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Enhancing the Performance of CZTS Thin Film Solar cell by SCAPS 1D

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Abstract—**Kesterite Copper-Zinc-Tin-Sulphide (Cu_2ZnSnS_4)** is a non toxic and earth abundant semiconductor compound with optimum band gap (1.3-1.5eV) and high absorption coefficient (10^4 cm^{-1}). In this work firstly the modeling of CZTS solar cell is done by SCAPS 1D software and then layer parameters have been optimized and cell parameters like V_{oc}, J_{sc}, FF and η are recorded for the best performance of solar cell. The cell structure simulated in this work is **Mo/CZTS/CdS/i-ZnO** in which CZTS works as an absorber layer, CdS works as buffer layer, i-ZnO as window layer and Mo is a back metal contact. We have optimized the effect of band gap (E_g), thickness of CZTS absorber layer. The effect of temperature is also studied in this work. The optimized values of CZTS thickness and band gap for the above structure are found to be 2.5µm and 1.4eV. The optimum temperature is 300K. By using these values the best performing solar cell in this work gave V_{oc}= 0.44V, J_{sc}= 45.70 mA/cm^2, FF=63.6% and η= 12.85%.

Keywords: Absorber layer CZTS, Efficiency, SCAPS-1D, Simulation

I. INTRODUCTION

Sunlight is one of the most effective and efficient source of energy. The consumption of oil and other fossil fuels is increasing day by day all around the world. These sources are rapidly running out and require millions of years to replenish. Sunlight is the huge source of energy which can fulfill world's energy demand and human can use it to convert it to an electrical energy. Globe consumes energy at the rate of $4.7x10^{20}$ watts per year, which is equal to 15 terawatts of total global power [1]. Solar cells and other solid-state electronics may convert solar energy into heat and power. Solar cells are very effective at converting sunlight into electricity, and energy can be turned to a useful form of energy without damaging the environment [2]. Researchers are developing and exploring new technologies and materials to manufacture solar cell cost effective and efficient. One such technology is thin film solar cells. For several decades, thin-film photovoltaic materials have garnered a lot of interest due to their potential to create large-area thin-film solar cells that are both inexpensive and highly efficient [3]. These materials include $Cu(InGa)Se_2$ and CdTe which have given an efficiency of about 22.1% and 23.3% respectively [4]. The commercial production of these technologies is limited as Ga and In are very costly materials and Cd is very toxic material. Kesterite material is a favourable material when used as an absorbing layer. It can be utilised as CZTS (Cu_2ZnSnS_4), CZTSe (Cu_2ZnSnS_e) and their alloys [5]. Copper-Zinc-Tin-Sulphide uses the materials which are low cost and earth abundant. It is a p-type semiconductor having optimum band gap (1.3eV to 1.5eV) and strong absorption coefficient (10^4 cm^{-1}) in visible spectrum [6] [7]. Several techniques have been used to fabricate CZTS thin film solar cell. Those are physical and chemical vapour deposition methods including sputtering and chemical based approach. Very first CZTS thin film solar cell was fabricated by Ito and Nakazawa with an efficiency of 0.66% using atom beam sputtering [8]. The highest conversion efficiency is achieved by Wang et al. by using hydrazine pure solution process and it is 12.6% [9]. The aim of this work is to model and analyse the solar cell structure Mo/CZTS/CdS/i-ZnO by using Solar Cell Capacitance Simulator (SCAPS 1D). The parameters affecting efficiency of solar cell have been optimized.

II. DEVICE STRUCTURE AND SIMULATION

SCAPS 1D is simulation software used to model thin film solar cells. Ii is developed at the Department of Electronics and Information System (ELIS) University of Gent, Belgium. This software is freely available for PV researchers. This software can model seven semiconductor layers. It can calculate I-V curve, C-V curve, Quantum Efficiency, Band Structure, Recombination profile, Power Conversion efficiency, Open Circuit Voltage, Short Circuit Current and other physical parameters. The function of SCAPS 1D depends upon three sets of equations [10].

