Numerical Modeling and Parameter Optimization of Kesterite Based Thin Film Solar Cell by SCAPS 1D

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Abstract A non-toxic and plentiful semiconductor compound, copper-zinc-tin-sulfide (Cu_2ZnSnS_4) has a high absorption coefficient (10^4 cm^{-1}) and an ideal band gap (1.3-1.5eV). Using SCAPS 1D software, the CZTS solar cell is first modelled in this work. Layer parameters are then improved and cell characteristics such as V_{oc}, J_{sc}, FF, and η are recorded for optimal solar cell performance and compared with experimental findings. The cell structure simulated in this work is CZTS/CdS/i-ZnO/ZnO: Al. In this structure CZTS works as an absorber layer, CdS as buffer layer, i-ZnO as window layer and ZnO:Al as Transparent conducting oxide (TCO) for transport of electron. We have optimized the CZTS layer's thickness, Bang Gap of CZTS (E_g), CdS thickness, Acceptor carrier density (N_a) for absorber layer and donor carrier density for buffer layer. This work also examines the impact of working temperature. The optimized values of CZTS thickness, band gap and acceptor carrier density for the above structure came out to be 2.5µm, 1.45eV and 1×10^{16} /cm^3 respectively. The optimized values of thickness and donor density of the buffer layer found to be 75µm and 1×10^{18} /cm^3. The optimum temperature is 300K. By using these optimized parameters in the SCAPS 1D software, the best performing solar cell in this work produced V_{oc}= 0.44V, J_{sc}= 45.87 mA/cm^2, FF=63.44% and η= 12.90%. These results are then compared with the experimental results. The experimental result gave the efficiency of about 6.2% when CZTS thin films are grown by co-sputtering for the same cell structure.

Keywords- CZTS solar cell, SCAPS 1D, efficiency, simulation, absorber layer.

1. Introduction These days world is using energy at the rate of 10^{20} Joule/year which is equal to world power consumption of 15 Terawatts [1]. The world population is increasing exponentially and so the energy demand is also increasing. This demand is fulfilled by oil and fossil fuels which are limited in nature and take millions of years to replenish. Fossil fuels also produce harmful gases like CO_2, NO_2, CO and SO_2 etc which create pollution in our environment [2]. But sunlight is most powerful, efficient and endless source of energy which can fulfill world's increasing energy demand. Solar energy can be transformed into electricity and heat using solar cells and other solid-state devices. Energy may be transformed into a useful form of energy without harming the environment because of solar cells' exceptional ability to convert sunlight into electricity [3]. More than 80% present photovoltaic industry is based on silicon which is indirect band gap absorber material and uses a thick layer of material to absorb more photons coming from solar radiation. Researchers are looking for new materials and technologies to manufacture cost effective and efficient solar cells. Since last several decades thin film solar cell technology have attracted so much interest as they are capable of giving large area solar cell which can fulfil our demand [4]. Among these materials are $Cu(InGa)Se_2$ and CdTe, which have respective efficiency values of roughly 22.1% and 23.3% [5]. The production of these solar cell technologies is also limited as Cd and Se are toxic in nature and In and Te are expensive and not abundantly available in nature [6]. One such material whose components are earth abundant and non toxic is Kesterite which is an alloy of Cu, Zn. Sn , S and Se and used as CZTS ($Cu_2 ZnSnS_4$), CZTSe (Cu_2 ZnSnSe) [7]. CZTS is a p-type semiconductor having band gap 1.3eV to 1.5eV which is good for solar cell applications [8] It is a direct band gap semiconductor and has strong absorption coefficient (10^4 cm^{-1}) in visible spectrum which makes it cost efficient as thin layer of material is enough to absorb solar radiation [9]. CZTS thin-film solar cells have been made using a variety of methods, which include sputtering and chemical-based approaches, as well as physical and chemical vapour deposition techniques. Using atom beam sputtering, Ito and Nakazawa created the first CZTS thin film solar cell with an efficiency of 0.66% [10]. Wang et al. use the hydrazine pure solution procedure to achieve the maximum conversion efficiency, which is 12.6% [11]. In the present work the modelling of CZTS solar cell is done and then we have optimized the layer parameters for the solar cell structure with the help of Solar Cell capacitance Simulator (SCAPS 1D).

