3]. Amorphous Si, CIGS(Cu(lnGa)Se), CdTe are the second-generation solar cells. Third generation solar cells are perovskite, CZTS (Cu_2ZnSnS_4), etc. [4-6]. Si can be considered as most widely used absorber materials. Though it's low throughput and high cost, it has an efficiency of 26.7 ± 0.5 % [7]. Second generation CIGS and CdTe solar cell efficiency is achieved upto 23% and 21% respectively [8]. But these two materials inherit high toxicity for cadmium and selenium. Other than that tellurium and indium are less available [9]. To overcome these problems researchers have been considering CZTS (Cu_2ZnSnS_4) as a good absorbing material for the past decade. Main objective of this study is to improve efficiency of CZTS solar cell aided with WS_2 additional layer. Focus was to improve the efficiency more than 12% [8]. In this paper we have studied CZTS/WS_2 based solar cell structure with the help of SCAPS-1D solar cell simulation and modeling software. We have observed the effect of variation in WS_2 layer thickness, CZTS layer thickness and temperature. We have also taken into consideration of the effect of shallow acceptor density of CZTS absorber material and shallow donor density of the WS_2 buffer layer. Based on the simulation an optimum design for CZTS/WS_2 structured solar cell is proposed. Generally, CdS is used as a buffer layer of a CZTS solar cell.

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II. Related Works

CZTS (Copper Zinc Tin Sulfide) is a compound semiconductor. This has non-toxic earth abundant materials. It exhibits photovoltaic properties like CIGS and CdTe. It has an absorption coefficient above 10^4 cm^{-1} and direct band gap ranges from 1.4 to 1.6 eV [10-11]. For the buffer layer of CZTS solar cell many researchers are using CdS, ZnS and CdZnS [12]. Cadmium sulfide. CZTS (Copper Zinc Tin Sulfide) is a compound semiconductor. This has non-toxic earth abundant materials. It exhibits photovoltaic properties like CIGS and CdTe. It has an absorption coefficient above 10^4 cm^{-1} and direct band gap ranges from 1.4 to 1.6 eV [10-11]. For the buffer layer of CZTS solar cell many researchers are using CdS, ZnS and CdZnS [12]. Cadmium sulfide (CdS) proved to be most potential buffer layer for CZTS absorber layer for its suitable bandgap and interface enhancing properties. But CdS has high toxic component and can affect the environment with its wastage [13]. Besides maximum efficiency for CZTS solar cell has been reported less than 12% [14]. Lately, the TMDCs (transition metal di-chalcogenides), mainly MoS_2 (Molybdenum disulfide) and WS_2 (Tungsten disulfide) postured specific concerns for the solar cell material researchers because of their unique optoelectronic properties as