II.I. TRANSPORT EQUATIONS FOR ELECTRONS AND HOLES

$$\frac{1}{q}\frac{dJn}{dx} = G_n - R_n \text{ and } \frac{1}{q}\frac{Jp}{dx} = G_p - R_p$$

Here J_n and J_p are electron and hole current densities. G_n and G_p are electron and hole generation rate. R_n and R_p are electron and hole recombination rate.

II.II. POISSON EQUATION

$$\frac{d^2 V}{d x^2} = \frac{q}{\varepsilon_0 \varepsilon_r}\{p(x) - n(x) + Nd - Na + \rho p - \rho n\}$$

Here V is electrostatic potential, n(x) and p(x) are electron and hole concentration N_a and N_d are acceptor and donor concentration, ρ_n and ρ_p are electron and hole distribution.

II.III. DRIFT AND DIFFUSION EQUATION

$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{dV}{dx} \text{ and } J_p = D_p \frac{dp}{dx} + \mu_p p \frac{dV}{dx}$$

Here D_n and D_p are diffusion coefficient, μ_n and μ_p are electron and hole mobilities.

The cell structure which is used in this work is Mo/CZTS/CdS/i-ZnO. This is shown in Figure 1. In this structure Mo is used as a back metal contact. p- CZTS and n- Cds is used as an absorber layer and buffer layer and make a p-n junction which is the most important part of solar cell. For these different layers various types of electrical and optical parameters are used. These parameters are taken from various research papers and articles [11], [12], [13], [14], [15]. In some cases some reasonable estimates have also been made. These parameters are given in Table 1.

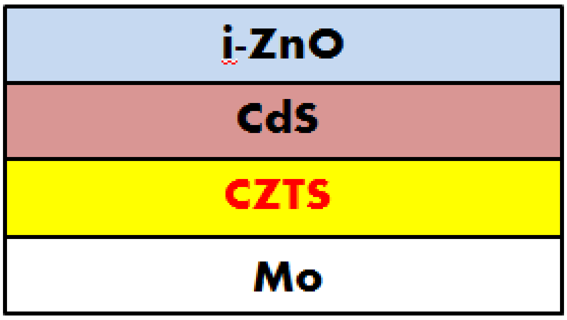


Figure 1. Structure of Solar Cell for simulation

Table 1. Material parameters used in solar cell simulation

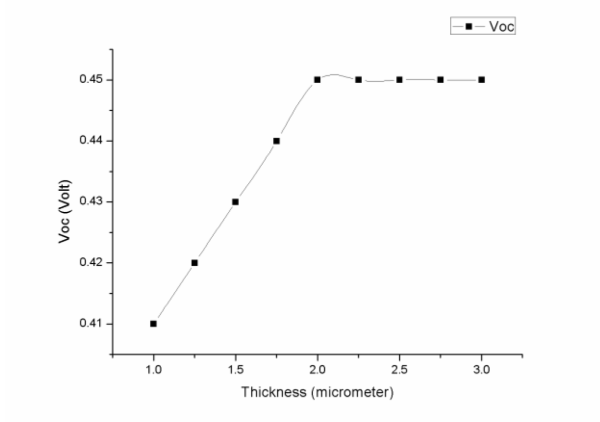
Parameters	**i-ZnO**	**Cds**	**CZTS**	**Mo**
Thickness (µm)	0.1	0.05	1-2.5	0.1
Band Gap (eV)	3.3	2.4	1.3-1.5	1.7
Electron Affinity (eV)	4.6	4.2	4.5	4.2
Dielectric Constant (χ)	9	10	10	13.6
C.B Density of States (cm^{-3})	$2.2x10^{18}$	$1.8x10^{19}$	$2.2x10^{18}$	$2.2x10^{18}$
V.B Density of States (cm^{-3})	$1.8x10^{19}$	$2.4x10^{18}$	$1.8x10^{19}$	$1.8x10^{19}$