2. Mathematical Modeling of SCAPS 1D

A simulation program called SCAPS 1D is used to model thin-film solar cells. Ii is created at the University of Gent in Belgium's Department of Electronics and Information Systems (ELIS). PV researchers can use this program for free. Seven semiconductor layers can be modelled by this software. In addition to other physical parameters, it can compute the I-V and C-V curves, band structure, recombination profile, power conversion efficiency, open circuit voltage, short circuit current, and quantum efficiency. It uses a variety of standard and other spectra including AM0. AM 1.5D, AM 1.5G and monochromatic etc. SCAPS is designed such that it is used to simulate practical circumstances but it can give superficial results if unrealistic input is given. The functioning of SCAPS 1D software depends upon three sets of equations [12].

(a) Transport equations for charge carriers:

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

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.

(b) Poisson Equation

$$\frac{d^2\,V}{d\,x^2} = \frac{q}{\varepsilon_0\,\varepsilon_r}\{p(x) - n(x) + N_d - N_a + \rho_p - \rho_n\}$$

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.

(c) Drift and Diffusion Equation for electron and hole

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

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

3. Numerical Simulation and Device Modeling

Figure 1 shows the solar cell structure CZTS/CdS/i-ZnO/ZnO: Al simulated in this work. For the layers of this solar cell structure various electrical and optical parameters are used which are given in Table 1 [13], [14], [15], [16], [17], [18]. These parameters are extracted from a number of articles and research papers. At some places some estimates have also been made.

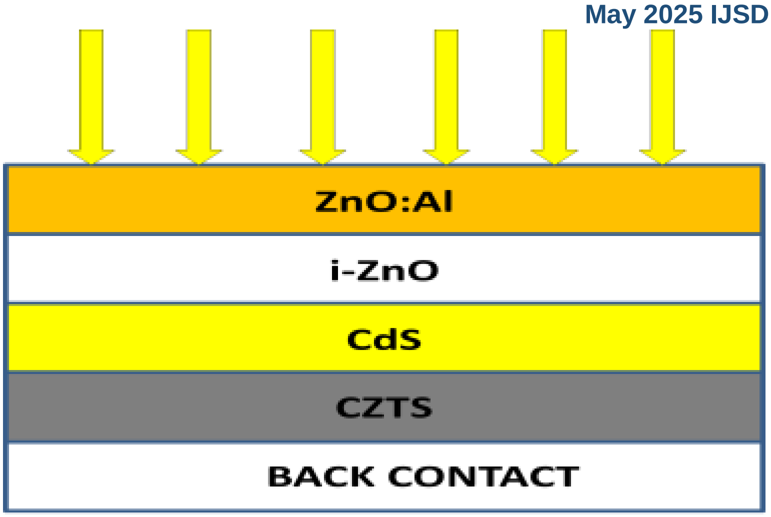

Figure: 1

Table 1

Parameters	**ZnO:Al**	**i-ZnO**	**Cds**	**CZTS**
Thickness (μm)	0.45	0.1	0.05	1-2.5
Band Gap (eV)	3.3	3.3	2.4	1.3-1.5
Electron Affinity (eV)	4.6	4.6	4.2	4.5
Dielectric Constant (χ)	9	9	10	10
C.B Density of States (cm^{-3})	$2.2x10^{18}$	$2.2x10^{18}$	$1.8x10^{19}$	$2.2x10^{18}$
V.B Density of States (cm^{-3})	$1.8x10^{19}$	$1.8x10^{19}$	$2.4x10^{18}$	$1.8x10^{19}$
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	100	50	100
Hole Mobilty (cm^2 /V-sec)	25	25	20	25
Donar Concentration (cm^{-3})	$1x10^{18}$	$1x10^{18}$	$1x10^{17}$	10
Acceptor Concentration (cm^{-3})	0	0	10	$1x10^{16}$

4. Results and Discussions The solar cell structure used in this study is illuminated with standard AM 1.5 spectrums and incident power density is fixed at 1000 Watt/m^2.