B. Validation of Structure

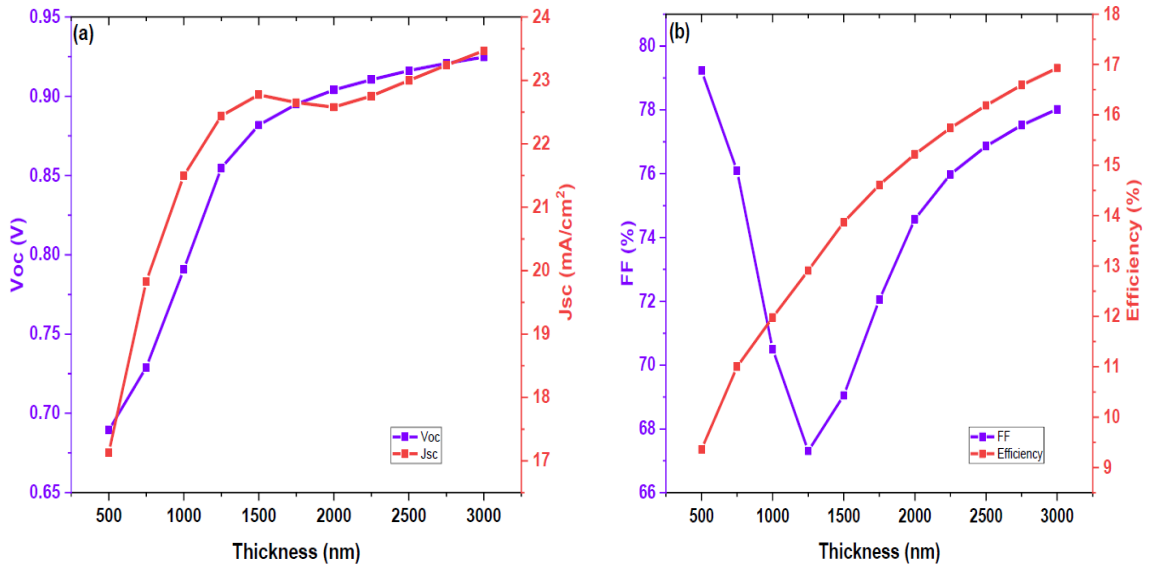

Fig.2 Absorber layer thickness variation (a) Voc, Jsc; (b) FF, Efficiency.

PV cell performance can be analyzed by J-V characteristic curve. We will validate the proposed structure by this J-V characteristic curve. Other than that, we will also make discussion over quantum efficiency. The fundamental equations that run the solar cell characteristics like Voc, Jsc, FF and efficiency can be expressed as

$$I = I_{ph} - I_o e^{\left(\frac{qV}{nk_BT}\right)} \quad \text{..... (1)}$$

$$I_{sc} = I_o \left[e^{\left(\frac{qV_{oc}}{nk_BT}\right)} - 1 \right] \text{... ... ...(2)}$$

$$V_{oc} = \frac{nk_BT}{q} \ln\left(\frac{I_{ph}}{I_o}\right) \quad \text{..... (3)}$$

Where, I_{ph} is photo-generated current, I_o is reverse saturation current, n & k_B is the ideality factor and Boltzmann constant respectively. Using voltage current density curve, we can determine the I_{sc} (short-circuit current) at V=0 and V_{oc} (open circuit voltage) at I=0. We can calculate these from equation (2) and (3).

C. Simulation Software & Material Parameter

In this research simulation software named SCAPS-1D (Solar Cell Capacitance Simulator) is used to do the simulation. SCAPS-1D is one-dimensional solar cell simulation software, is developed by the dept. of EIS, University of Gent, Belgium. Material properties like band gap, electron and hole mobility, dielectric permittivity, electron affinity and other properties for different layer can be attuned in the layer properties panel [29]. SCAPS functionality depends on three differential equations. One of the equations is known as Poisson's equation and other two are continuity equation for electron and hole. The equations are respectively

$$\frac{\partial}{\partial x}\left(\varepsilon(x)\frac{\partial \Psi}{\partial x}\right) = -\frac{q}{\varepsilon_o}\left[-n + p + N_D - N_A + \frac{1}{q}\rho_{def}(n,p)\right] \text{... ... ...(4)}$$

$$\frac{1}{q}\frac{\partial J_n}{\partial x} + G - R_n(n,p) = \frac{\partial n}{\partial t} \text{... ... ... (5)}$$

$$-\frac{1}{q}\frac{\partial J_p}{\partial x} + G - R_p(n,p) = \frac{\partial p}{\partial t} \text{..... (6)}$$

Where, Ψ & Є are electrostatic potential and dielectric constant and $Є_o$ is the permittivity in vacuum., n, p are carrier concentration of electron and hole respectively. N_D and N_A are donor and acceptor density and ρ_{def} is the defect density. R_n, R_p are combination rate of electron and hole, G is the generation rate and J_p & J_n are the current density of hole and electron.

