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Solar cell performance enhancement with optimized CIGS absorber bandgap and buffer layer

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Abstract. In the past years, copper-indium-gallium-diselenide (CIGS) based solar cells have improved the efficiency records reaching to 22.6%. This result shows that CIGS absorbent is idealistic for thin-film solar cells. The most attractive feature in CIGS is the tunable bandgap of the absorber layer that varies from 1.06 eV to 1.7 eV according to the gallium fraction in the absorber layer. As a result of this feature, the solar spectrum can be best matched. In the presented work, the influence of the bandgap of the absorber is investigated using solar cell capacitance simulator (SCAPS). An optimum bandgap of 1.39 eV results in a maximum efficiency of 24.288%. In order to get a Cd-free CIGS thin film solar cell, In₂S₃ has been used as a buffer layer instead of CdS. The results show that In₂S₃ is a proper alternative that does not degrade the cell performance.

1. Introduction
Now multiple researches are based on thin film solar cells materials because of their high efficiency/cost ratio. Chalcopyrite solar cells are featured by their 2 μm absorbent layer thickness that is appropriate in absorbing the solar spectrum useful part. Compared to silicon solar cells that require a 200 μm absorbent layer thickness, chalcopyrite solar cells possess an convenient performance with a relatively high efficiency. The cost of the solar cells is also reduced as result of the material reduction [1-4]. CIGS solar cells are highly attractive in the thin film technology market as they have the highest efficiency [5]. Cu(In₁₋ₓ, Gaₓ)Se₂ has good advantages that it has a direct tunable band gap which can be changed from 1.06 eV to 1.7 eV due to the change in the indium to gallium ratio [6], with high absorption coefficient reaching 10⁵ cm⁻¹ [7], also they have excellent outdoor stability.

A number of studies have been done to report the variation of the optical bandgap of the absorbent on the solar cell performances [8-10]. They concluded that with the reduction of the absorbent layer bandgap energy, the short-circuit current density increases. Conversely, the increase in bandgap energy of the absorber layer increases the open circuit voltage. So that, to best optimize the CIGS bandgap, there is a trade-off between high short circuit current density at low bandgap energy and high open circuit voltage at high bandgap energy. Several parameters in the absorbent layer are affected by the variation of the gallium fraction such as optical bandgap, optical absorption of the incident solar spectrum and also concentration of defects that in turn affect solar cell performance. In the presented
study, the badgap of the absorber is varied to examine the solar cell performance, while keeping all other parameters without any change. Then the used cadmium sulfide (CdS) in the buffer layer is substituted by indium sulfide (In$_2$S$_3$). In$_2$S$_3$ is a good alternative to achieve Cd-free CIGS solar cells, because of the toxicity of the cadmium metal that is very harmful for humans and the environment [11, 12]. In the shadow of the proposed work, it is expected to have a notable increase in the cell performance of Cd-free free CIGS thin film solar cell.

2. Methodology

2.1. Structure of CIGS cell

As seen in Figure 1, the CIGS thin film solar cells are consist of various layers. First, the soda lime glass substrate layer is deposited which is mostly used in the CIGS solar cells. Then the Molybdenum (Mo) back contact layer which is responsible for reflecting most of the unabsorbed photons back to the absorber layer due to its high electron affinity that forms an ohmic contact with the CIGS. Next, the absorbent CIGS (Cu (In$_{1-x}$, Ga$_x$) Se$_2$) is deposited that is the most important layer. It has a direct bandgap material. The bandgap value can range from 1.06 eV to 1.7 eV according to the ratio of indium (In) to the gallium (Ga) concentration. Above the absorbent layer the n-CdS buffer layer is deposited. The main purpose of the buffer layer is the creation of hetero-junction with the p-CIGS absorbent layer where the creation of the electron-hole pairs occurs. A thin intrinsic zinc oxide (i-ZnO) layer is sputtered over the CdS surface. Depending on its high resistivity; it can prevent shunt paths from being created through the device. Then Aluminum-doped zinc oxide (ZnO:Al) is deposited using a transparent conducting oxide (TCO). Its main role is to collect the electrons out from the solar cell. Both i-ZnO and ZnO:Al together form a bi-layer called window layer. Before the deposition of the front-contact, an anti-reflection layer is added made of MgF$_2$ which is used to minimize the number of reflected photons.