4.1 Effect of CZTS layer thickness The thickness of absorber layer is varied from 0.5μm to 3.5μm at fixed band gap value of 1.4 eV. The thickness of buffer layer is fixed at 50 μm. Then we analyze the effect of layer thickness on open circuit voltage (V_{oc}), short circuit current density (J_{sc}), Fill Factor (FF) and Efficiency (η). These cell parameters increases with increase in thickness and this variation is shown in Fig 2. The number of photons absorbed and hence the electron-hole pair absorbed by the absorber layer increases with increase in thickness. The optimum thickness of CZTS layer is found to be 2.5μm. The maximum efficiency 12.86% is obtained at 2.5 μm layer thickness.

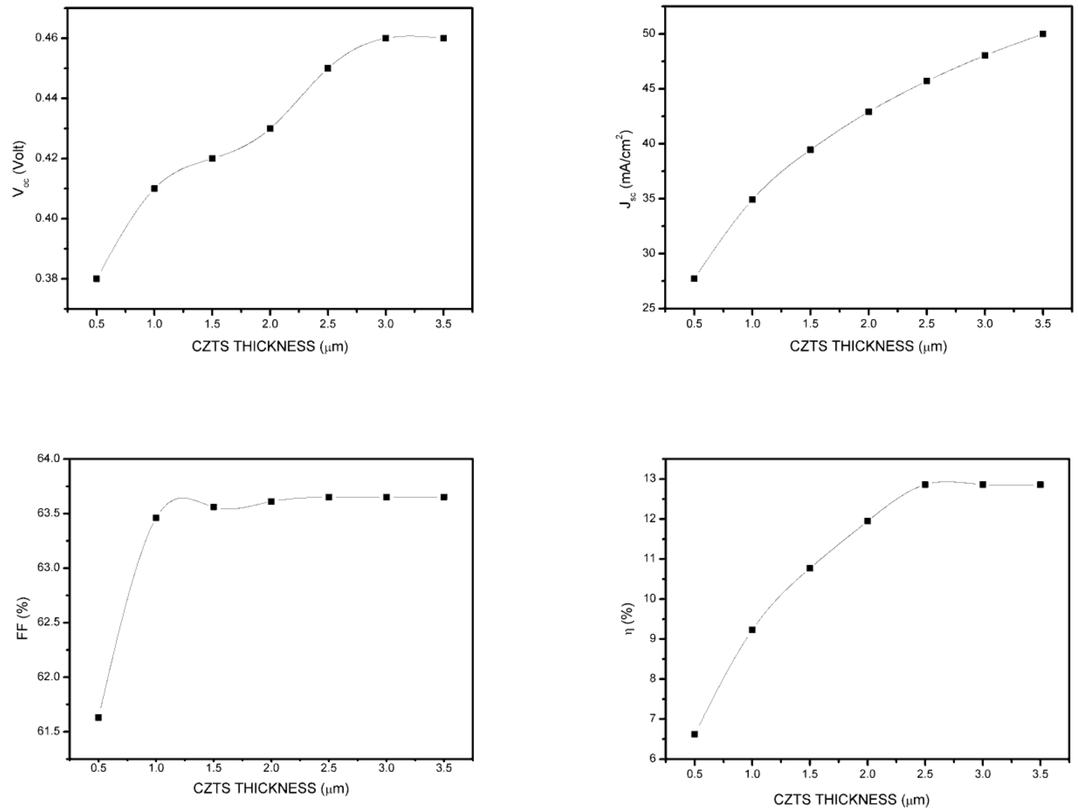

Figure 2 – Effect of CZTS thickness on V_{oc} , J_{sc} , FF and η

4.2 Effect of CZTS Band Gap The band gap of CZTS absorber layer is varied from 1.3 eV to 1.5 eV and analyze the effect of this variation on V_{oc} , J_{sc} , FF and η. This variation is shown in Fig. 3. From the graph we can see that the open circuit voltage increases with increase in thickness of CZTS layer. This is due to the fact that the potential difference between the valence and conduction bands grows as the band gap of any material increases. As a result, voltage also rises. The short circuit current density decreases with increase in band gap. A larger band gap causes the material to absorb less light and produce fewer electron-hole pairs, which lowers the short circuit current. The fill factor increases with increase in band gap because of less short circuit current due to less absorption at higher band gap. Due to the defects present in the absorber layer the efficiency of this cell structure decreases with band gap variation. At 1.45 eV the open circuit voltage, short circuit current, fill factor and efficiency 12.61%. So 1.45 eV is the optimum band gap for absorber layer.