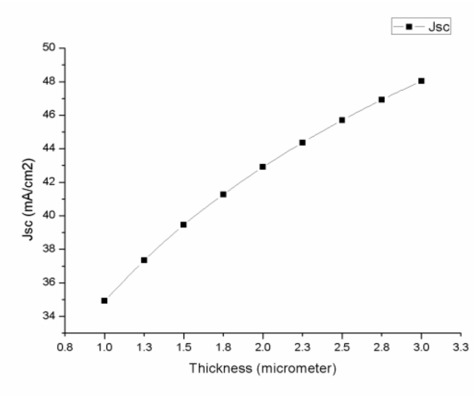
Electron thermal velocity (cm/sec)	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$
Hole Thermal velocity (cm/sec)	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$
Electron Mobility (cm^2 /V-sec)	100	50	100	100
Hole Mobilty (cm^2 /V-sec)	25	20	25	25
Donar Concentration (cm^{-3})	$1x10^{18}$	$1x10^{17}$	10	0
Acceptor Concentration (cm^{-3})	0	10	$1x10^{16}$	$1x10^{16}$

III. RESULTS AND DISCUSSIONS

For the present work in the SCAPS 1D the standard illumination spectrum AM 1.5 is used to illuminate solar cell. The incident light power has fixed to be $1000W/m^2$. The solar cell structure Mo/CZTS/CdS/i-ZnO has been considered in this study.

3.1 Effect of absorber layer thickness: First of all the effect of absorber layer thickness has been studied. For this the band gap of absorber layer has taken to be 1.4 eV value and buffer layer thickness is 50µm. Both of these parameters have been fixed and thickness of absorber layer is increased from 1µm to 3µm and studied the effect of layer thickness on open circuit voltage (V_{oc}), short circuit current (J_{sc}), Fill Factor (FF) and Efficiency (η). The variation of these parameters with thickness is shown in Figure 2. These graphs show that all these parameters increases with increasing thickness. This is because by increasing the thickness of absorber layer the number of photons absorbed by layer increases and more electron- hole pairs are created and as a result all parameters increases. The maximum efficiency 12.85% is obtained at 2.5µm of layer thickness. At this value of thickness V_{oc} is 0.44 Volt, short circuit current density is 45.70 mA/cm^2. Fill Factor is 63.6 %.





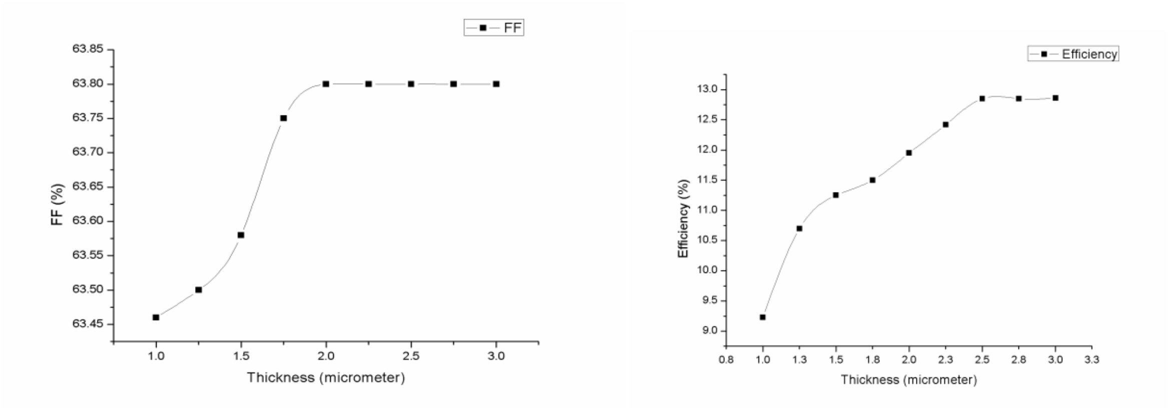


Figure 2. Variation of cell parameters with absorber layer thickness

3.2 Effect of Band Gap variation: In this simulation work we have also simulated the effect of band gap on the cell parameters. The band gap of CZTS is varied from 1.3eV to 1.5eV. The variation of V_{oc} , J_{sc} , FF and η with the band gap is shown in Figure 3. Figure shows that with increase in band gap the open circuit voltage increases. This is because with increase in band gap of any material the potential difference between the conduction band and valence band increases. Due to which voltage also increases. Also the short circuit current density decreases with increases in band gap. At lager band gap, the absorption of light in the material decreases and less number of electron-hole pair will generate which results in less short circuit current. The fill factor in this case increases with increase in band gap due to less short circuit current which is due to less absorption at higher band gap. The efficiency of this cell decreases with increase in band gap. It can be due to the defects which are present in the absorber layer. The optimized value of band gap has come out to be 1.4eV at which efficiency is 12.8 %.

