Simulation and Investigation of Cd-free SnS-based Solar Cells with a ZnSe as a Buffer Layer using SCAPS-1D

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Abstract:- Using SCAPS-1D software, a highly efficient SnS thin film solar cell has been explored and simulated in this study. A promising material for thin-film solar cells, Tin Sulfide (SnS) is non-toxic, abundant on Earth, inexpensive, and readily available. The optical characteristics that make up an excellent absorber layer, such as a band gap of roughly 1.6 eV and a high absorption coefficient more than 104 cm-1, etc. This study analyzes how the thickness of the buffer and absorber layers affects the efficiency of solar cells. Due to its significant hazardous impact on the environment, this article aimed to discourage the use of cadmium in the production of solar cells. Numerous photovoltaic parameters have been determined using ZnSe as a buffer layer. Efficiency (η), Fill Factor (FF), Open-circuit Voltage (Voc), Short-circuit current (Jsc), Voltage vs Junction Capacitance characteristics and other parameters have been examined in this work by altering the thickness of the absorber layer between 3 and 8 µm and the thickness of the buffer layer between 0.05 and 0.5 µm. When the absorber layer thickness is 8 µm and the buffer layer thickness is 0.5 µm, the optimized solar cell exhibits an efficiency of 24.24%. This work also looks into the impact of temperature on SnS thin film solar cells. I-V Characteristics Curve of SnS has also been measured in this study.

Keywords:- *SnS, ZnSe, SCAPS-1D, I-V Measurement, C-V Curve, Temperature, Resistance.*

I. INTRODUCTION

To address the main issues of global warming, there is a demand for a sustainable, renewable, affordable, and clean energy in today's globe. Geothermal, solar, biomass, wind energy and mechanical vibrations are examples of renewable energy sources. Among all the ambient renewable energy sources, solar energy has a lot of potential in a variety of uses. Materials play a key role in the creation of highly efficient solar cells. Researchers have discovered a few solar energy materials with excellent light absorption and sufficient physical characteristics to raise solar cell efficiency. A few materials explored for solar cell application is SnS, ZnSe [1], Cu_2O [2], Cu_2SnS_3 [3], Cu_2GeS_3 [4], GeSe [5], Sb2S3[6], Sb_2Se_3 [7] etc. These materials have demonstrated suitable physical qualities for PV cells. Sb_2S_3, Sb_2Se_3 absorber-based solar cells, which have demonstrated comparatively greater PV efficiency of roughly 6.5%, have received substantial interest from the scientific community.

A semiconductor made of Tin and sulfur is known as SnS. These materials are essential for terrestrial applications due to their high efficacy, long-lasting excellent performance, and affordable pricing. These semiconductors are suitable for use as a thin film absorber layer material due to their p-type conductivity, high absorption coefficient, and direct band-gap [8-9]. A thin film solar cell with polycrystalline SnS absorber layers performs better and has higher efficiency when compared to wafer-based crystalline solar cells. Better radiation hardness, robust stability, greatest efficiencies, and excellent film factor are all features of the SnS based solar cells [10-13]. The SnS is a compound semiconductor material which lessens the necessity of extensive minority carrier diffusion length of solar cells. Due to the high absorption coefficient this p type semiconductor material is the most promising materials now a day for thin film photovoltaic technology. In this simulation-based work, a layer called the buffer layer has been used between the absorber layer and the window layer. The window layer has been used in this case for a specific function, namely to stabilize the device's structural integrity and to correct the electrostatic circumstances inside the absorber layer. The well-known compound substance CdS might be employed in solar cells as a buffer layer. But the author used Tin selenide (ZnSe) because of its negative environmental effects.

A thin film of SnS based solar cells has been presented in this work using SCAPS to evaluate photovoltaic parameters such as η, FF, Jsc and Voc at 300K. The impact of absorber layer and buffer layer on the performance of SnS based solar cells has been simulated using SCAPS-1D.