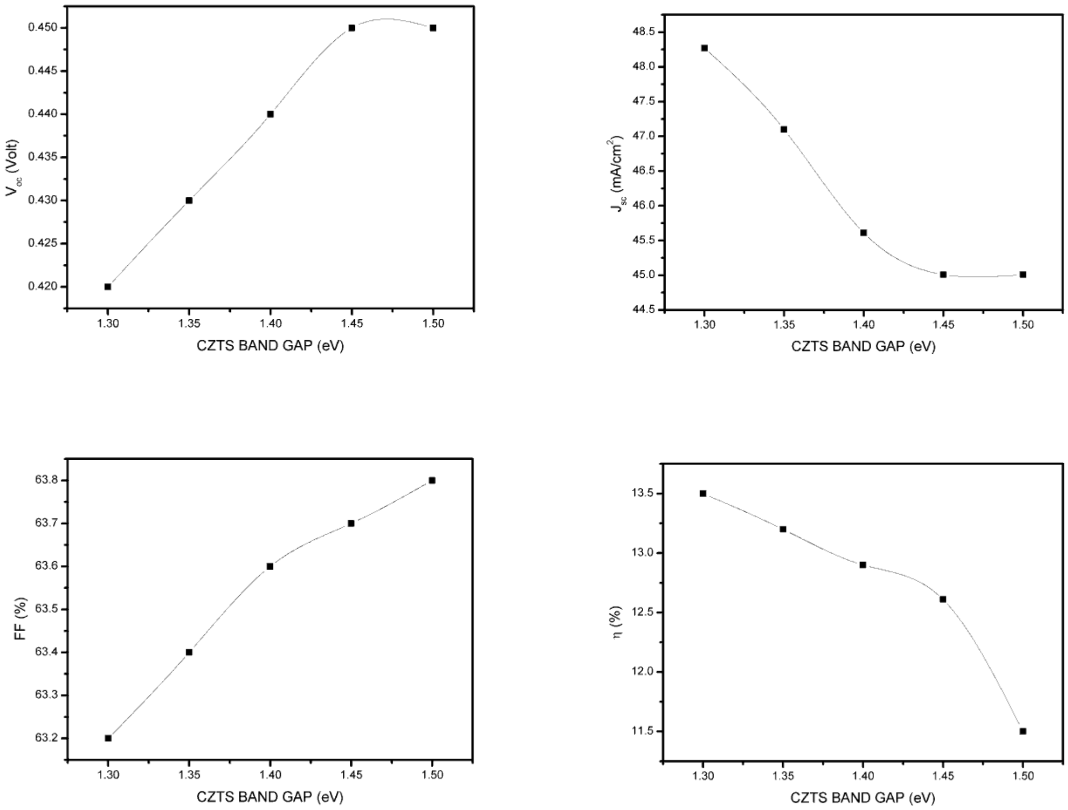

Figure 3 Effect of CZTS Band Gap on V_{oc} , J_{sc} , FF and η

4.3 Effect of Cell Temperature The effect of increasing working temperature on cell parameters is shown in Fig 4. We can see that all the cell parameters decreases with increase in working temperature. Increase in temperature reduces the band gap and increase the recombination of charge carrier due to which the cell parameters decreases. The cell parameters at 300K are 0.45 Volt, 48.3 mA/cm^2, 63.7% and 12.80%. So 300 K is the simulated temperature for the given structure.