The light illumination was through the n-ITO layer side with 1.5 global air mass spectrums with 1000W/m^2 at 298 K. We have included two types of single layer defects in CZTS for the simulation. Neutral type defect and single donor defect was considered for the CZTS material to perform the simulation and get more practical result. The simulation is performed in several steps. At first, the absorber layer thickness (500 nm - 3000 nm) was varied and then the buffer layer thickness (50 nm -150 nm). Next, the doping concentration was taken into consideration for both absorber and buffer layer. The shallow acceptor density of the CZTS material and shallow donor density (5.5×10^{12} to 5.5×10^{18} cm^{-3}) of the WS_2 material (1×10^{15} to 1×10^{20} cm^{-3}) was varied during the simulation. All other simulation results like QE (Quantum Efficiency), generation-recombination, band diagram of the proposed structure and J-V characteristics graph have been observed and analyzed. All the physical

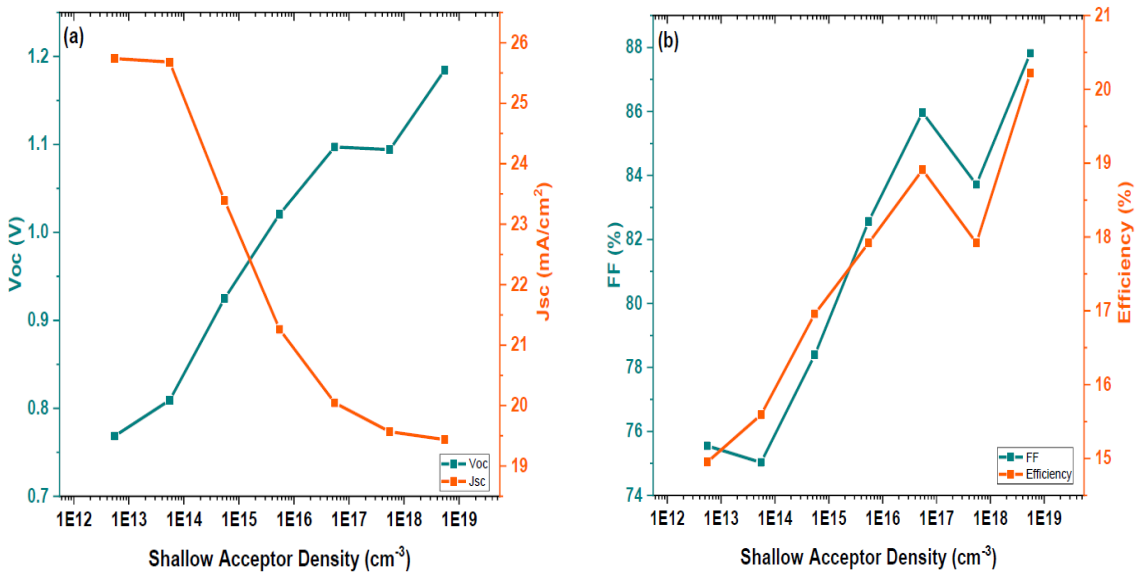

Fig.4. Shallow acceptor density variation of absorber layer (a) V0c, Jsc; (b) FF, Efficiency

70 nm the Voc starts to increase and at 150 nm the Voc becomes 0.9253 V. Fig. 3(a) shows the Voc variation graph of buffer layer thickness variation. But the scenario for the Jsc is quite different. The short circuit density decreases from 23.46 mA/cm^2 to 23.16 mA/cm^2. The change in Jsc is very low. So, it can be said that the variation of thickness of the buffer layer didn't affect the Jsc very much. The fill factor increases if the thickness of the buffer layer is increased but the rate of increment is very low. It remains between 78.0 % and 78.8%. But the efficiency of the solar cell depends on the thickness of the buffer layer. In general, the thickness of the buffer layer is50 nm if we use CdS as a buffer layer. But in this research, we have observed that efficiency starts to increase at first but after 70 nm to 90 nm it remains constant. But if we increase the thickness of the buffer layer more, the efficiency starts to decrease. We have taken our optimum buffer layer thickness to 90 nm because at this thickness the efficiency was at pick and the fill factor was also reasonable.

