Efficiency enhancement of thin-film solar cell by implementation of double-absorber and BSF layers: the effect of thickness and carrier concentration

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Abstract
A back surface field CIGS multilayer solar cell structure is simulated by SCAPS 1D, in which a CZTSSe layer is added between BSF and CIGS layers as a second absorber layer. To achieve the best performance for the proposed structure, the thickness of different layers and the related carrier concentration varied. The 1 µm and 0.05 µm thickness for CZTSSe and CIGS leads to the best performance of the device. The optimum thickness for the rest of layers is also calculated. The effect of the carrier concentration on the performance of the proposed solar cell is also studied. After optimization, a solar cell with a privileged power conversion efficiency of 35.1% was achieved.

Keywords Thin film · BSF, CIGS, CZTSe · Thickness · Efficiency

1 Introduction
Due to special features such as high-power conversion efficiency (PCE) and low deposition cost on large areas, thin-film solar cells are very promising candidates for energy harvesting applications. In this regard, approaching a new structure to improve the power/cost ratio is always a strong purpose for scientists. Thus, various thin-film materials such as CIGS, CZTS and CdTe have been studied for the fabrication of solar cells [1–4]. Cu2ZnSnS4–xSex (CZTSSe) is an excellent candidate as absorber layer for thin-film solar cells. This material shows an appropriate direct bandgap of 1–1.4 eV that well fit the solar spectrum and can collect most of the incident photons. Besides, this compound is nontoxic and abundant in the earth crust. CZTSSe has a high absorption coefficient (more than 10⁴ cm⁻¹). This material also has a tunable bandgap that is controlled by S and Se contents in the material [5–9]. Copper–indium–gallium–diselenide (CIGS)-based solar cells are well known for their special features such as high efficiency, easy fabrication process, low cost, very high durability and stability, flexibility and lightweight. CIGS has a high absorption coefficient of 10⁵ cm⁻¹ in the visible solar spectrum and a direct bandgap that varies from 1.04 to 1.7 eV [10–13]. In the fabrication process of solar cells, using a back surface field (BSF) layer is a solution to boost the efficiency of the solar cell. BSF layer causes a rear pushing force at the highly doped back side of the solar cell and leads to deflection of the minority carries toward front depletion area. Hence, the BSF layer lowers the rear recombination of the solar cell, which accordingly improves the electrical characteristics of the solar cell. Lead sulfide (PbS) is a promising candidate as the BSF layer. It is low cost and abundant with higher electron affinity and better absorption coefficient than materials such as SnS, Al₂O₃ and MoSe₂ BSF [5, 14, 15]. In this study, we regarded an experimental work on a single-junction CIGS solar cell as the baseline [10] and regenerated the results through the numerical simulation followed by adding a CZTSSe layer as the second absorber layer and manipulated the thickness of the layers to achieve the optimum efficiency.
2 Simulation and analysis

Recently, simulation has been a great tool for optimizing and analyzing the performance of efficient solar cells. In this study, we use the solar cell capacitance simulator structures in 1 dimension (SCAPS 1D) package \[16, 17\] to simulate the proposed solar cell. SCAPS simulator can solve the Poisson and continuity equations of electron and holes. The equations are:

\[
\nabla^2 \psi = \frac{q}{\varepsilon} (n - p + N_A - N_D), \tag{1}
\]

\[
\nabla \cdot J_n - q \frac{\partial n}{\partial t} = qG, \tag{2}
\]

\[
\nabla \cdot J_p + q \frac{\partial p}{\partial t} = -qR, \tag{3}
\]

where \(\psi(x)\) is the electrostatic potential, \(q\) is electrical charge, \(\varepsilon\) is the effective permittivity, \(n\) and \(p\) are electron and hole concentrations, \(N_A\) is the acceptor-type and \(N_D\) is the donor-type impurities, and \(G\) and \(R\) are the generation and recombination rate \[18– 20\]. By combining the current contributions of the drift and diffusion effect, we obtain:

\[
\overline{T}_n = qn\mu_n \vec{E} + qD_n \nabla n, \tag{4}
\]

\[
\overline{T}_p = qp\mu_p \vec{E} - qD_p \nabla p, \tag{5}
\]

where \(\mu_n, \mu_p, E, D_n\) and \(D_p\) stand for electron mobility, hole mobility, diffusion coefficient of electrons and diffusion coefficient of holes, respectively. SCAPS 1D solves the above equations and calculates all point quasi-Fermi level and electrostatic potential for electrons and holes \[21\]. The Shockley–Read–Hall (SRH) and Auger recombination mechanisms were considered in our calculations. Based on our calculations, Au, Ag and Al are very suitable for anode and cathode. However, because of the stability against oxidation, Au contact with work function of 5.1 eV was used as the back and forward contact. All the simulations are conducted under 1.5 AM solar spectrum and at 300 K Table 1.

