A novel design of CTZS/Si tandem solar cell: a numerical approach

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Received: 8 March 2021 / Accepted: 10 June 2021 / Published online: 16 July 2021
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Abstract
Multijunction or tandem solar cells can split the solar spectrum over several subcells with different bandgaps to convert sunlight into electricity more effectively than single-junction solar cells. The monolithic tandem design of third generation silicon solar energy materials is auspicious for photovoltaics. In this paper, the simulation-based studies of copper zinc tin sulfide/silicon (CZTS/Si) tandem cells based on CZTS as an upper subcell and silicon as a lower subcell absorber layer have been performed using SCAPS-1D. This study aims to evaluate the CZTS tandem cells’ performance based on the fact that both subcells are simulated to produce the best efficiency recorded at its bandgap. The simulation and optimization of the single-junction CZTS and Si solar cells were initially performed to fit the state-of-the-art records efficiency of 11.65% and 18.7%, respectively. Further, both the upper and lower cells have been evaluated at different thicknesses for tandem configuration after validation. Also, to obtain the same current for tandem structure, the upper subcell’s performance is investigated at different thicknesses ranged from 0.1–1 µm while keeping the lower subcell thickness at 80 µm. Thus, at optimized upper absorber thickness of 0.191 µm and lower subcell 80 µm at transmitted spectrum the same current was obtained and gave an efficiency of 10.6% and 11.9%, respectively. The maximum efficiency of ~ 23 is obtained for tandem design with enhancing open circuit voltage 1.4 V.

Keywords CZTS · Tandem · Solar cell · Simulation · SCAPS-1D

Abbreviations
BSF Back surface field
CZTS Copper zinc tin sulfide
CZTGS Copper zinc tin germanium sulfide
TiN Copper zinc tin sulfide
Voc Open-circuit voltage
Jsc Short-circuit density
FF Fill factor
EFF Efficiency

1 Introduction
Numerous studies have been conducted to improve the efficiency of single-junction solar cells [1, 2]. Theoretically, infinite junction stacking under AM1.5 illumination can produce efficiency of 65.4%, and under a concentrated incident spectrum, it can enhance the efficiency up to 85% [3]. Typically, tandem structures of III–V/a-Si solar cells are manufactured to improve efficiency, and in fact, the cells with an efficiency of 46% and 13.6% have been illustrated that exceed single-junction solar cell efficiency [4].

In tandem device, various bandgap $p$–$n$ junction solar cells are to be stacked in a particular arrangement in which the upper cell absorbs high-energy photons equal to their absorber bandgap and the bottom subcell absorbed the remaining low-energy photons similar to their corresponding absorber band gaps [5]. This requirement brings numerous restrictions and obstacles to the development of a tandem solar device. A transparent tunnel junction connects the subcells, allowing the transmission of carriers and unabsorbed photons from the upper subcell through the tunnel junction with minimal loss. Also, except for the significantly lower subcell, the upper subcells should be thinned appropriately to achieve the same current between the subcells. In theory, the subcells in the tandem structure are electrically considered to be in a series connection, which means that the lowest current density subcell becomes the current limiting cell.
Thus, ensure the most efficient tandem device by matching the subcells’ current density [6–8].

Few studies have been conducted on Cu₂ZnSnS₄ (CZTS)-based tandem solar cells than a-Si or III–V solar cells. Crystalline-silicon solar cell’s efficiency is an approach to the upper limit predicted by this material’s fundamental properties [9–11]. As a result, the Si (bottom cells)-based tandem solar cells are essential because they are the direct way to go beyond the single-junction efficiency limit. CZTS represents an exciting candidate for the upper subcell absorber because it consists of an abundant, non-toxic component and shows no stability problem under normal sunlight conditions [12]. A theoretical study of tandem Cu₂ZnSn(S/Se)₄ junction solar cells has been reported by Goutam Kumar et al. with maximum efficiency of 21.7% [13]. Also, Adeyinka et al. developed a monolithic tandem device based on (Cu₂ZnGeS₄) CZTGS/CZTS and achieved 17.51% efficiency [14]. Recently, the first functioning monolithic CZTS/Si tandem cells have been ensured using a different intermediate connection between the subcells with Vₜ at around 948 mV and an efficiency of 3.5% [15]. Further, it was proposed to develop bottom Si cell protection strategies to obtain functioning monolithic CZTS/Si tandem cells. A comparative analysis of monolithic CZTS/Si tandem cells generates using different diffusion barrier layers based on titanium nitride (TiN), and solar cells are achieved, which have an open-circuit voltage (Vₜ) of 1.06 V, with good efficiency of 3.9% [16].