ISSN No:-2456-2165

II. MATHEMATICAL MODELING AND MATERIAL PARAMETERS

A solar cell consisting of p-type absorber layer and n-type buffer layer has been shown in this work. Tin Sulfide (SnS) has been used here as absorber layer and Zinc Selenide (ZnSe) has been used here as buffer layer which is shown in Fig.1. i-ZnO has been used as a window layer in this solar cell configuration. To simulate and analyze the SnS based solar cell, the author used Solar Cell Capacitance Simulator Structures (SCAPS-1D) [14]. SCAPS-1D is a one dimensional solar cell device simulator invented by University of Gent, which is available for the PV research community freely all over the world.

Basic semiconductor equations, the continuity equation and the Poisson equation can be solved by SCAPS easily for electron and holes [15].

$$\frac{d^2}{dx^2}\Psi(x) = \frac{e}{\varepsilon_0\varepsilon_r}(p(x) - n(x) + N_D - N_A + \rho_P - \rho_n) \ldots\ldots\ldots (1)$$

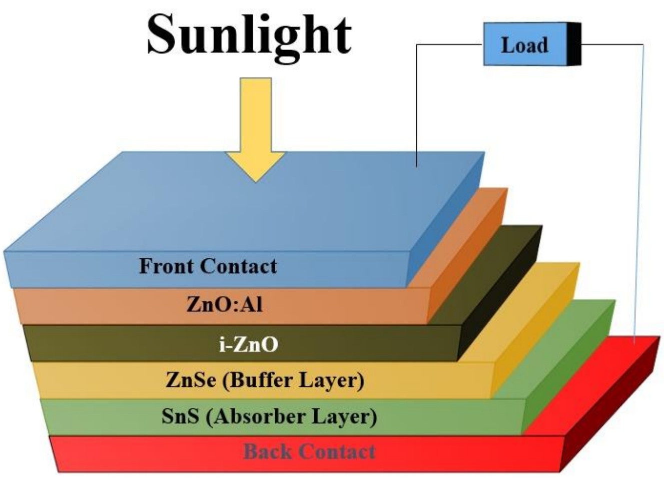


Fig 1:- schematic diagram of SnS based solar cell.

From equation 1 it can easily be said that Ψ is electrostatic potential, e is electrical charge, ε_0 is the vacuum permittivity, ε_r is the relative permittivity, p and n are hole and electron concentrations, N_D is charged impurities of donor and N_A is acceptor type. There are also holes and electrons distribution ρ_P and ρ_n in this equation.

The following equations 2 and 3 are the continuity equations for electrons and holes:

$$\frac{dJ_n}{dx} = G - R \ldots\ldots\ldots (2)$$

$$\frac{dJ_p}{dx} = G - R \ldots\ldots\ldots (3)$$

J_n and J_p represents the electron and hole current densities, R represent the recombination rate and G is the generation rate. Carrier transportation happened by drift and diffusion in the semiconductor and can be expressed in the following equations:

$$J_n = D_n\frac{d_n}{d_x} + \mu_n n\frac{d\varphi}{d_x} \ldots\ldots\ldots (4)$$

$$J_p = D_p\frac{d_p}{d_x} + \mu_p p\frac{d\varphi}{d_x} \ldots\ldots\ldots (5)$$

The solution of the basic equations of semiconductors has been done using SCAPS in 1 dimension and steady state conditions. The parameters used in this SnS based solar cells are given below in table 1.

Parameters	**SnS**	**ZnSe**	**ZnO:Al**	**i-ZnO**
E_g(eV)	1.6	0.08	3.5	3.3
ε_r	13	10	9	9
χ(eV)	4.1	2.9	4.2	4.5
μn($cm^2V^{-1}S^{-1}$)	15	50	10^2	10^2
μp($cm^2V^{-1}S^{-1}$)	100	20	25	25
N_D (cm^{-3})	0	$1.5*10^{18}$	2.2×10^{18}	1×10^{18}
N_A (cm^{-3})	10^{16}-10^{19}	0	1.8×10^{19}	1×10^{17}
V_t(cm/s)	1×10^7	1×10^7	1×10^7	1×10^7
V_t(cm/s)	1×10^7	1×10^7	1×10^7	1×10^7

Table 1:- The parameters for the SnSbased solar cell at 300K

III. RESULT

The main goal of this study is to see how changing parameters of the absorber layer affect the light conversion efficiency of SnS based thin film solar cells. The use of the optimized data will allow us to establish a set of criteria for real-time solar photovoltaic device design with the highest efficiency. This in-depth investigation allowed us to measure the Efficiency (η), Fill Factor (FF), Open-circuit Voltage (Voc) and Short-circuit current (Jsc) in the SnS-based thin film solar cell, allowing the research community to develop more efficient solar cell devices [14]. In this paper SnS/ZnSe/i-ZnO/ZnO:Al thin film solar cell we found the efficiency 24.24% as shown in table 2.

