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Development and Simulation of Cd-free Sb_2Se_3-based Solar Cells with ZnS Buffer Layers

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Abstract:- This paper explores the development and simulation of cadmium-free solar cells based on Antimony tri-selenium (Sb2Se3) absorber materials, with the integration of zinc sulfide (ZnS) buffer layers. The aim is to replace cadmium-based materials with environmentally friendly alternatives while maintaining or improving the efficiency of thin-film solar cells. We utilize the SCAPS-1D (Solar Cell Capacitance Simulator) software to model and simulate the electrical and optical characteristics of the proposed solar cell structure. This work used SCAPS-1D software to construct and quantitatively analyze solar cells made of high-efficiency Antimony tri-selenium (Sb_2Se_3) and Zinc sulfide (ZnS). This study examines how the thickness of the absorber surface and the buffering layer affects the efficiency of solar cells. Cadmium has been avoided because of its significant toxicity to the environment, for making solar cells which is suitable and efficient. Various photovoltaic parameters have been determined using ZnS as a buffer layer. By varying the depth of the absorber layer from 0.6µm to 0.5µm and the thickness of the buffer layer from 0.06 µm to 0.2 µm author tried to investigate the properties of solar cell. At the time of 5µm thickness of absorber surface and 0.08 µm of buffer surface the optimized efficiency of 22% of solar cell has been found.

Keywords:- *SCAPS-1D, Sb_2Se_3 Solar Cell, ZnS, Absorber Layer, Buffer Layer.*

I. INTRODUCTION

Materials are critical in the production of high-efficiency solar cells. Antimony tri-selenium (Sb_2Se_3) is an antimony and selenium semiconductor material. These materials are critical for terrestrial applications due to their high efficiency, long-term performance, and low cost. Many materials for thin film solar cells, such as CZTS [1], CTS [2], CIGS [3], SnS [4], and Sb_2S_3 [5], have been proposed and investigated as alternatives. Due to the electrical conductivity p-type materials, significant absorbing capacity, and uniform band-gap, these kinds of semiconductors are ideal for usage as thin film absorber material substances [6-7]. In comparison to Crystalline semiconductor wafers Sb_2Se_3 thin film solar cells, the absorber layers' function better and are more efficient. Antimony tri-selenium-based solar cells have higher radiation hardness, higher stability, higher efficiencies (22.04%), and a higher film factor (75.78%) [8-11]. The chemical compound having the formula Sb2Se3 is known as antimony tri selenide. Antimonselite, a sulfosalt mineral that crystallizes in an orthorhombic space group, is the only known form of the substance that reduces the need for long minority carrier diffusion lengths in solar cells. One of the most promising materials for thin film solar technology today is this p type semiconductor substance due to its significant absorbency rate. Between the layer that acts as an absorber and the entrance layer during this simulation-based technique, there was a layer that served as an intermediate termed the buffer surface. The window layer was utilized for a genuine purpose, which is to offer the appliance's structural integrity as well as to stabilize the electrostatic conditions inside the absorber layer. CdS, a well-known mixed component, which may be used as a buffer layer in solar cells. However, because of its negative environmental effect, the authors have chosen Zinc sulfide (ZnS). This paper presents a thin film of antimony tri-selenium-based solar cells that were evaluated using SCAPS at 300k temperature for PV parameters. SCAPS-1D was used to simulate the effect of the buffer layer on the performance of Sb2Se3 solar cells. Using ZnS as a buffer layer, the Current-Voltage (I-V) characteristic was estimated for improved performance and efficiency.

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II. THE MATERIAL VARIABLES AND COMPUTATIONAL MODELING

Figure 1 shows a substance called Antimony tri-sulfide (Sb_2Se_3)-based solar cell with a p-type Sb_2Se_3 absorber layer and an n-type ZnS buffer layer. In this solar cell arrangement, the opening surface, i-ZnO was employed. The Sb_2Se_3-based solar cell was simulated and analyzed using SCAPS-1D [12]. A single-dimensional solar cell unit simulator called SCAPS was created at the University of Gent and made available to the world's PV research community. SCAPS has the capability of rapidly resolving fundamental silicon equations such as the equation for continuity and the Poisson equation for electrons and holes [13].