![Figure 1. Cross Section of the CIGS solar cell.](image)

2.2. SCAPS simulation and material properties

In our numerical simulation, we used SCAPS (Solar Cell Capacitance Simulator) software version 3.3.06. SCAPS is a one-dimensional simulator developed by the University of Gent, Belgium [13]. It developed primarily for CdTe and CIGS solar cell families. SCAPS depends on the fundamental equations of the solar cells like Poisson's equation, the continuity equations for the electrons and the continuity equations for the holes in steady state condition. The equation of Poisson's that is commonly used for semiconductor device is [14]
where, \( n \) and \( p \) are the free electrons and holes concentrations, \( N_D \) and \( N_A \) are the donors and acceptors charged impurities concentrations, \( q \) is the electron charge, \( \varepsilon_s \) is the permittivity of silicon, \( \varepsilon_0 \) is the permittivity of free space, \( \Psi \) is the electrostatic potential, \( \rho_{ds} \) is the deep state charge density, which depends in a nonlinear way on the electron and hole concentrations. While, the continuity equations for electrons and that of holes in steady state conditions are

\[
\frac{1}{q} \frac{d}{dx} J_n = R_n x - G(x),
\]

\[
\frac{1}{q} \frac{d}{dx} J_p = G x - R_p x ,
\]

where, \( J_n \) is the electrons current density, \( J_p \) is the holes current density, \( q \) is the electron charge. Whereas, \( R_n \) is the recombination rate of the electrons, \( G \) is the generation rate of the charge and \( R_p \) is the recombination rate of the holes. Simulations can be done under dark or light conditions with different illuminations and temperatures. In our simulation, it was illuminated under global AM1.5 solar spectrum, temperature of 300 K, and incident light power of 1000 W/m\(^2\). The material properties of each layer and their defects are shown in Table 1.

The solar cell efficiency is defined as ratio between the maximum generated power and the solar incident power. It can be expressed as [15]

\[
\eta = \frac{P_{\text{max}}}{P_{\text{in}}} ,
\]

where \( \eta \) is the solar cell efficiency, \( P_{\text{in}} \) is the sunlight incident power. Whereas, \( P_{\text{max}} \) is the maximum delivered power from the solar cell and it is equal to \( V_{\text{oc}} I_{\text{sc}} \text{FF} \). While the open circuit voltage (\( V_{\text{oc}} \)) is the maximum voltage that can be delivered by a solar cell when the total current is equal to zero. It can be expressed as [15]

\[
V_{\text{oc}} = V_T \ln \frac{J_{\text{sc}}}{J_0} + 1 ,
\]

where \( V_T \) is the thermal voltage. It is equal to \( K_B T/q \), where \( K_B \) is the Boltzmann constant, \( T \) is the temperature and \( J_0 \) is the saturation current density. While, the photo-generated current density \( (J_{\text{sc}}) \) passes in a direction opposite to that of the dark current density. It is defined as the maximum current density delivered when the voltage across the solar cell is equal zero. The generation and collection of the photo-generated carriers results in the formation of the photo-generated current density. For a p-n junction solar cell under illumination the J-V characteristics can be expressed as [15]

\[
J_{\text{light}} = J_D - J_{\text{ph}} = J_0 \exp \frac{qV}{K_B T} - \frac{1}{K_B T} J_{\text{ph}} ,
\]

where \( J_D \) is the current density at dark, and \( J_{\text{ph}} \) is the photocurrent density. While at zero voltage, short-circuit current density \( J_{\text{sc}} \) is equal to the photo-generated current density. In the case of a solar cell with no surface recombination and uniform generation, \( J_{\text{ph}} \) can be determined as [15]
\[ J_{\text{ph}} = qG(L_N + W + L_P), \]  

where \( W \) is the depletion region width, \( L_N \) is the electrons diffusion lengths and \( L_P \) is the holes diffusion lengths.

The fill factor measures the squareness of the \( J-V \) characteristics and it is the ratio between the generated maximum power \( (P_{\text{max}} = J_{\text{mpp}}V_{\text{mpp}}) \) and the product of \( J_{\text{sc}} \) with \( V_{\text{oc}} \) of the solar cell. It can be expressed as [15]

\[ FF = \frac{J_{\text{mpp}}V_{\text{mpp}}}{J_{\text{sc}}V_{\text{oc}}}, \]

where the subscript \( \text{mpp} \) denotes the maximum power point of the solar cell, i.e. the point on the \( J-V \) characteristic curve, where the maximal output power can be achieved by the solar cell.