Figure 1 shows our purposed double-absorber layer solar cell structure (Al/ITO/AZO/i-ZnO/CdS/CIGS/CZTSSe/PbS/Mo) with a p-type CIGS absorber layer, a p-type CZTSSe absorber layer and an n-type CdS buffer layer. A PbS layer as the BSF layer is added to the structure between the absorption layer and Mo back contact.

To verify the simulation process, results related to an experimental work \[10\] was simulated and the calculated values are summarized in Table 2. It is seen that the calculated values almost match the reported values \[10\].

### Table 1 Physical parameters of the proposed solar cell \[7, 10, 13, 22\] including \(d\) (thickness), bandgap \(E_g\), electron affinity \(\chi\), dielectric constant \(\varepsilon\), conduction/valence band density of states \((N_c/N_v)\), electron/hole mobility \((\mu_e/\mu_h)\), thermal velocity of electron/hole \((v_{thn}/v_{thp})\) and donor/acceptor concentration \((n/p)\)

| Parameter | p-CIGS | n-CdS | i-ZnO | Al–ZnO | p-PbS | CZTSSe |
|-----------|--------|-------|-------|--------|-------|--------|
| \(d (\mu m)\) | 1.5    | 0.05  | 0.05  | 0.2    | 0.15  | 1.0    |
| \(E_g (eV)\) | 1.3    | 2.4   | 3.4   | 3.4    | 1.4   | 1.0    |
| \(\chi (eV)\) | 4.5    | 4.2   | 4.5   | 4.6    | 4.35  | 4.6    |
| \(\varepsilon\) | 13.6   | 10    | 9     | 9      | 10    | 13.6   |
| \(N_c (m^{-3})\) | \(2.2 \times 10^{18}\) | \(2.4 \times 10^{18}\) | \(2 \times 10^{18}\) | \(2 \times 10^{18}\) | \(2 \times 10^{18}\) | \(2.2 \times 10^{18}\) |
| \(N_v (m^{-3})\) | \(1.8 \times 10^{19}\) | \(2.6 \times 10^{19}\) | \(1.8 \times 10^{19}\) | \(1.8 \times 10^{19}\) | \(2 \times 10^{18}\) | \(1.8 \times 10^{19}\) |
| \(\mu_e (cm^2/Vs)\) | 200    | 340   | 100   | 100    | 25    | 100    |
| \(\mu_h (cm^2/Vs)\) | 100    | 50    | 25    | 25     | 100   | 25     |
| \(v_{thn} (cm/s)\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) |
| \(v_{thp} (cm/s)\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) | \(1.0 \times 10^7\) |
| \(n (cm^{-3})\) | 0      | 0     | 0     | 0      | 5.5 \(\times 10^{16}\) | 1.5 \(\times 10^{15}\) |
| \(p (cm^{-3})\) | \(5.1 \times 10^{16}\) | 0     | 0     | 0      | 0     | 0      |
3 Effect of the thickness of CZTSSe as the second absorber layer on the performance of the proposed solar cell

Initially, it is shown that by applying a PbS layer as BSF, recombination of the solar cell is decreased, and accordingly, efficiency is increased. By adding a CZTSSe layer as the second absorber layer and varying the thickness from 0.1 to 4.5 µm, the photovoltaic parameters are calculated. It is obvious that all photovoltaic parameters (\(V_{oc}\), \(J_{sc}\), FF and \(\eta\)) are increased. However, the increase of \(V_{oc}\) and FF is not remarkable. Also, the significant change occurs in the thicknesses thinner than 1 µm for CZTSSe layer. It is seen that the photovoltaic parameters for 1 µm CZTSSe layer are more improved than the other thicknesses (Figs. 2 and 3). So, the thickness of CZTSSe layer is taken as 1 µm for the next step of simulation. Comparing this choice with Barman’s optimum structure shows more than 4.5% increase in \(\eta\).

### Table 2 Photovoltaic parameters of the proposed solar cell with and without PbS layer in comparison with those reported in [10]

| Parameters | \(V_{oc}\) (V) | \(J_{sc}\) (mA/cm²) | FF (%) | \(\eta\) (%) |
|-----------|-----------------|-------------------|--------|-------------|
| Source    | Ref [10] | This work | Ref [10] | This work | Ref [10] | This work | Ref [10] | This work |
| Without PbS | 0.81  | 0.78  | 33.96 | 33.52 | 82.35 | 82.71 | 22.67 | 21.63 |
| With PbS   | 0.83  | 0.81  | 35.22 | 35.84 | 82.29 | 83.90 | 24.22 | 24.23 |

![Fig. 2 Variations of \(J_{sc}\) and \(V_{oc}\) of the proposed solar cell as a function of CZTSSe layer thickness](image2)

![Fig. 3 Variations of the FF and \(\eta\) for the proposed solar cell as a function of CZTSSe layer thickness](image3)