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

Ψ is electrostatic potential from equation 1 it can easily be said that, 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 continuity equations for electrons and holes are given by equations 2 and 3:

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

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

Jn and Jp 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:

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

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

SCAPS was used in only a single dimension under constant-state situations to solve the fundamental mathematical problems of electronics.

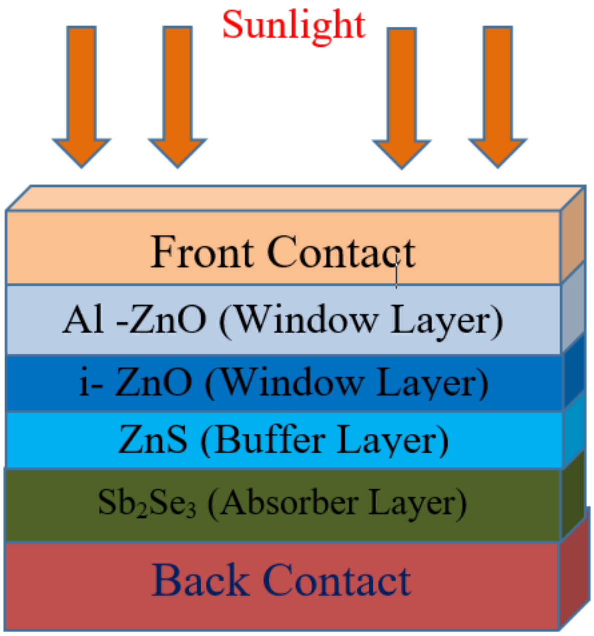

FIG.1 SCHEMATIC DIAGRAM OF SNSBASED SOLAR CELL.

Table 1 below lists the variables employed in these Sb_2Se_3-based solar cells.

Table 1. The Sb_2Se_3-based solar cell's properties at 300K temps.

Parameters	**Sb_2Se_3**	**ZnS**	**i-ZnO**	**ZnO:Al**
Bandgap	1.62	0.08	3.3	3.5
Relative dielectric constant	7.08	10	9	9
Exciton binding energy	3.7	2.9	4.5	4.2
$\mu n(cm^2V^{-1}S^{-1})$	9.8	50	10^2	10^2
$\mu p(cm^2V^{-1}S^{-1})$	10	20	25	25
$N_D\ (cm^{-3})$	0	$1.5*10^{18}$	$1*10^{18}$	$2.2*10^{18}$
$N_A\ (cm^{-3})$	$5.7*10^{15}$	0	$1*10^{17}$	$1.8*10^{19}$
$V_t(cm/s)$	$1*10^7$	$1*10^7$	$1*10^7$	$1*10^7$
$V_t(cm/s)$	$1*10^7$	$1*10^7$	$1*10^7$	$1*10^7$

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III. RESULT

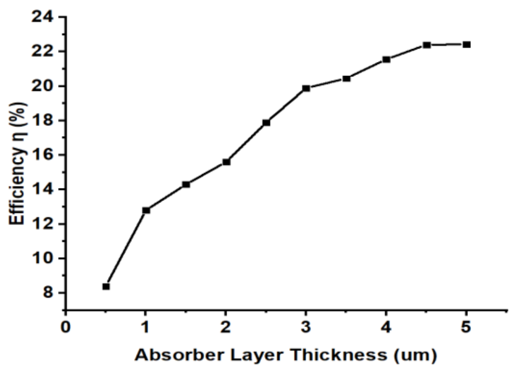
The main goal of this simulation based work is to determine how characteristics are affected by the light conversion efficiency of Sb2Se3-based thin film solar cells changing absorbing surface. As a consequence of this thorough investigation, we were able to assess the PV characteristics in the Sb2Se3-based thin film solar cell, enabling the research community to create more effective solar cell devices [14]. The photovoltaic characteristics for the Sb2Se3-based solar cell are shown in Table 2.