Device Structure	**Open circuit Voltage V_{OC}(V)**	**Current Density J_{SC} (mA/cm^2)**	**Fill Factor FF (%)**	**Efficiency η (%)**
SnS/ZnSe/i-ZnO/ZnO:Al	1.22	24.98	79.93	24.24

Table 2:- Photovoltaic parameters for the SnS based solar cell

ISSN No:-2456-2165

➢ *Effect of absorber layer and buffer layer thickness on efficiency in* SnS *based solar cell*

The analysis of the simulated results shows that best photovoltaic parameters are found by using ZnSe as a buffer layer. To achieve the best performance of the SnS based solar cell, absorber layer and buffer layer thickness of the cell should be optimized. The impact of absorber layer thickness on solar cell parameters such as open circuit voltage (Voc), short circuit current (Isc), fill factor (FF), and efficiency (%) is thoroughly investigated in this work. Simulated characteristics can be seen in Fig. 2 , 3, 4, 5 for absorber layer from 3 µm to 8 µm and buffer layer from 0.05 µm to .5 µm. The increase of efficiency with increasing thickness represents the increase in the generation of the electron hole pairs in the absorber layer. The efficiency gradually improves as recombination lowers and the extraction rate of electron and hole pairs increases. The rise in optical density is the fundamental cause for the increase in efficiency with increasing thickness. [17].

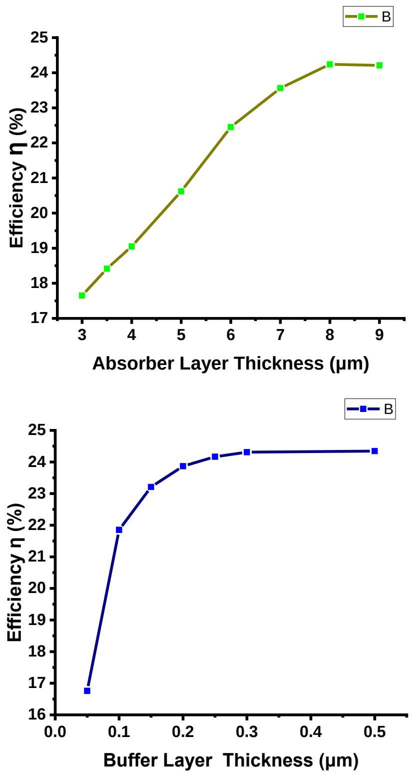


Fig 2:- Effect of absorber layer and buffer layer thickness on Efficiency

This paper attempted to take values of different parameters by changing the values of thickness of absorber layer in the range from 3 µm to 8 µm. In this paper found efficiency 22.24% when the absorber layer thickness is 8µm shown in Fig. 2. and buffer layer thickness is 0.08µm which is shown in Fig. 2. Fig. 2. Indicates that, as the thickness of the buffer layer is increased, the efficiency begins to rise. This is because a thinner buffer layer collects the majority of the produced carriers. Short-wavelength photons are absorbed at a greater distance between the window and the absorber junction as the thickness increases [18]. According to the simulation results, if the absorber layer is too thin, it will not be able to absorb all of the incoming light, resulting in low efficiency. Similarly, when the thickness is greater than the optimum value, the photo produced carrier's travel path is too long, resulting in higher recombination of the generated carrier. When the absorber layer thickness is increased, the carrier recombination rate increases in comparison to the carrier generation rate, resulting in a constant efficiency.