In this work, the CZTS/Si tandem device’s potential efficiencies have examined using the SCAPS-1D simulation tool. Initially, the simulation of single-junction CZTS-based absorber layer solar cells and Si-based absorber layer solar cells has been performed and validated against the simulated data. Further, the study has expanded for tandem solar cell structures to achieve improved photoconversion efficiencies. In tandem structure, the same current has been achieved with the variation in both subcells absorber layer thickness to enable the upper and lower subcells to have the same current density (Jₑ). The efficiency of tandem solar cells has limited by the relatively lower Jₑ of the upper subcells. Therefore, it must enhance CZTS solar cells’ efficiencies in advance to illustrate a CZTS/Si tandem solar cell that exceeds the device performance from an optimized single-junction solar cell.

2 Methodology

The optoelectronic performance of the considered tandem solar cell has been studied by using Solar Cell Capacitance Simulator (SCAPS-1D, version 3.3.07) software under AM1.5 illumination. SCAPS is a one-dimensional simulation tool with seven input semiconductor layers developed at the Department of Electronics and Information Systems, University of Gent, Belgium [17]. Furthermore, this software can measure precisely the open-circuit voltage, short-current density, quantum efficiency, fill factor, the band structure of heterojunctions, power conversion efficiency, spectral performance, electric field distribution, temperature, capacitance–voltage, generation and recombination profile, light bias, lighting from either the n-side or p-side, and frequency spectroscopy [18] as compared to other simulation software such as Aestimo [19], PC1D [20], GPVDM [21], and AFORS-HET [22].

The material considered for the comprehensive study of a single-junction and tandem configuration is CZTS and Si with a bandgap of 1.55 eV and 1.1 eV, respectively. The upper subcell structure consists of an efficient layer such as ZnO:Al, i-ZnO, ZnMgO, and CZTS as shown in Fig. 1a. A p-type CZTS semiconductor is used as an absorber layer for producing a carrier with the least absorbed light reflection and the lowest transmission losses [23]. The ZnO serves as a window layer because of its high n-type conductivity and wide bandgap [24], and n-type ZnMgO is used as a buffer layer. Thus, a buffer layer creates a junction along with the absorber layer to reduce absorption losses and direct the produced carrier to the electrodes. At the same time, the buffer layer will minimize surface losses along with the window layer [25]. Moreover, ZnMgO has a wide bandgap and, as a buffer layer, leads to reduce the recombination [26]. Also, ZnMgO as buffer layer has a perfect lattice match with the i-ZnO and ZnO:Al window layer [27, 28]. Similarly, the bottom subcell consists of front contact, n-Si, p-Si, p⁺⁺-Si/back contact, as shown in Fig. 1b. TiN is used as front contact of lower subcell with work function of 4.3 eV because of its excellent chemical and thermal stability and quasi-metallic conductivity and as a copper diffusion barrier for interconnect technologies [29, 30]. A highly doped Back Surface Field (BSF) p⁺⁺-Si was used to minimize carrier recombination losses on the rear surface. The band structures of the considered material are shown in Fig. 2.

