Optimization of electrical and optical properties of tin sulfide for thin film photovoltaics using SCAPS

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Abstract. Tin sulfide (SnS), being a binary metal chalcogenide, can be a potential absorber material for the thin film photovoltaics because of its optimum direct bandgap (1.3 eV) and high absorption coefficient (>10⁴ cm⁻¹). In the present work, the electrical and optical properties of SnS thin film solar cells have been optimized and analyzed by Solar Cell Capacitance Simulator (SCAPS). The effect of thickness and optical band gap of SnS absorber layer on the J-V curve have been investigated to obtain better device performance. The maximum photovoltaic (PV) efficiency achieved by the PV device is 22.3 % with VOC = 756 mV, JSC = 34.9 mAcm⁻² and FF = 84.4 %. The VOC value is higher than the reported values for kesterite CZTSSe absorber based solar cells. Consequently, the SnS can be a potential contender for the contemporary thin film solar cells.

1. Introduction
Solar energy is considered as a clean and efficient source of renewable energy source. Harvesting solar energy by photovoltaic effect (conversion of light energy to the electrical energy) has the potential to counter global warming, a worldwide, concern. In order to harness solar energy, PV materials have been explored since six decades. In the exploration, many materials such as Si, CIGSSe, CdTe, CZTSSe, Perovskites etc. have been emerged as potential absorbers for solar cells. Presently, PV market is dominated by Si solar cells [1]. These solar cells are still far away from household purposes due to the high processing cost of Si wafers. CIGSSe and CdTe solar cells have shown better efficiency in the thin film solar cell category [2,3]. Due to scarcity of indium (In) in CIGSSe and toxicity of cadmium (Cd) in CdTe have limited the widespread use of these solar cells. CZTSSe based chalcogenide has been adopted as an alternative to CIGSSe solar cells. CZTSSe absorber based solar cells have been saturated to the maximum efficiency of 12.4% [4] due to the presence of stable secondary phases and cation disordering in CZTSSe. Perovskite (a hybrid organic and inorganic compound) solar cells, classified as emerging photovoltaics, have shown a substantial increase of PV efficiency up to 22% in a decade. The stability of PV efficiency over a long period is a major concern in the perovskite solar cells [5].

In recent years, tin-sulphide has emerged as a potential binary absorber material for heterojunction solar cells [6–9]. Tin sulfide is one of the favorable material because of earth-abundant and nontoxic constituents which is an advantage to a cost-effective and eco-friendly thin film solar cells. Moreover, due to the binary SnS compound, unlike CZTSSe the possibility of formation of secondary phases can be avoided. The characteristic properties of SnS are p-type conductivity, optical band gap 1.3 eV, absorption coefficient ~10⁴ cm⁻¹ which makes it a suitable absorber material for thin film solar cells. Several attempts have been made to fabricate SnS absorber based heterojunction thin film solar cells.
The maximum PV efficiency achieved till date is below 5% which is far below the Shockley–Queisser detailed balance limit for a single p-n junction solar cells [15]. The efficiency can be improved by modifying device structure from hetero- to homo-junction SnS solar cells. SnS is an intrinsically p-type semiconductor due to the tin vacancy. There are few reports available on the synthesis of n-type [16–18]. Replacing the buffer layer by n-SnS can serve a better approach to obtain high-efficiency solar cells.

In the current article, device modelling is carried out on the SnS homo-junction based thin film solar cell. Device modelling provides a deeper understanding of the transport of charge carriers in thin film solar cells. In the modelling, basic transport equations (continuity equation and Poisson’s equation) are solved numerically. There have been many device modelling programs developed such as SCAPS [19], AMPS [20], PC-1D [21] etc. In the present work, device modelling is carried out using SCAPS-3.3.05 simulation program. SCAPS (Solar cell CAPacitance Simulator) is a 1D solar cell simulation program developed by Marc Burgelman et. al.[19]. The current-voltage (J-V) characteristics of SnS solar cell has been analyzed by varying thickness and bandgap of SnS.

2. Device modelling

The device modelling is carried out on Mo/p-SnS/n-SnS/WL thin film solar cells (shown in Fig. 1) using 1D-SCAPS program. WL is the window layer and its properties are proposed in Table 1. The device is simulated in the substrate configuration where the light falls on the substrate after passing through all the layers. The properties of the layers used as parameters for modelling the device are given in Table 1. The device is illuminated by AM1.5 G light with intensity of 100 mWcm⁻². The surface work function of back contact (Mo) is considered as 5.5 eV with surface recombination velocity (SRV) of 10⁷ cm/s and 10⁵ cm/s for electron and hole respectively.