➢ *Effect of absorber layer and buffer thickness on Fill Factor in* SnS based solar cell

As shown in Fig. 3. The fill factor for SnSsolar cells improves as the thickness of the absorber layer increases, while it remains constant at thicknesses above 4µm. When the absorber layer thickness is increased, the internal resistance rises. As resistance rises, depletion rises as well so the fill factor leads to constant. In SnS based solar cells, the use of a ZnSe as buffer layer is required for a reliable and effective hetero-junction. In Fig. 3 the effect of buffer layer thickness on fill factor has been shown. It can be seen that maximum fill factor has been found when the buffer layer thickness is 0.5 µm. After 0.5µm fill factor tends to constant.

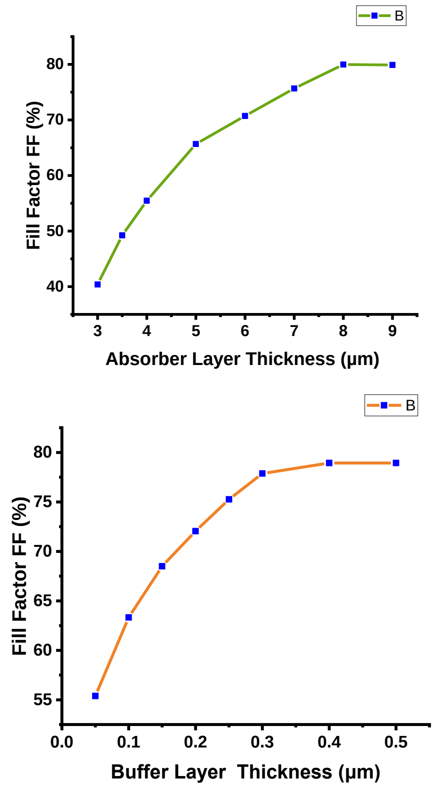


Fig 3:- Effect of absorber layer and buffer layer thickness on Fill Factor

➢ *The Effects of absorber layer and buffer thickness on Current Density in SnS based solar cell*

The carrier recombination rate increases as the absorber layer thickness grows in comparison to the carrier generation rate, as shown in Fig.4 The current increases from 3 µm to 8 µm thickness of absorber layer, however the current tends to saturate after 8 µm thickness of absorber layer. The current density start to increase with the increase in SnS thickness because the thicker SnS layer will absorb more photons and generates more electron–hole pairs [19].The effect of buffer layer thickness on current density has been shown in Fig.4. Maximum current density 24.98 mA/cm^2 has been found when the buffer layer thickness is 0.5 µm. But the current density is 23.5 mA/cm^2 when the buffer layer thickness is 0.5 µm. The decrease in current density results due to the less production of electron–hole pair as less number of electron–hole pair can reach the absorber layer with increase in buffer layer thickness [20].

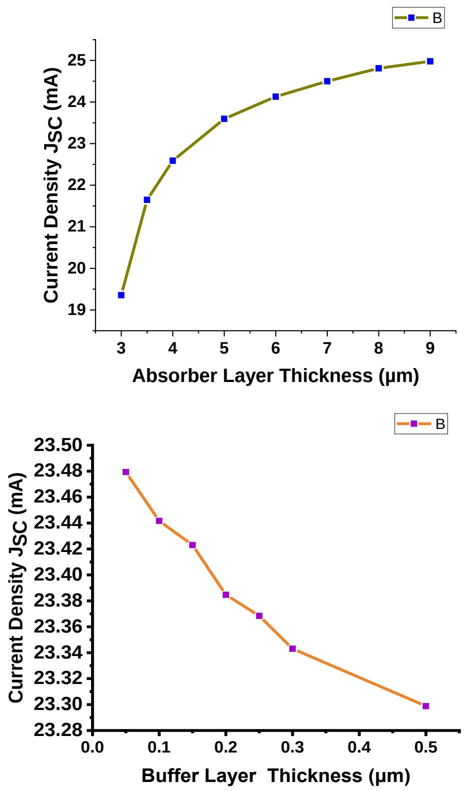
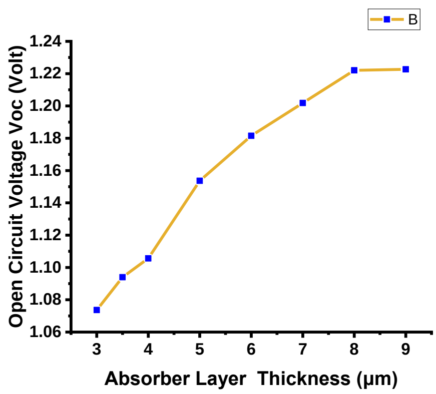