C. Shallow Acceptor Density Variation

As it is known that doping creates a depletion layer in the p-n junction photovoltaic solar cell. So, the variation of doping concentration creates different depletion layer width which creates different electric field for photons generated carrier for flowing. In this part we have kept the thickness of the CZTS layer at 3000 nm and the thickness of the buffer layer at 90 nm. But we have varied the acceptor density of the CZTS layer because the CZTS layer is working as a p-type material where the hole of the material is ready to create recombination with electron. The acceptor density varied from 5.5 × 10^{12} cm^{-3} to 5.5 × 10^{18} cm^{-3}. The effect of the variation of acceptor density is shown in Fig. 4. Voc increases almost linearly from 5.5 × 10^{12} cm^{-3} to 5.5 × 10^{16} cm^{-3} of acceptor density. This time, it increases from 0.75 V to 1.06 V and after that it remains constant for a further increment of the density. But after 5.5 × 10^{17} cm^{-3}, it starts to increase again. Jsc show different scenario for acceptor density variation. Short circuit current density decreases from 25.73 mA/cm2 to 19.43 mA/cm^2 as the acceptor density of the absorber layer increases. If the acceptor density of the CZTS layer increased, the simulation data shows that, fill factor and efficiency both increase for increasing density. The graph shows that the efficiency and fill factor both increases linearly at the density variation from 5.5 × 10^{12} cm^{-3} to 5.5 × 10^{16} cm-3 after that it decreases a bit and again starts to increase. At 5.5 × 10^{16} cm^{-3} FF becomes 86% and the efficiency becomes 18.90%. Fig. 4(b) shows the graph of fill factor and efficiency. We have selected our shallow acceptor density 5.5 × 10^{16} cm^{-3} because to have more practical oriented data.

D. Shallow Donor Density Variation

We have also analyzed the shallow donor density variation of the WS_2 buffer layer to optimize our device structure. WS_2 is the high doped n-type layer. The practical density can be achieved up to 1.0 × 10^{20}cm^{-3}. The donor density was varied from 1.0 × 10 ^{15} cm^{-3} to 1.0 × 10^{20} cm^{-3}. At this time the shallow acceptor density of the absorber layer was kept at 5.5 × 10^{16} cm^{-3}. Fig. 5 shows the graph of various electrical parameter of the solar cell device. Open circuit voltage (Voc) of the device increases from 0.98V to 1.09V because of increasing the donor density of the layer up to 1.0 ×10^{18}cm^{-3}. After that it remains at this level upto the donor density of 1.0 × 10^{20}cm^{-3}. Jsc also increase from 18.50 mA/cm^2 to 20.04 mA/cm^2 at the layer donor density increase from 1.0 × 10^{15} cm^{-3} to 1.0 × 10^{18} cm^{-3}. After that it starts to decrease. Fig. 5(a) shows the data graph of Voc and Jsc. same scenario happened for the fill factor and efficiency of the solar cell device.

have seen that low temperature (4ºC -9ºC) improves the conversion rate [37].

VII. Conclusion

In this study numerical simulation of CZTS solar cell with WS_2 buffer layer was carried out by SCAPS-1D software to study the solar cell performance. Solar cell parameters were observed by varying the absorber layer thickness, buffer layer thickness, shallow acceptor density, shallow donor density. The J-V curve confirms the proposed structure and exhibit 18.90 % efficiency. High open circuit voltage dominates the J-V curve. As we can observe from the simulated data substituting CdS by WS_2 as a buffer layer improves the efficiency about 6%. Increasing the carrier concentration, the performance parameter can be improved. We have also showed the temperature variation of our proposed structure and this case solar cell performance decreases for increasing working temperature. Nevertheless, it has been observed from our study that introducing WS_2 as a buffer layer of a CZTS solar cell improves the cell performance.

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