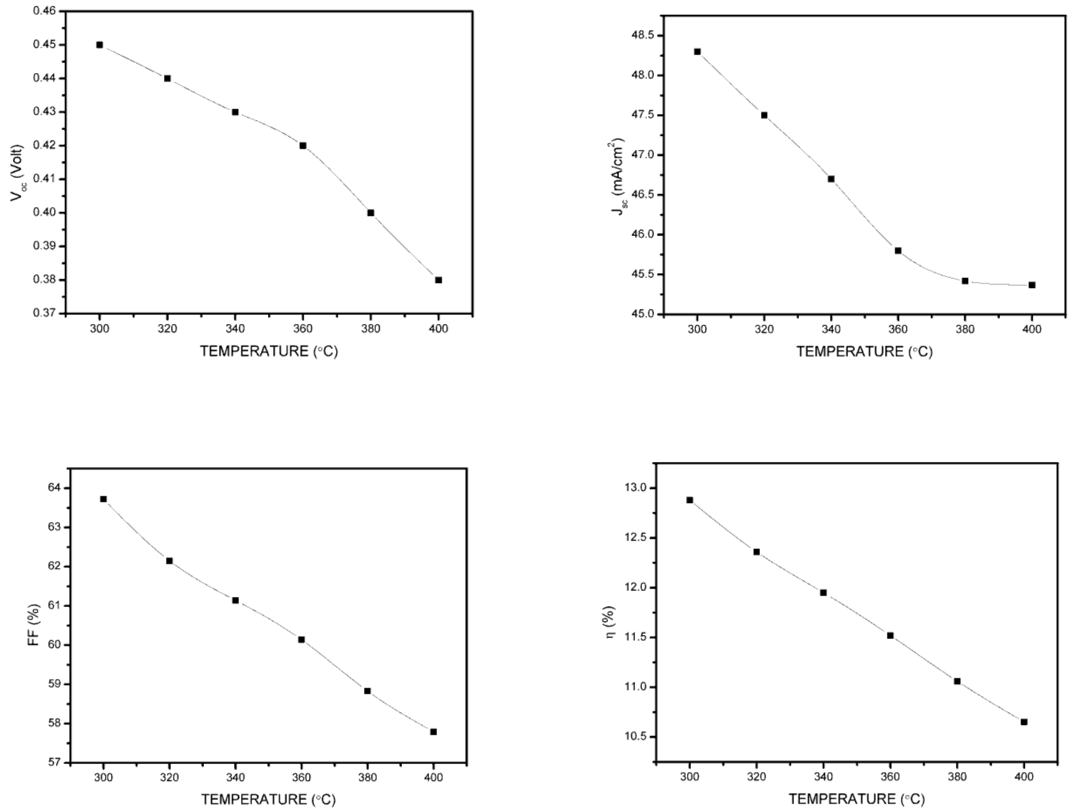

Figure 4- Effect of CZTS cell temperature on V_{oc} , J_{sc} , FF and η

4.4 Effect of Buffer Layer Thickness Simulation was done on the structure shown in Figure 1 to investigate the effect of buffer layer thickness variation on the cell parameters. The thickness of CdS is varied from 50 µm to 200 µm. At 75 µm, the open circuit voltage is 0.45 Volt, the short circuit current density is 48.66 mA/cm^2, fill factor is 63.56% and efficiency is 12.88%. So 75 µm is chosen to be the optimum thickness. A thick CdS buffer layer reduces the number of photons to reach the absorber layer which limits the value of V_{oc} and J_{sc}. A thick layer absorb more photons and reduce carrier transport so the cell performance is degraded with increase in buffer layer thickness and FF and η decreases.. This effect is shown in Fig. 5.

4.5 Effect of acceptor concentration in absorber layer The simulation results for varying acceptor concentration are shown in Fig. 6. The acceptor carrier concentration is increased from $1x10^{15}$ cm^{-3} to $1x10^{18}$ cm^{-3} .With increase in acceptor carrier concentration saturation current increases so V_{oc} also increases. Moreover the recombination process increases and generation process reduces which decreases the J_{sc}. The fill factor and efficiency increases with increases in carrier density in CZTS layer. The highest efficiency of 12.8% is obtained at $1x10^{16}$ cm^{-3} of acceptor concentration.