![Fig. 4 Variation of \(J_{sc}\) and \(V_{oc}\) of the proposed solar cell with the thickness of CIGS layer](image4)

4 Determination of the optimum thickness of CIGS layer

After finding the optimum thickness of CZTSSe layer, the corresponding thickness for CIGS layer is also calculated. To perform that, the thickness of CIGS layer is changed from 0.05 to 1 µm. Results show an overall increase in photovoltaic parameters (Figs. 4 and 5) and the efficiency of the cell increased more than 3%. This trend can be linked to: (a) the reduction in the series resistance of the cell stemming from shorter length of CIGS layer and (b) decrease in recombination of the charge carriers traveling in shorter paths. For the next step of optimization, the structure with 0.05 µm CIGS layer is considered.
When we calculate the photovoltaic parameters for a structure with 0.05 µm AZO and 1 µm CZTSSe, $V_{oc}$ (0.8336 V), $J_{sc}$ (45.006305), FF (85.72%) and $\eta$ (32.16%) are achieved. These values are very promising as compared to the values of the baseline structure. The J–V characteristic and the QE of this structure is shown in Figs. 6 and 7, respectively.

### 5 The effect of carrier concentration on the performance of the proposed solar cell

Another key parameter that has a drastic effect on the performance of a solar cell is the carrier concentration of different layers. Initially, the variation of the carrier concentration of CIGS layer is studied (Fig. 8). It is clear that as the carrier concentration increases from $10^{11}$ to $10^{16}$ cm$^{-3}$, $J_{sc}$ and $\eta$ increase, while $V_{oc}$ and FF decrease. Meanwhile, when the carrier concentration of CZTSSe layer rises from $10^{14}$ to $10^{20}$ cm$^{-3}$, $J_{sc}$ increases rapidly up to $10^{17}$cm$^{-3}$ followed by trivial increase for the higher concentrations (Fig. 9). Contrarily, the other parameters decrease in this range. This implies that higher carrier concentration of the second absorber layer causes narrowing of the depletion zone leading to decrease of $V_{oc}$. Also, this can be due to the high recombination of the photogenerated carriers in the CZTSSe absorber layer.

With the optimum value of 1 µm for thickness and $10^{17}$ cm$^{-3}$ for carrier concentration of CZTSSe layer, the highest $\eta = 32.17\%$ is achieved. The effect of carrier concentration of PbS (Fig. 10) and CdS layer (Fig. 11) on the performance of the proposed solar cell is also studied. It is seen that all output parameters of the sell increase with the carrier concentration of PbS layer up to $10^{17}$ cm$^{-3}$. This trend can be assigned to the reduction of the photogenerated charge carrier recombination.

On the other hand, at high carrier concentration, the Fermi level of PbS at HTL (hole transport layer) shifted toward the valence band, thus forming a nearly ohmic contact with back metal electrode caused the efficient collection of holes. For CdS layer, the carrier concentration is changed from $10^{16}$ to $10^{20}$ cm$^{-3}$. As it is clearly shown in Fig. 11, except FF, the other output parameters increased by carrier concentration. The increase in the efficiency of the cell can be related to the better collection a photogenerated electrons on the optimized buffer layer.

The optimum performance of the designed structure was achieved at 0.05 µm thickness and $9 \times 10^{19}$ cm$^{-3}$ carrier concentration of CdS layer where $\eta = 35.1\%$. The
Fig. 8  Variation of photovoltaic parameters of the proposed solar cell with carrier concentration of CIGS absorber layer
corresponding $V_{oc}$, $J_{sc}$ and FF are 0.89 V, 45.6 mA cm$^{-2}$ and 87%, respectively.

6 Conclusion

In summary, a thin-film solar cell with double-absorber layer and BSF layer was proposed and the effect of the thickness of different layers and carrier concentration was studied. The optimum thickness for CZTSSe and CIGS layers was found 1 and 0.05 microns, respectively. Using a BSF layer improved the photovoltaic properties of the device drastically. The optimum carrier concentration of each layer was determined through optimization process. After the determination of the optimum values, the final structure was simulated. Calculations revealed a privileged power conversion efficiency of 35.1%. This result makes our modeled structure as a promising candidate for thin-film solar cells.

Fig. 9 Variation of photovoltaic parameters of the proposed solar cell with carrier concentration of CZTSSe as the second absorber layer
Fig. 10  Variation of photovoltaic parameters of the proposed solar cell with carrier concentration of BSF layer
Enquiries about data availability should be directed to the authors.

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**Data availability**  All data are available whenever were asked.

**Code availability**  The code will be available whenever is asked.

**Declarations**

**Conflict of interest**  The authors have not disclosed any competing interests.

**Consent for publication**  I, the undersigned, give my consent for the publication of identifiable details, which can include photographs and details within the text to be published in the above Journal and Article.

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