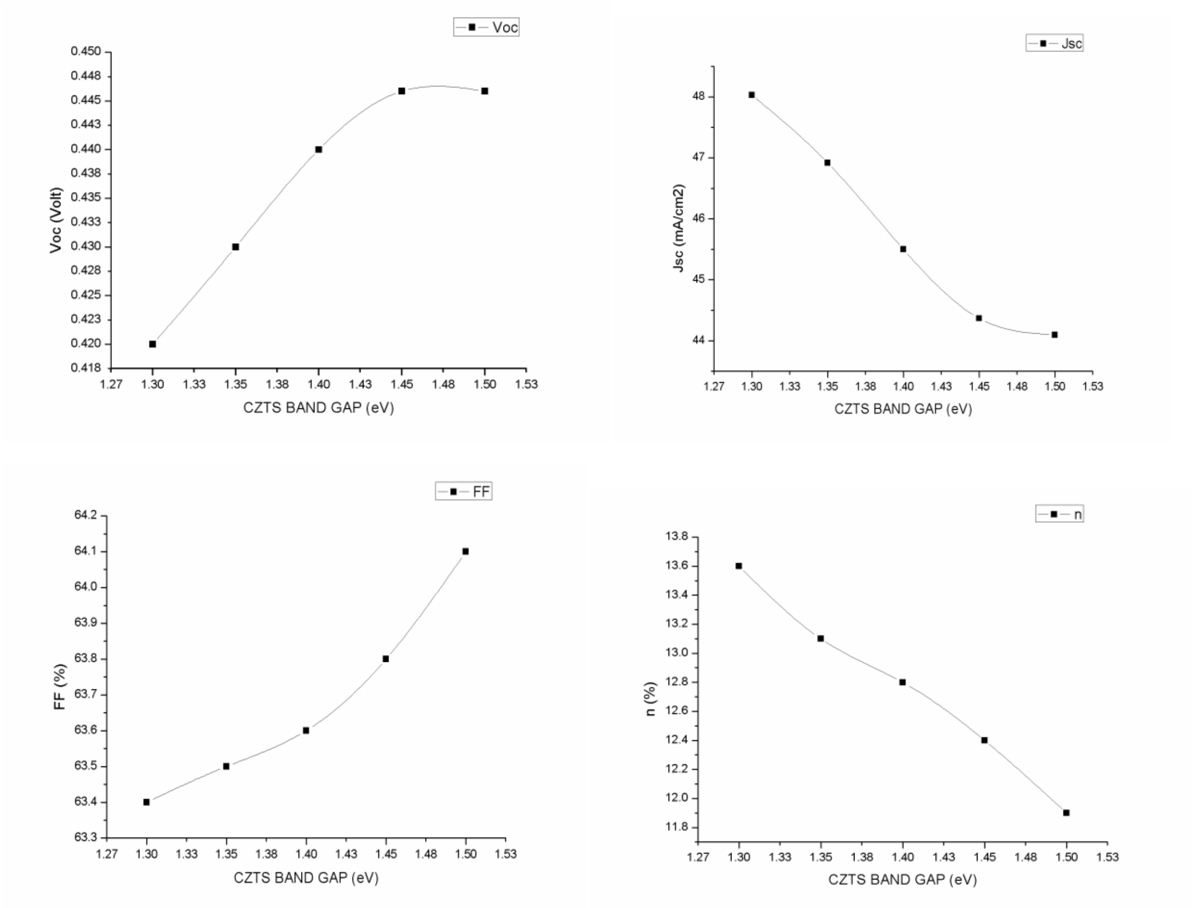


Figure 3. Variation of cell parameters with band gap of CZTS

3.3 Effect of working temperature: In the next step the working temperature of cell has been varied from 250°C to 450°C. At 300°C the efficiency is 12.5%, which is the maximum optimized value. The simulated results for working temperature Vs cell parameters are shown in Figure 4