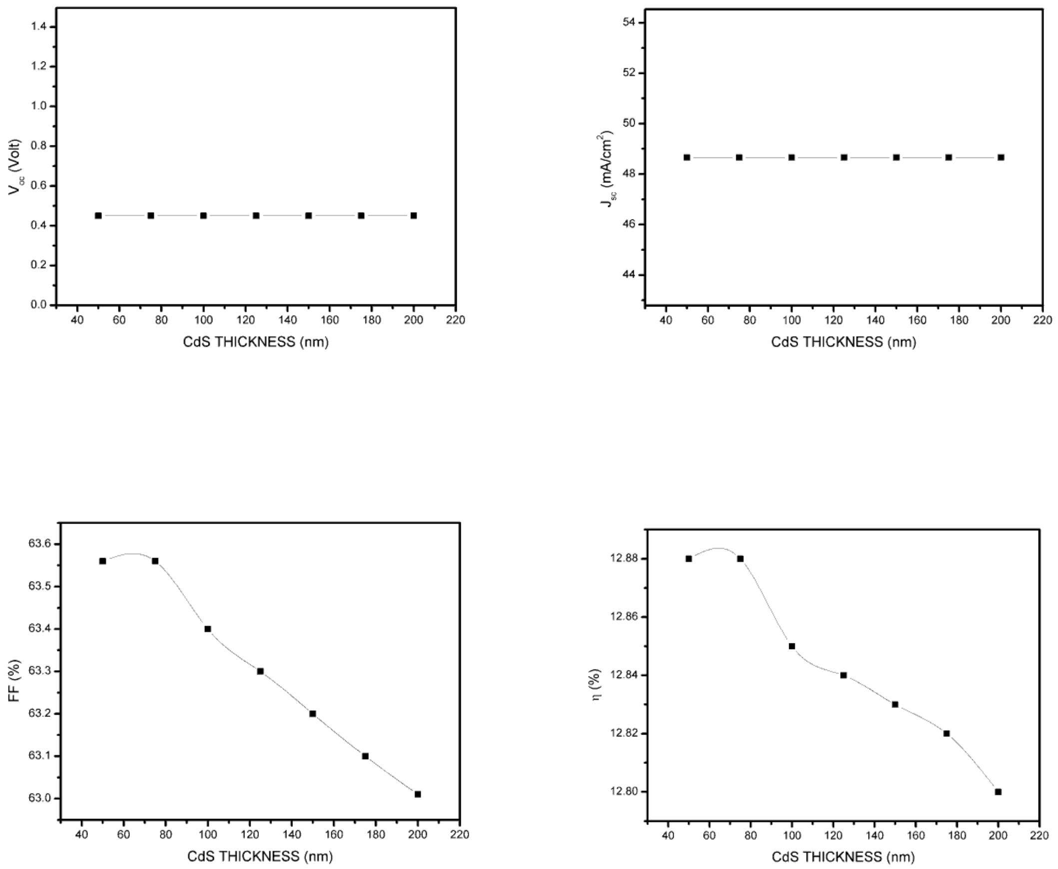

Figure 5 - Effect of CdS buffer layer thickness on V_{oc} , J_{sc} , FF and η

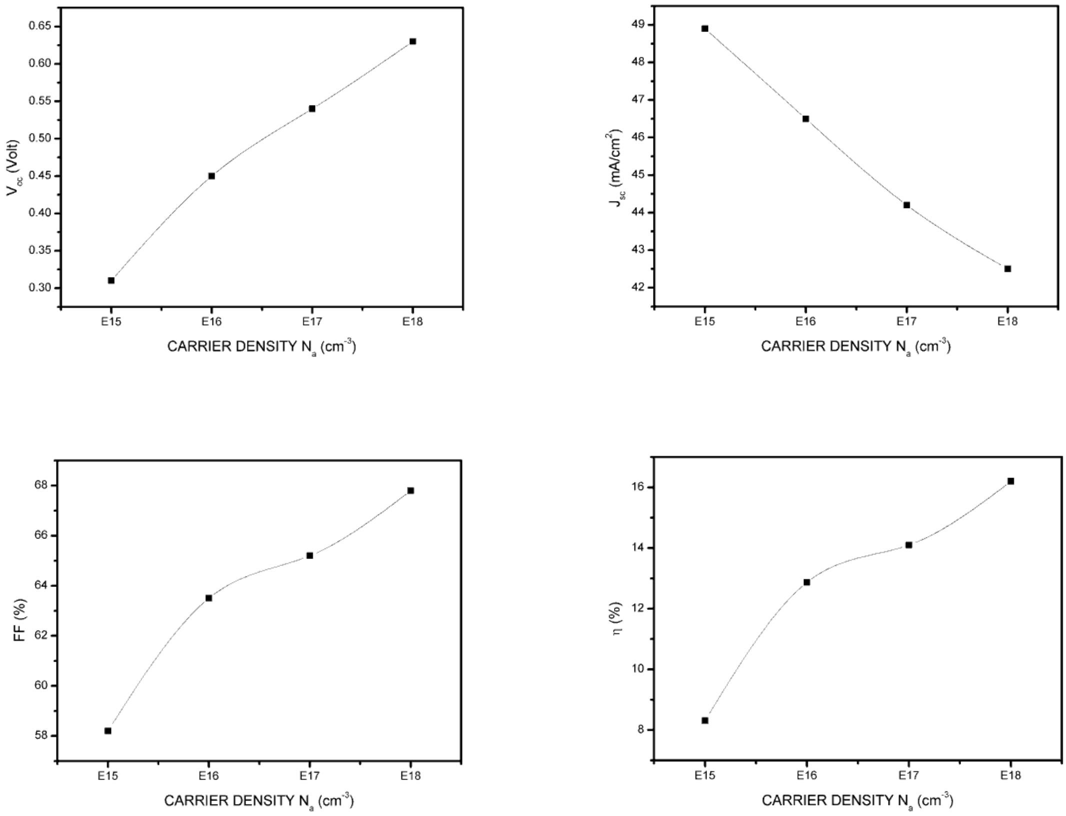

Figure 6 - Effect of acceptor concentration on V_{oc} , J_{sc} , FF and η

4.6 Effect of Donor concentration in buffer layer The variation of donor concentration with all the cell parameters is shown in Fig. 7. In this simulation the donor concentration is varied from $1x10^{15}$ cm^{-3} to $1x10^{18}$ cm^{-3}. The open circuit voltage and short circuit current density remains constant with donor concentration while the fill factor and efficiency first increases and then becomes constant. At donor concentration of $1x10^{18}$ cm^{-3}, the cell parameters are 0.45 eV, 46.6 mA/cm^2 , 46.6% and 12.6%. So it has been found to be the optimum value to donor concentration.