Fig 4:- Effect of absorber layer and buffer layer thickness on current density

- *Effect of absorber layer and buffer thickness on Open Circuit Voltage in SnS based solar cell*

As shown in Fig.5. The change in Voc increases as the absorber layer thickness increases due to the effective enhancement of holes mobility. In Fig.5. the effect of buffer layer thickness on open circuit voltage has been shown. Fig.5 shows that open circuit voltage starts increasing with the increase in buffer layer thickness.



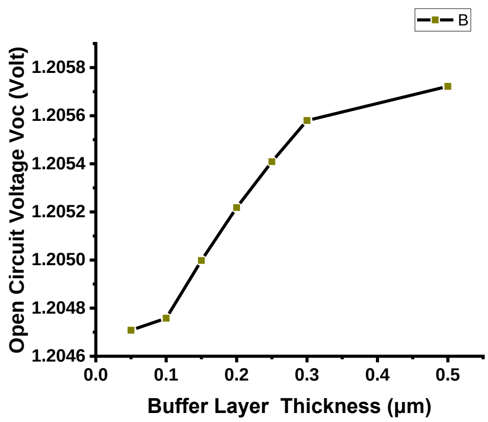


Fig 5:- Effect of absorber layer and buffer layer thickness on open circuit voltage

- *I-V Characteristics Curves of SnS based solar cell*

Fig.6 depicts the simulated I-V characteristics of a solar cell based on SnS. The four photovoltaic parameters of a SnS based solar cell I_{sc}, V_{oc}, η and FF has been found from this I-V characteristics curve.

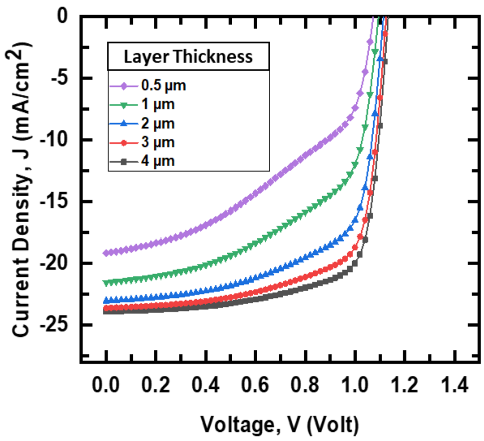


Fig 6:- I-V Characteristics Curve of SnS based solar cell.

According to the diagram, solar cells containing ZnSe as a buffer layer have high conversion efficiency. The maximum efficiency obtained is 24.24% for *SnS* thin film solar cell.

- *Voltage and Junction Capacitance Characteristics Curves of SnS based solar cell*

An ideal Schottky diode's capacity increases with the bias voltage and is frequency independent. The relationship between capacitance C and polarization voltage V to the Schottky diode is shown in Fig.7. for several types of solar cell architectures where there is a jump capacity after V = 0.7 V, with shift curves to higher order capacities containing the superior performance structures.

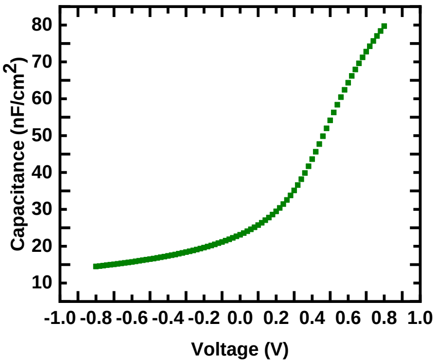


Fig 7:- Voltage vs Junction Capacitance Characteristics Curve of SnS based solar cell.