Table 2: PV parameters for the Sb_2Se_3 based solar cell

Device Structure	Voltage in open circuit V_{OC} (V)	J_{SC} for Current Density (mA/cm^2)	Factor of Fill FF (%)	Efficiency η (%)
ZnO:Al/i-ZnO/ZnS/Sb_2Se_3	1.43	25.89	75.78	22.03

- *Effect of thickness of different layers on Sb2Se3 based device*

The absorber surface's depth and buffer surface depth is critical in calculating the performance of a solar cell. The influence of absorber surface depth on PV cell characteristics is thoroughly investigated in this research. It is possible to see modeled qualities in Fig.2 (a, b), 3(a, b), 4(a, b), 5(a, b) for .09 µm as a buffer layer. Table 2 shows various photovoltaic characteristics such as JSC, V_{OC}, FF, and for the Sb_2Se_3-based solar cell with various buffer layers.



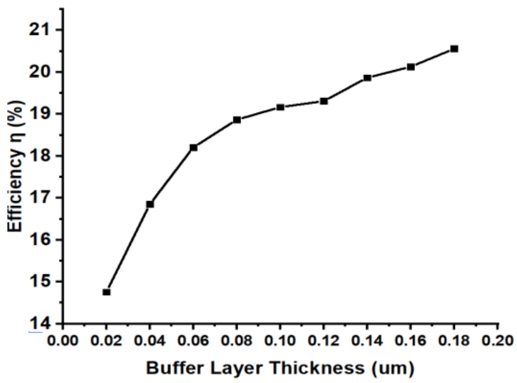
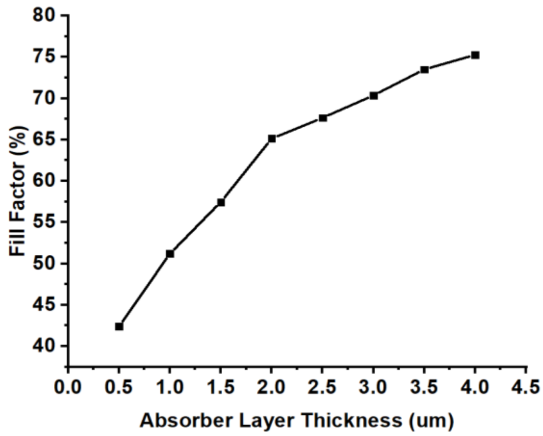


Fig.2. Effect (a) absorption layer thickness on efficiency (b) buffer layer thickness on efficiency.

- *The Impact of the Solar Cell's FF on the Absorber Surface and Buffer Depth*

As seen in Figure 3(a). The FF for Sb_2Se_3 solar cells increases with absorber layer depth, but stays stable above 4m. Internal resistance increases as the absorber layer depth grows. As resistance goes up, depletion increases, causing the fill factor to remain constant. A ZnS buffer layer is necessary for a stable efficient heterojunction in Sb^2Se^3-based solar cells. It is shown how buffer surface depth affects fill factor in Fig. 3(b). Optimized value is found for FF at the time of 0.09 µm depth for buffer surface. The FF tries to be stable after 0.09 µm.



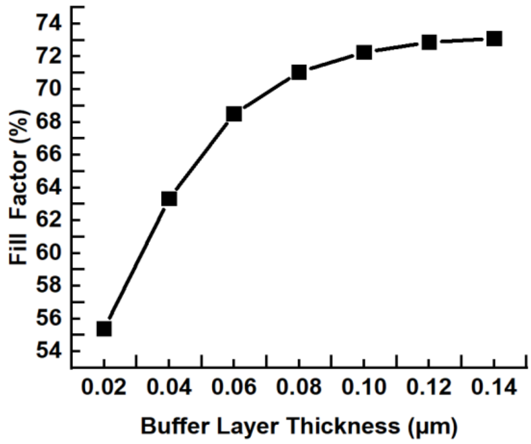


Fig.3. (a) A's thickness of the absorber layer's impact on FF and (b) buffer layer thickness on fill factor

- *The Effect of thickness of different layers on current density in Sb_2Se_3 based solar cell*

As demonstrated in Fig.4 (a), the carrier integration rate goes up when the depth of absorbing layer increases in contrast to the carrier creation rate. The current grows from 0.5 µm to 4 µm depth of absorber layer, but after 4 µm depth of absorber layer, the current begins to saturate. Figure 4 (b) depicts the influence of buffer layer depth on current density. Current density at its peak 25.89 mA/cm2 has been found when the buffer layer thickness is 0.04 µm. But the current density is 25.89 mA/cm2 when the buffer layer thickness is 0.16µm.