In the first step, the simulations of single-junction CZTS and Si solar cells were performed under the standard AM1.5 spectrum, and results are validated against the simulated data reported by Bahfir et al. [31] and Kim et al. [32]. Further, the tandem design CZTS/Si is presented in Fig. 1c. The CZTS/Si tandem device has an ideal tunnel junction to have the same current density value in both subcells. However, because of the limitations of the SCAPS-1D simulator, between the upper and lower subcells, the ideal tunnel junction without optoelectric losses has been presumed. It is essential to achieve the same current between the cells to conduct the tandem design study. Thus, both cells have independently simulated with different illumination ranges. The upper subcell’s current density and the transmitted spectra for the lower subcell have been calculated by adjusting the
upper subcell absorber layer thicknesses ranged from 0.1 to 1 µm. The transmitted spectrum was then used as the lower Si subcell of the input illumination spectrum. Next, the lower subcell $J_{sc}$ values are determined, and then, each of the current matching points was calculated. A similar method is commonly used for reporting tandem design simulation using the SCAPS-1D [13, 32]. The material properties in Table 1 are taken from the literature and are used to simulate the photovoltaic response of the considered single and tandem solar cell [27, 33–40], whereas the optical absorption coefficients of CZTS taken from file [41], and other from SCAPS-1D are presented in Fig. 3. Table 2 shows the basic equations for the SCAPS-1D and transmitted spectrum [42, 43].

3 Results and discussion

This section is categorized into three subsections: The standalone performance of the single-junction upper and lower subcell is presented in Sect. 3.1. The impact of absorber layer thickness on the photovoltaic performance of upper and lower subcells is introduced in Sect. 3.2. The performance of the CZTS–Si tandem solar cell is addressed in Sect. 3.3.

3.1 The standalone performance of the single-junction upper and lower subcell

In this section, the upper and lower subcell’s validation with the numerically simulated solar cell reported in the previously published data is presented. The current density voltage ($J$–$V$) characteristics of the single-junction upper...
\[ \text{Table 1 Material parameters used in single-junction tandem solar cell simulation} \]

| Material properties | Window layer ZnO | i:ZnO | ZnMgO | CZTS | Si (n) | Si (p⁺) | Si(P++) |
|---------------------|------------------|-------|-------|------|--------|--------|---------|
| Thickness \( d \) (µm) | 0.01 | 0.02 | 0.02 | Variable | 0.02 | 80 | 0.1 |
| Bandgap (eV) | 3.37 | 3.3 | 3.32 | 1.55 | 1.1 | 1.1 | 1.1 |
| Electron affinity \( \chi \) (eV) | 4.45 | 4.6 | 4.53 | 4.5 | 4.05 | 4.05 | 4.05 |
| Relative permittivity \( \varepsilon \) | 9 | 9 | 9 | 10 | 11.9 | 11.9 | 11.9 |
| Conduction band effective density of states (cm\(^{-3}\)) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) | \(2.8 \times 10^{19}\) | \(2.8 \times 10^{19}\) | \(2.8 \times 10^{19}\) |
| Valence band effective density of states (cm\(^{-3}\)) | \(1.8 \times 10^{19}\) | \(1.8 \times 10^{19}\) | \(1.8 \times 10^{19}\) | \(2.6 \times 10^{19}\) | \(2.6 \times 10^{19}\) | \(2.6 \times 10^{19}\) |
| Electron mobility \( \mu_n \) (cm\(^2\)/Vs) | 1.00 \(\times 10^2\) | 1.00 \(\times 10^2\) | 1.00 \(\times 10^2\) | 1.041 \(\times 10^3\) | 1.041 \(\times 10^3\) | 1.041 \(\times 10^3\) |
| Hole mobility \( \mu_p \) (cm\(^2\)/Vs) | 2.5 \(\times 10^1\) | 2.5 \(\times 10^1\) | 2.5 \(\times 10^1\) | 3.5 \(\times 10^1\) | 4.21 \(\times 10^2\) | 4.21 \(\times 10^2\) |
| Donor density \( N_D \) (cm\(^{-3}\)) | 1.0 \(\times 10^{20}\) | 1.0 \(\times 10^{20}\) | 1.0 \(\times 10^{20}\) | 8.0 \(\times 10^{20}\) | 1.0 \(\times 10^1\) | 1.0 \(\times 10^1\) |
| Acceptor density \( N_A \) (cm\(^{-3}\)) | 0.0 \(\times 10^0\) | 0.0 \(\times 10^0\) | 1.0 \(\times 10^0\) | 1.0 \(\times 10^{17}\) | 1.0 \(\times 10^1\) | 5.0 \(\times 10^{18}\) |

\[ \text{Table 2 Basic equations for the SCAPS-1D, transmitted spectrum and computing efficiency} \]