### Table 1. Material properties for CIGS solar cell.

<table>
<thead>
<tr>
<th>Layers properties</th>
<th>CIGS</th>
<th>CdS</th>
<th>i-ZnO</th>
<th>ZnO:Al</th>
</tr>
</thead>
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<tr>
<td>( w ) (( \mu m ))</td>
<td>2</td>
<td>0.05</td>
<td>0.08</td>
<td>0.35</td>
</tr>
<tr>
<td>( E_g ) (eV)</td>
<td>( E_g(x) )</td>
<td>2.4</td>
<td>3.3</td>
<td>3.3</td>
</tr>
<tr>
<td>( \chi ) (eV)</td>
<td>4.1</td>
<td>3.8</td>
<td>4</td>
<td>4</td>
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<tr>
<td>( \varepsilon_r )</td>
<td>13.6</td>
<td>10</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>( N_e ) (cm(^{-2}))</td>
<td>2.2x10(^{10})</td>
<td>2.2x10(^{11})</td>
<td>2.2x10(^{18})</td>
<td>2.2x10(^{18})</td>
</tr>
<tr>
<td>( N_v ) (cm(^{-3}))</td>
<td>1.8x10(^{10})</td>
<td>1.8x10(^{19})</td>
<td>1.8x10(^{19})</td>
<td>1.8x10(^{19})</td>
</tr>
<tr>
<td>( \mu_e ) (cm(^2)/Vs)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>( \mu_h ) (cm(^2)/Vs)</td>
<td>25</td>
<td>25</td>
<td>13</td>
<td>13</td>
</tr>
<tr>
<td>( N_D ) (cm(^{-3}))</td>
<td>0</td>
<td>1.1x10(^{13})</td>
<td>5.6x10(^{18})</td>
<td>5.6x10(^{20})</td>
</tr>
<tr>
<td>( N_A ) (cm(^{-3}))</td>
<td>2x10(^{15})</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Defects of the layers

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Donor</th>
<th>Acceptor</th>
<th>Donor</th>
<th>Donor</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_e ) (cm(^{-2}))</td>
<td>5x10(^{-13})</td>
<td>1x10(^{-17})</td>
<td>1x10(^{-12})</td>
<td>1x10(^{-12})</td>
</tr>
<tr>
<td>( \sigma_h ) (cm(^{-2}))</td>
<td>1x10(^{-15})</td>
<td>1x10(^{-12})</td>
<td>1x10(^{-15})</td>
<td>1x10(^{-15})</td>
</tr>
<tr>
<td>( N_i ) (cm(^{-2}))</td>
<td>1.1x10(^{12})</td>
<td>4x10(^{15})</td>
<td>1x10(^{17})</td>
<td>1x10(^{17})</td>
</tr>
</tbody>
</table>
3. Results and Discussions

3.1. The influence of the CIGS absorber layer bandgap

To avoid mismatching the solar spectrum, the absorber bandgap has to be tuned from 1.06 eV up to 1.7 eV depending on the Ga fraction in the CIGS layer, that corresponds to the Ga/(In+Ga) (x) ratio that varies from 0 to 1. All the other electrical properties of the cell are kept as in Table 1, so the variation effect can be noticed. As can be seen from Figure 2, the behavior of this cell conformity the photovoltaic general trend as expected. High current density is achieved for low bandgap energy, while high voltage is achieved for high bandgap energy. As shown in Figure 3, the $J_{sc}$ decreases as a result of the increase in recombination rate and hence the decrease in carrier lifetime. In addition to the degradation of the spectrum absorption which can be noticed from QE curve (Figure 4) at large bandgap values. Contrarily, the $V_{oc}$ and FF increase with the increase of the bandgap. A maximum efficiency of 24.288% is achieved at an optimum bandgap of 1.39 eV in which the cell has a high fill factor without sacrificing its short circuit current density or even its open circuit voltage. These results is consistent with the theoretical considerations submitted by Loferski based on Shockley-Queisser limit which stated that the theoretically the maximum efficiency that can be obtained by a solar cell is for absorber layer band gap in the range of 1.2 eV to 1.5 eV [16].

![Figure 2. J-V curves of different CIGS bandgaps.](image)
Figure 3. Influence of (a) the Jsc, (b) the Voc, (c) the FF and (d) the η as a function of CIGS bandgap.
3.2. The influence of changing the CdS buffer layer

After deciding the optimum CIGS bandgap of 1.39 eV, the CdS buffer layer is replaced by In$_2$S$_3$ in order to achieve Cd-free CIGS thin film solar cell. As can be noticed from Figure 5 and Table 2, almost there is no difference between both structures, but it is better to get rid of the toxic cadmium material. This result shows that In$_2$S$_3$ is a prominent candidate that does not degrade the cell performance.

![Figure 4. Quantum efficiency of different CIGS bandgaps.](image1)

![Figure 5. Comparison of (a) JV and (b) QE of CIGS structure with different buffer layers.](image2)
4. Conclusion
In the presented study, a numerical simulation of CIGS-based thin film solar cell was presented using SCAPS. The influence of the absorbent bandgap on the performances of the CIGS solar cell has been investigated. An optimum bandgap of 1.39 eV resulting in a maximum efficiency of 24.288%, a short-circuit current of 31.3686 mA/cm², an open-circuit voltage of 0.904 V, and a fill factor of 85.62%. These results can be further improved by studying other effective parameters that need to be investigated in further studies. Also, the CdS buffer layer in the CIGS based solar cell is replaced by In$_2$S$_3$. The results show that In$_2$S$_3$ is a proper alternative that does not degrade the cell performance.

Acknowledgments
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References