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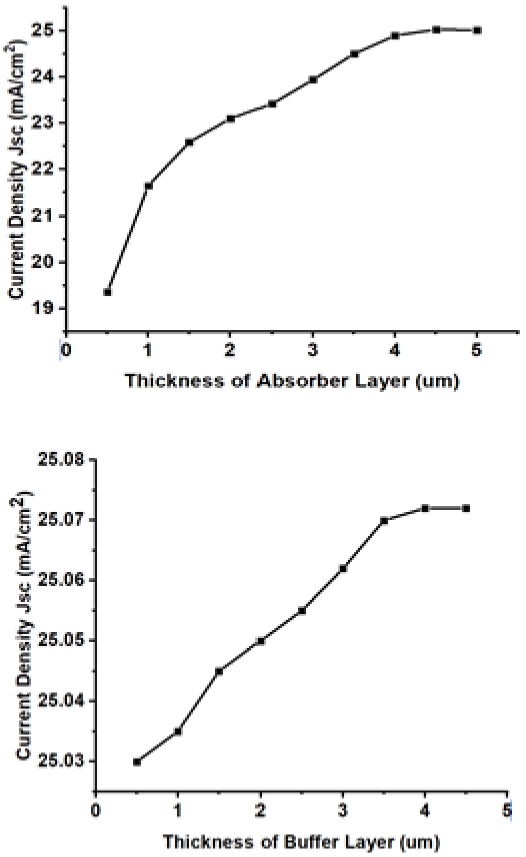

Fig.4. Current density is impacted by (a) the thickness of the absorber layer and (b) buffer surface depth on current density.

The paper's author attempted to obtain values for various parameters by varying the depth of the absorbing surface in a variety of 0.6 µm to 5 µm. The author got optimum efficiency of greater than 22% if the absorber layer is 4 µm thick, as indicated in Fig. 2(a) Furthermore, the buffer layer has a 0.08 µm thickness, as indicated in Fig. 2(b). The results of the simulation show that if the layer covering the absorber is too thin, it won't be able to completely soak up the light that comes in, leading to poor efficiency. The photo produced carrier's journey route is excessively lengthy when the thickness is larger than the ideal value, leading to more recombination of the generated carrier. The efficiency remains constant as the depth of the absorber sheet grows because the carrier recombination rate rises relative to the carrier production rate.

- *The Effect of absorber layer and buffer thickness on Open Circuit Voltage in Sb2Se3 based solar cell*

As shown in Fig. 5 (a), the effective amplification of holes' mobility causes the change in Voc to grow as the absorber layer thickness increases. The impact of buffer layer thickness on open circuit voltage is seen in Fig. 5(b). Open circuit voltage begins to rise with an increase in buffer layer thickness, as seen in Fig. 5(b).