**One- dimensional semiconductor equation**

\[
\begin{align*}
\frac{d}{dx} \left( \varepsilon(x) \frac{d\Psi(x)}{dx} \right) &= -q \left( P - n + N_D^+ - N_D^- + P_t - n_t \right), \\
J_n &= -\frac{\mu_n}{q} \frac{d\Psi}{dx}, \\
J_p &= \frac{\mu_p}{q} \frac{d\Psi}{dx},
\end{align*}
\]

**Beer–Lambert model**

\[ S(\lambda) = S_i(\lambda) \cdot \exp \left( \sum_{i=1}^{3} \left( a_i(\lambda) \cdot d_i \right) \right) \]

**FF and efficiency of solar cell**

\[
\begin{align*}
\text{FF} &= \frac{V_{oc} \cdot J_{sc}}{V_{oc} \cdot J_{sc} \cdot FF \times 100}, \\
\eta &= \frac{V_{oc} \cdot J_{sc} \times \text{FF} \times 100}{E_{in}}
\end{align*}
\]

is 20.5 mA/cm\(^2\) and 36.9 mA/cm\(^2\) while the \(V_{oc}\) in the individual cells is 0.7 V and 0.639 V. The photovoltaic parameters are summarized and compared against the previously published simulated data in Table 3.

### 3.2 Impact of absorber layer thickness on the photovoltaic performance of upper and lower subcells

The upper and lower solar cells are investigated first with different absorber layer thicknesses to evaluate the CZTS–Si tandem device’s performance. The \(J–V\) characteristic of upper and lower subcells with different absorber layer thicknesses is depicted in Fig. 5 under AM1.5 illuminations. It is obtained that an increase in the thickness of the active layer of the upper subcell substantially increases the current density shown in Fig. 5a. This enhancement is due to improved optical absorption that further leads to increased production of electron–hole pairs. The \(J_{sc}\) of the device is increased by the resultant separation of produced electron–hole pairs.

\[ \text{Fig. 3 Absorption coefficient profile of upper subcell used for transmitted spectrum} \]

and lower cell are obtained in this respect and are stated in Fig. 4. The results presented in Fig. 4 show that the short-circuit current density of upper and lower subcells in Fig. 5a. This enhancement is due to improved optical absorption that further leads to increased production of electron–hole pairs. The \(J_{sc}\) of the device is increased by the resultant separation of produced electron–hole pairs. It
is observed that at lower thicknesses, the improvement in $J_{sc}$ is substantial; however, it begins to saturate at greater thicknesses as depicted in Fig. 5a. Quantitatively, improvement of 17.9%, 14.9%, and 9.5% in $J_{sc}$ was computed when raising the upper cell’s thickness from 0.1 to 0.2 µm, 0.2 to 0.3 µm, and 0.3 to 0.4 µm, respectively, whereas 2.1%, 1.8%, and 1% rise in $J_{sc}$ are evaluated in lower subcell thickness. Figure 5b depicts that there is no major effect of thickness on the $J_{sc}$ of the lower subcell; however, a slight increase in thickness is observed approaching the optimum value of $J_{sc}$ for CZTS.

Furthermore, both devices’ PV parameters are computed at different absorber layer thicknesses to summarize their performance, and the results are plotted in Fig. 6. It has been found that $V_{oc}$ of CZTS increases with increasing thickness from 0.1 to 0.2 µm and saturates with a further increase in thickness while the Si-based solar cell does not have a major thickness impact on $V_{oc}$ and a marginal increase with thickness is observed. The $J_{sc}$ of CZTS-based solar cell shows a significant increase with the absorber layer’s thickness, while in Si-based solar cell $J_{sc}$ does not show a significant increase with thickness. Also, FF shows the same behavior as the $V_{oc}$ of both cells. It is evaluated that both cells conversion efficiency is improved from 2.8% (upper subcell) and 21.3% (lower subcell) to 18% (upper subcell) and 21.4% (lower subcell) by increasing the thickness from 0.1 to 1.0 µm for upper subcell and 10 to 250 µm for lower subcell, respectively.