- ➢ *Effect of temperature on photovoltaic parameters of SnS based solar cell*

As shown in Fig.8, the influence of operation temperature on the photovoltaic performance of the proposed Cd-free SnS based Solar Cell is explored when the buffer layer thickness is 0.5 µm with an absorber layer thickness of 8 µm. To achieve the stability of the Cd-free SnS-based Solar Cell, the working temperature has been changed from 250K to 450K. With an increase in operating temperature, Voc dropped dramatically from 1.25V to 0.82V. It is observed in Fig.8 that, Jsc barely increased as the temperature rise. The fill factor increased from 69.5% to 76% with the increase in temperature 250K to 425K but at 450K fill factor tries to decrease. Efficiencies of 24.24% at temperature 250K have been fallen to 15.05% at temperature 450K which is shown in Fig.8. The performance of a solar cell device is also influenced by temperature. A solar cell device's testing temperature is usually 300°K, however the working temperature is higher than 300°K in real-world situations [23]. The temperature of the simulated model was adjusted from 300K to 450K to understand the influence of temperature on the electrical performance of a solar cell. Figure 9 depicts the changes in the features. The temperature is dropping, with a reduction of 5.42 percent. Increasing temperature may lead to the more stress and deformation resulting in increased interconnectivity between the layers. As the diffusion length decreases, the series resistance rises, lowering the fill factor and efficiency [23]. The simulated model's optimum temperature is adjusted to 300K to ensure high efficiency. The model's maximum possible efficiency is 30.35 percent at this temperature, with a fill factor of 74.94 percent, Jsc= 59.78 mA/cm2, and Voc=0.6774 V.

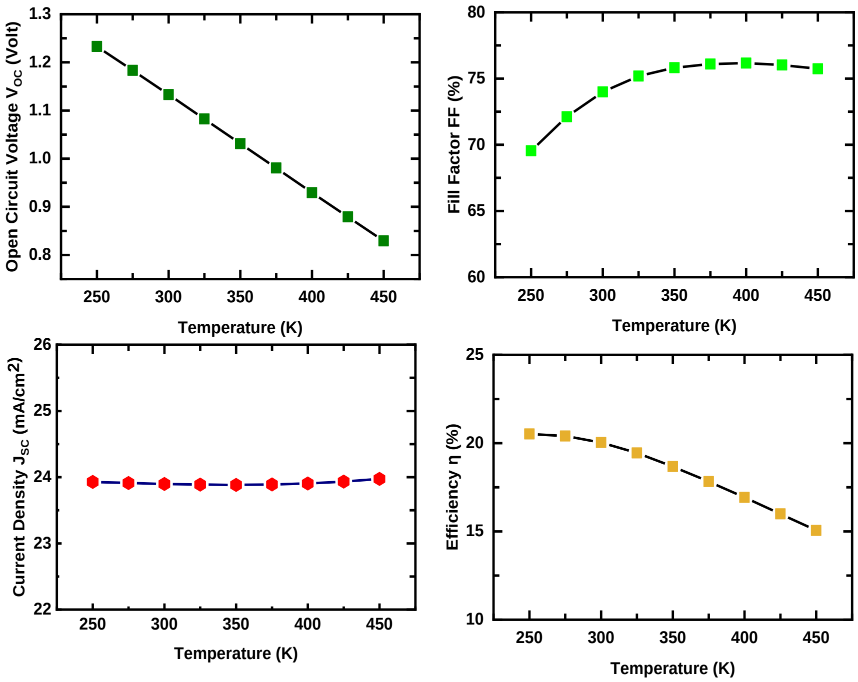


Fig 8:- Effect of temperature on photovoltaic parameter

IV. CONCLUSION

The performance of SnS based solar cell has been investigated in this research work using SCAPS-1D. The thickness of the absorber in relation to the buffer layer has a significant impact on the efficiency and other photovoltaic parameters of the solar cell, according to the findings. The effect of variation in concentration of defect density has been investigated in this paper. In this simulation based work the Efficiency (η), Fill Factor (FF), Open-circuit Voltage (Voc) and Short-circuit current (Jsc) have been investigated and found maximum efficiency of greater than 24.24% when the absorber layer thickness is 8µm and buffer layer thickness is 0.5µm. The researchers will be able to enhance better efficiency of SnS based solar cell which is based on a simulation analysis and optimized parameters.

ACKNOWLEDGEMENTS

We thankfully acknowledge to Dr. Marc Burgelman of the University of Gent in Belgium who has generously provided the SCAPS simulation program.

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