![Fig. 1 Device structure of SnS absorber based thin film solar cell](image-url)
Table 1. Parameters of p-SnS, n-SnS, WL used for modelling the solar cell

|                      | p-SnS | n-SnS | WL   |
|----------------------|-------|-------|------|
| Thickness (µm)       | Varied| 0.05  | 0.2  |
| Electron affinity (eV)| 3.52  | 3.52  | 4    |
| Band gap (eV)        | Varied| 1.15  | 2.75 |
| Dielectric permittivity (relative) | 12.5  | 12.5  | 9    |
| CB DOS (N_c) (cm⁻³)  | 1×10¹⁹| 1.00×10¹⁹| 1.00×10¹⁹|
| VB DOS (N_v) (cm⁻³)  | 1×10¹⁹| 1.00×10¹⁹| 1.00×10¹⁹|
| e mobility (µ_e) (cm²/V/s) | 50    | 50    | 100  |
| h mobility (µ_h) (cm²/V/s) | 20    | 20    | 20   |
| Acceptor density (N_A) (cm⁻³) | 1.00×10¹⁵| -------- | -------- |
| Donor density (N_D) (cm⁻³) | -------- | 1×10¹⁷  | 1×10²⁰ |
| Absorption (A) (cm⁻¹ eV¹/²) | 1×10⁵  | 1×10⁵  | 1×10⁵  |
| e thermal velocity (V_{th,n}) (cm/s) | 10⁷   | 10⁷   | 10⁷   |
| h thermal velocity (V_{th,h}) (cm/s) | 10⁷   | 10⁷   | 10⁷   |

3. Results and discussion
SnS solar cell modelling is carried out by varying thickness and optical band gap of SnS. The thickness of SnS is varied from 400 nm to 2 µm and the optical band gap is varied from 1 eV to 1.4 eV. Fig. 2 (a) shows that the short circuit current density (J_sc) increases with the thickness of the absorber layer (SnS) due to the absorption of more photons and consequently generation of large number electron-hole pairs. It is observed from the figure that J_sc decreases with the increase of bandgap of SnS. This is due to the decrease of absorption coefficient of the absorber layer as the bandgap of the layer increases.

The behavior of V_OC with thickness and bandgap is presented in Fig. 2 (b). It shows that band V_OC depends prominently on bandgap of the absorber layer. At a higher bandgap, the V_OC is large. The behavior can be understood using Eq. 1 [12]

\[ V_{OC} = \frac{E_g}{q} + \frac{k_B T}{q} \ln \left( \frac{I_L + I_0}{I_0 e^{\frac{E_g}{k_B T}}} \right) \]  Eq. 1

where, \( E_g \), \( k_B \), \( T \), \( q \), \( I_L \) and \( I_0 \) is optical band gap of SnS, Boltzmann constant, temperature, electron charge, current under illumination and reverse saturation current.
The equation suggests that the maximum $V_{OC}$ can be equal to the bandgap of the absorber layer. The $V_{OC}$ is limited by reverse saturation current embedded in the second term of equation 2. Thus, the $V_{OC}$ is found to be lower than the bandgap of the absorber layer. $V_{OC}$ can also be approximated to the splitting of quasi-Fermi levels in the energy band diagram as shown in Fig. 3.

The fill factor ($FF$) and photovoltaic efficiency ($\eta$) of the solar cell is presented in Fig. 2 (c) and Fig. 2 (d) respectively. The $FF$ and $\eta$ of a solar cell is given by

$$ FF = \frac{J_{max}V_{max}}{J_{SC}V_{OC}} $$ \hspace{1cm} \text{Eq. 2} \\
$$ \eta = \frac{J_{max}V_{max}}{P_{in}} = \frac{J_{SC}V_{OC}FF}{P_{in}} $$ \hspace{1cm} \text{Eq. 3} \\

where, $J_{max}$, $V_{max}$ and $P_{in}$ are current density (at maximum power), voltage (at maximum power) and input power (100 mWcm$^{-2}$). It is noted from the figure that the $FF$ and $\eta$ is high in the region of higher thickness and higher band gap region.
Fig. 3 Energy band diagram of SnS absorber based solar cell illuminated under AM1.5 G light. The horizontal axis is the thickness of layers in the solar cell. $x = 0$ is the interface of the substrate and absorber layer.

The J-V characteristics of the SnS solar cell after optimizing thickness and optical bandgap of the absorber layer is illustrated in Fig. 4. The optimum value of thickness and bandgap obtained after the simulation are 2 µm and 1.36 eV. The maximum photovoltaic efficiency corresponding to the optimized parameters is 22.3 % with $V_{oc} = 756$ mV, $J_{sc} = 34.9$ mAcm$^{-2}$ and FF = 84.4 %. It is also noteworthy that there is no JV cross-over distortion between dark and illuminated curves. The distortion of the JV curve is generally due to the large offsets at the interface of the substrate/absorber and absorber/buffer interfaces. The inclusion of n-type SnS (formation of homojunction) helps in the reduction of the offsets formed across the junction.

Fig. 4 JV characteristics of of SnS absorber based solar cell under AM1.5 G illumination. Red and black curves are the JV characteristics of the cell obtained in dark (without light) and AM1.5 G illumination.
4. Conclusion

SnS absorber based homo-junction solar cell (Mo/p-SnS/n-SnS/WL) in substrate configuration is investigated using SCAPS-1D numerical simulation program. The device is optimized by varying thickness and optical band gap of absorber layer (SnS). The efficiency of the optimized cell is 22.3% with $V_{OC} = 756$ mV, $J_{SC} = 34.9$ mAcm$^{-2}$ and FF = 84.4%, respectively. The incorporation of n-SnS layer in the cell results in proper band alignment and thus there is no J-V crossover from the fourth quadrant to the first quadrant. The results highlight that the application of homo-junction SnS solar cell can serve a better approach to achieve maximum PV efficiency.

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