### Table 3  Comparison of the photovoltaic parameter of single-junction CZTS and Si solar cell

|                          | $V_{oc}$ (V) | $J_{sc}$ (mA/cm²) | FF (%) | PCE (%) | Refs. |
|--------------------------|--------------|-------------------|--------|---------|-------|
| CZTS-based absorber layer solar cell | 0.70         | 20.52             | 80.74  | 11.65   | Present work |
| CZTS-based absorber layer solar cell | 0.78         | 21.32             | 68.78  | 11.42   | [31]   |
| Si-based absorber layer solar cell       | 0.6433       | 35.04             | 83.39  | 18.8    | Present work |
| Si-based absorber solar cell             | 0.639        | 36.9              | 79.4   | 18.7    | [32]   |

![Fig. 4](image.png)  
**Fig. 4** $J$–$V$ of single-junction upper and lower subcell at AM1.5 illumination

![Fig. 5](image.png)  
**Fig. 5** $J$–$V$ curve of upper and lower cell variation with the thickness of absorber layer
3.3 CZTS–Si tandem solar cell

A tandem solar cell simulation was performed by employing a wide bandgap CZTS-based subcell on the narrow bandgap silicon-based subcell, separated by TiN which is the front contact of the lower subcell. For simulating CZTS/Si tandem solar cells, a straightforward technique was used. In this section, the AM1.5 sun spectrum as shown in Fig. 7a is used to incident on the upper cell’s front surface. The transmitted spectra from the upper subcell are computed by using Beer–Lambert law with the help of thickness and absorption coefficient of each layer of the upper cell presented in Table 2. The upper subcell was initially simulated by changing the absorber layer thickness from 0.1~1 µm, while the other layer thickness in the upper subcell remains fixed. The transmitted spectrums filtered by the upper subcell with different absorber layer thicknesses are shown in Fig. 7b. These transmitted spectrums are then used to illuminate the lower subcell to achieve the same current. Two-terminal tandem devices operate electrically as two diodes connected in series, so the same current must pass from each subcell because of this arrangement’s electrical properties. In contrast, the total voltage drop equals the sum of each cell’s voltage drop across the tandem device [44]. The tandem $J_{sc}$ follows the lower value of subcell connected in series [45]. When the upper subcell thickness increases beyond the optimized value, the $J_{sc}$ of the upper subcell increases, whereas the lower cell $J_{sc}$ is reduced. This is due to the absorption of more photons by thicker upper subcell and less light is transmitted to the lower subcell. Thus, the overall current density of tandem cells decreases [14]. The same phenomenon happens when the upper subcell thickness is less than the optimized value; less absorption occurs in the upper subcell, which reduces the overall tandem current density. Because of the mentioned phenomena above, the same current in upper and lower subcells is obtained to acquire the same $J_{sc}$ value. This was done through the calculated transmitted spectrum with different absorber layer thicknesses in the upper subcell, as depicted in Fig. 7b. The calculated transmitted spectrums at different upper subcell thicknesses are illuminated on the lower subcell’s front surface and evaluate the lower subcell PV parameters. Furthermore, adjusting the lower subcell thickness has been done by varying, the lower cell thickness from 10 to 250 µm to
find the optimal value. Thus, the upper subcell thickness at 0.191 µm and lower subcell thickness at 80 µm the same current established where both upper and lower subcells have same $J_{sc}$ value of 19.3 mA/cm² as shown in Fig. 7c.

Additionally, the remaining PV parameters under the filtered spectrum from the lower subcell are also obtained, as shown in Fig. 8a–d. Figure 8a shows that the value of $J_{sc}$ is higher at the low thickness of the upper subcell, which begins to decrease as the absorber layer thickness increases and in between found the same current point. A slight influence on $V_{oc}$ and FF is also observed in Fig. 8b and d. The PCE under transmitted spectrum decreases with upper subcell thickness shown in Fig. 8d.