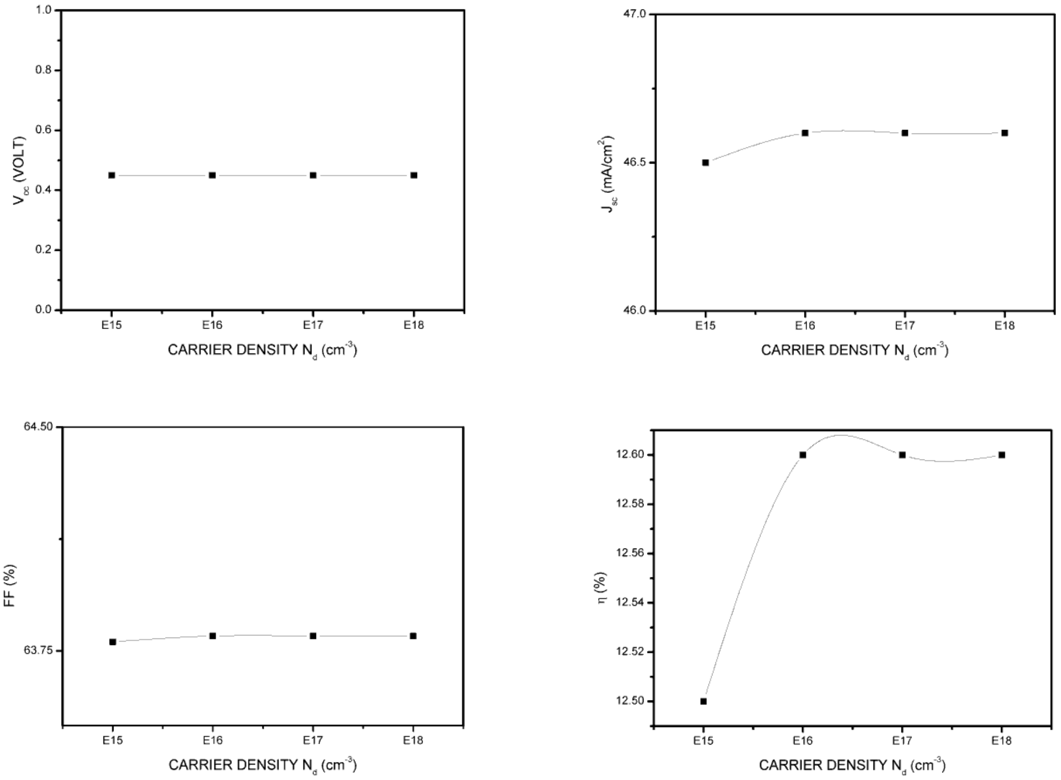

Figure 7 - Effect of donor concentration on V_{oc} , J_{sc} , FF and η

For the optimized material parameters the J-V characterstics are drawn, which are shown in Fig. 8. This graph gives the full insight of cell parameters. Comparisons between simulated and experimental results are summarized in Table 2.

Table 2

Solar Cell Structure	V_{oc}(V)	J_{sc}(mA/cm^2)	FF(%)	η (%)	Method
Mo/CZTS/CdS/ZnO:Al	0.61	17.9	62	6.77	Co-Sputtering
CZTS/CdS/i-ZnO/ZnO:Al	0.45	45.87	63.44	12.9	Simulated

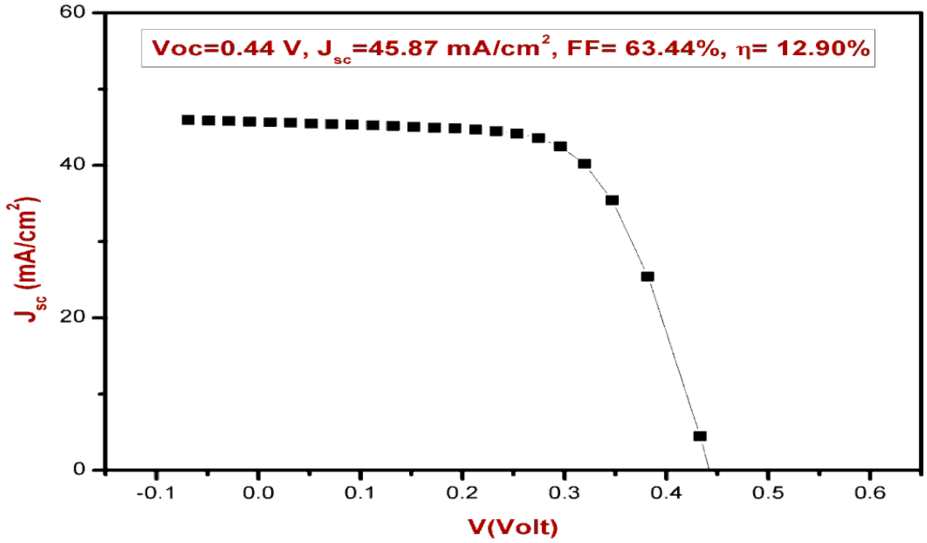

Figure 8 J-V curve for simulated cell structure

5. Conclusion The impact of different properties of CZTS solar cell on the cell performance is explored in this work. The simulation on device structure provided the optimum values of thickness of CZTS absorber and CdS buffer layer, band gap of CZTS layer, the acceptor and donor carrier densities and the working temperature. In this work parameters which affect the efficiency of cell are explained. The maximum efficiency of 12.90% is obtained for CZTS thickness of 2.5 μm, CZTS band gap of 1.45eV, CdS thickness of 75μm, acceptor and donor concentration of $1x10^{16}$ and $1x10^{18}$ cm^{-3}. These simulated results might be very useful for manufacturing of CZTS based solar cell. So we can say that simulated results might play important role to improve the performance of solar cell.

6. Acknowledgement The authors of this article are very thankful to Marc Burgelman, ELIS, University of Gent, Belgium for developing and providing the free access of this SCAPS 1D software.

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