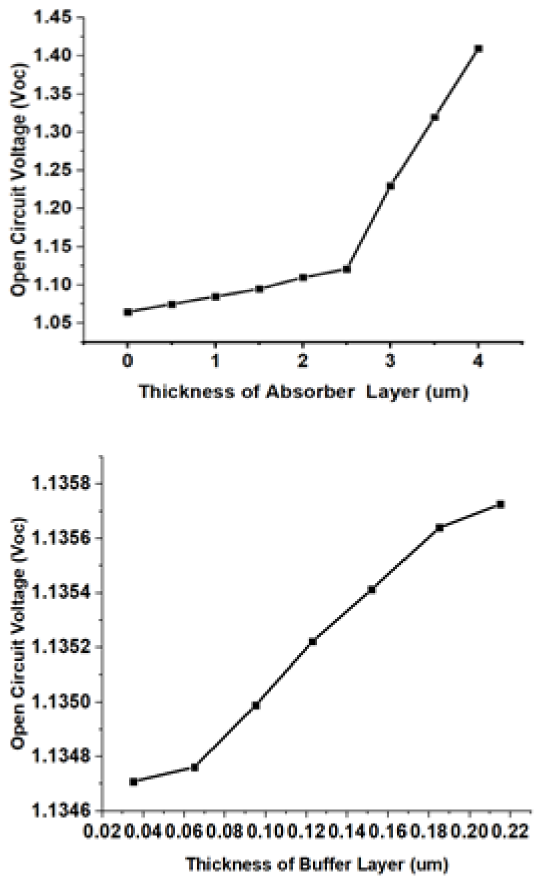

Fig.4. Effect of (a) absorber layer thickness on open circuit voltage and (b) buffer layer thickness on open circuit voltage.

- *The Effect of different layer depth on Jsc in Sb_2Se_3 based solar cell*

Because of the successful enhancement of holes' transportation, as illustrated in Fig. 5(a), the variation in Voc rises as the absorbing surface depth rises. Figure 5(b) illustrates how buffer layer depth affects Voc voltage. According to Fig. 5(b), Voc begins to rise as buffered layer depth rises.

- *Voltage- Current Performance Curve for Sb_2Se_3-based Solar Cell*

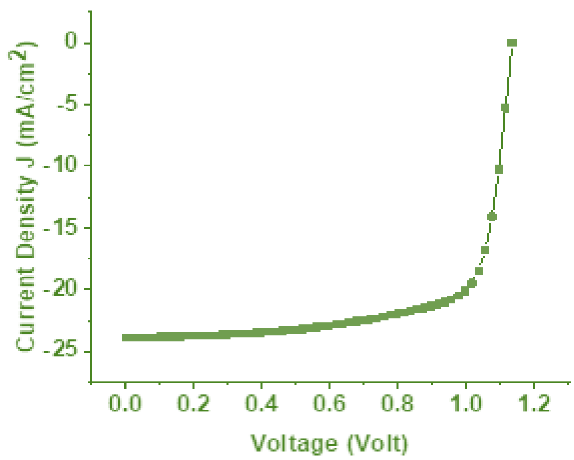

Fig 5: Sb_2Se_3-based solar cell's features of the I-V graph.

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Figure 5 displays the I-V simulations of features of a Sb_2S_3-based solar cell. This I-V characteristics graph yielded the four PV parameters of a Sb_2Se_3-based solar cell, Isc, Voc, and FF. Solar cells with ZnS as a buffer layer have a high conversion efficiency, according to the diagram. For Sb_2S_3, the maximum efficiency obtained is 22.03%.

IV. CONCLUSION

This thesis work used SCAPS-1D to investigate the performance of Sb_2Se_3-based solar cells. Compound materials such as Zinc Sulphide (ZnS) can substitute the typical buffer layer CdS. Because of its superior performance and availability, zinc sulphide (ZnS) has been chosen as an alternative to CdS in this study. The third-generation solar cell is tuned for numerous controllable parameters that affect performance, such as thickness, recombination, defect and acceptor density, and work function of back contact, within empirically acceptable ranges. According to study findings, the solar cell's efficiency and other photovoltaic characteristics are significantly influenced by the depth of the absorber in relation to the buffer layer. This thesis investigated the impact of changing the thickness of the buffer and absorber layers. The short-circuit current (Jsc), open-circuit voltage (Voc), fill factor (FF), efficiency (η), and were explored in this simulation-based work, and an optimal efficiency that is more than 22% was discovered when the layer of absorbent width is 4m and the buffer layer depth is 0.09 µm. Through this study, investigators will be able to create higher efficiency Sb_2Se_3-based earth abundant, non-toxic third generation solar cells based on simulation analysis and adjusted parameters.

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