The tandem cell’s $J$–$V$ curve at 0.191-µm-thick CZTS upper cell and 80-µm silicon lower cell is shown in Fig. 9, along with the upper and lower subcell in tandem structure with the same current. The $J$–$V$ curve of both upper and lower subcell, measured separately at the same current, is added together in series, i.e., $V_{oc}$ of both upper and lower subcell is summed at the same current to compute tandem device’s $J$–$V$ characteristics [32, 44]. Next, the tandem device’s FF and efficiency are calculated by using the formula represented in Table 2. The tandem device’s significance can be observed in terms of higher open-circuit voltage, which is the sum of the upper and lower cells’ open-circuit voltages. The maximum current in the tandem cell configuration is limited by the current in the CZTS upper subcell. This helped to achieve a higher $V_{oc}$ with an optimum current density for the complete tandem structure. The PV parameters of the upper cell, lower cell, and tandem device with the same current are shown in Table 4. For the optimized CZTS/Si tandem structure, the
Fig. 8. 3D contour plots for a lower subcell with the variation of silicon absorber layer thickness under transmitted spectra, a current density, b open-circuit voltage, c fill factor, d efficiency

Fig. 9  J–V curve of the optimized upper, lower, and tandem solar cell

Table 4  PV parameter of optimized upper, lower, and tandem solar cell configuration

| Solar cell                     | $V_{oc}$ (v) | $J_{sc}$ (mA/cm²) | FF (%) | PCE (%) |
|-------------------------------|--------------|-------------------|--------|---------|
| CZTS upper subcell in a tandem structure | 0.7098       | 19.38             | 76.66  | 10.6    |
| Si lower subcell in a tandem structure | 0.6992       | 19.34             | 83.48  | 11.93   |
| Tandem cell                   | 1.4          | 19.38             | 83.5   | 22.9    |
investigated device configuration’s maximum efficiency is achieved by approximately 23%.

Eventually, in Table 5, the comparative study of present work with those related in previous work has been shown. Our proposed model that consists of earth abundant and non-toxic Si and CZTS as an absorber layer and ZnMgO as a buffer layer rather than toxic CdS supports high voltage, current density, fill factor, efficiency.

Table 5 Comparison of PV parameter of present work with other tandem structures from the literature

| Structure     | $V_{oc}$ (V) | $J_{sc}$ (mA/cm²) | FF (%) | PCE (%) | Refs. |
|---------------|--------------|--------------------|--------|---------|-------|
| CIGS/Si       | 1.25         | 15.80              | 81.50  | 19.8    | [32]  |
| CZTS-Pero-sky- | 0.80         | 28.22              | 49.99  | 22.50   | [46]  |
| CZTS/CTS      | 1.41         | 24.85              | 62.04  | 21.77   | [47]  |
| CZTS/CTZSe    | 1.43         | 19.17              | 72.60  | 19.86   | [48]  |
| CZTG/S/      | 1.32         | 20.98              | 78.20  | 20.87   | [13]  |
| CZTS/Si      | 1.35         | 18.53              | 62.17  | 17.51   | [14]  |
| CZTS/Si      | 1.4          | 19.38              | 83.5   | 22.9    | Present work |

4 Conclusions

The investigation of CZTS/Si tandem solar cells, consisting of CZTS-based upper subcell and Si-based lower subcell was carried out by SCAPS-1D simulation tool. The upper and lower cell condition was simulated individually based on the state-of-the-art records with the conversion efficiency of 11.65% and 18.7%. Further, the upper and lower subcells are evaluated at different thicknesses ranged from 0.1–1 µm and 10–250 µm, respectively, for tandem arrangement. Moreover, adjust the absorber layer’s thickness in the upper subcell to achieve the same current in both subcell for a realistic tandem approach. Thus, at optimized upper subcell absorber layer thickness of 0.191 µm and lower subcell 80 µm at transmitted spectrum, the same current is obtained and gave an efficiency of 10.6% and 11.9%, respectively. The tandem cell’s J–V curve is obtained by adding the J–V curve of the upper subcell at AM1.5 and the lower subcell at transmitted spectrum at equal current. The current study showed the PV parameter $V_{oc}$ = 1.4 V, $J_{sc}$ = 19.38 mA/cm², FF = 83.5% with an optimum efficiency of about 23% for CZTS/Si tandem design. This present study demonstrates that a CZTS /Si tandem design improves the CZTS single-junction solar cell performance due to the absorption of more solar photons.

Acknowledgements This work was supported by the Research Program of the School of Physics, Dalian University of Technology, China. Authors are highly acknowledges Dr. M. Burgelman for providing SCAPS-1D simulator.

Data availability All data generated or analyzed during this study are included in this published article.

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