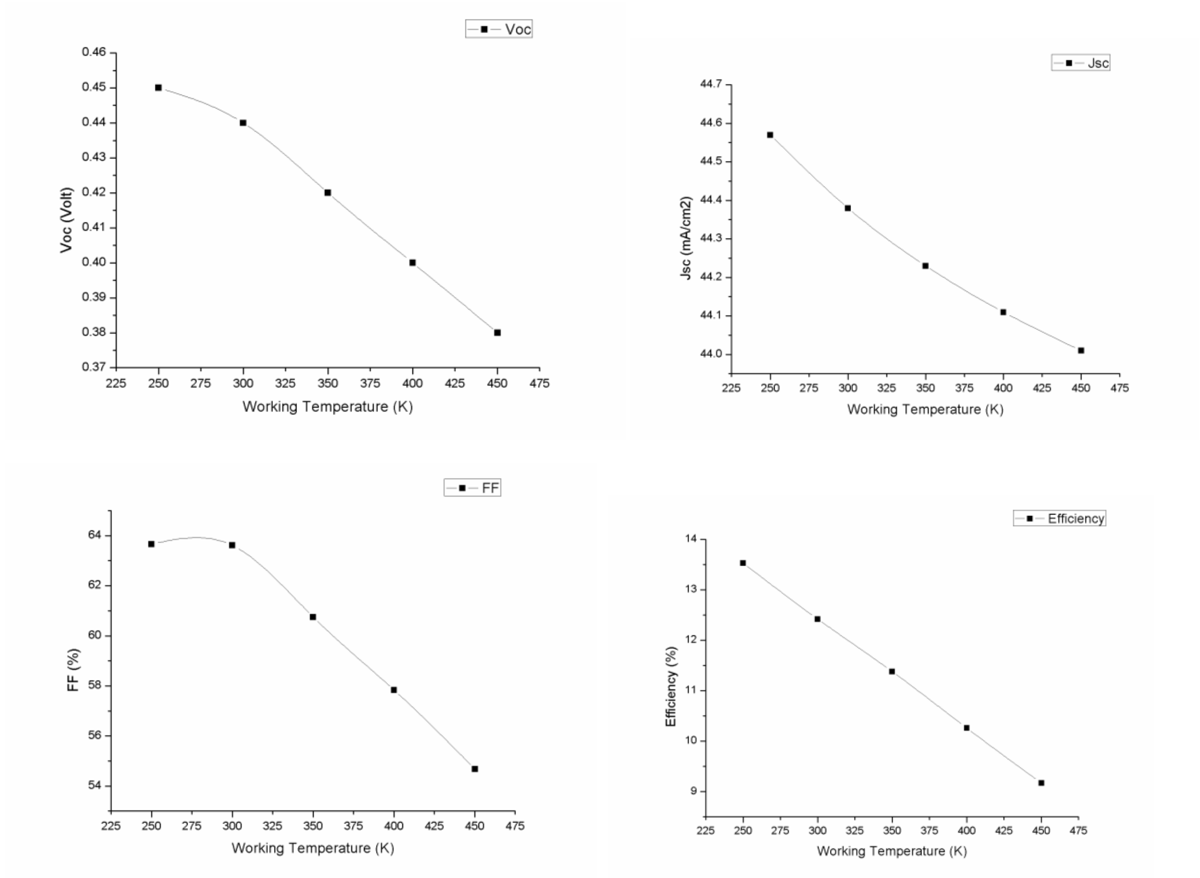


Figure 4. Variation of cell parameters with working temperature

IV. CONCLUSION

In this study we performed numerical simulation of CZTS thin film solar cell by SCAPS 1D and observed the performance of solar cell by simulating the thickness, band gap of absorber layer and working temperature of the cell. The simulated results shows that the optimum thickness of CZTS absorber layer is 2.5µm, the optimum band gap is 1.4eV and optimum working temperature is 300K. The cell simulated results gives open circuit voltage of 0.44eV, short circuit current density of 45.70 mA/cm^2, FF is 63.6% and efficiency is 12.85%. These results can be used in fabricating solar cell by doing some more simulations. In this way numerical modeling can guide the researches to make the solar cell of greater efficiency.

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