Simulation analysis of the effect graded Zn(O,S) on the performance of the ultra thin copper indium gallium diselenide (CIGS) solar cells

Chihi Adel*, Boujmil Mohamed Fethi and Bessais Brahim

Laboratoire Photovoltaïque, Centre des Recherches et des Technologies de l'Energie Technopole BorjCedria
B.P No. 95 2050 - Hammam Lif - Tunisie.

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This paper indicated a numerical modeling of ultra thin copper indium gallium diselenide (CIGS) solar cells. An optimum value of the thickness of the structure has been calculated and it is shown that by optimizing the thickness of the cell, efficiency has been increased and cost of production can been reduced. Numerical optimizations have been done by adjusting parameters such as thickness of the layers and the gap. It shows that by optimization of the considered structure, open circuit voltage (\(V_{oc}\)) increases and an improvement of conversion efficiency has been observed in comparison to the conventional CIGS system.

Key words: Graded pseudo copper indium gallium diselenide (CIGS)-Zn(O,S), solar cells, efficiency enhancement, solar capacitance simulator (SCAPS).

INTRODUCTION

Copper indium gallium diselenide (CuIn\(_{1-x}\)Ga\(_x\)Se\(_2\) or CIGSe) solar cells is a multilayer thin film technology which has been increasingly developed in the last decade; thanks to its relatively low cost combined with high efficiencies. CIGSe is a direct band gap semiconductor with a chalcopyrite structure, a p-type doping and band gap varying continuously with the gallium content x from about 1 eV for pure Cis to about 1.7 eV for CuGaSe. Presently, the highest conversion efficiency never reported in thin film technology, with a record value of 20.3% was recently reported by Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (Centre for Solar Energy and Hydrogen Research) (ZSW) (Jackson et al., 2011). Over the past decade, the CIGSe field experienced an increasing industrial development with the commercialization of high efficiency modules (Powalla et al., 2006). It is now considered as one of the most promising alternative technology to silicon-based solar cells. The p-CIGSe layer can be grown by several vacuum and non vacuum methods, such as co-evaporation (Repins et al., 2008; Thornton, 1984), sputtering (Thornton, 1984; Nakada et al., 1995), electrodeposition (Lincot et al., 2004) or nanoparticles based techniques (Vijay et al., 2003).

A numerical device model for the electronic and optical processes allows researchers for a good understanding
and also, efficient optimization of thin film solar cells. There were several numerical studies for investigation of thin film solar cells that reports to investigate most important parameters of cells such as grain boundary, defects density and thickness which contribute in performance of thin film solar cell.

Several numerical software have been developed by research groups to predict the thin film solar cell performance of the cell, a typical CIGS solar cell structure which composed of three layers, namely a transparent conductive oxide (TCO) contact which composed of n-doped graded Zn(O,S), n-doped CdS buffer layer, and p-doped CuIn\textsubscript{1-x}Ga\textsubscript{x}Se\textsubscript{2} layer.

In this paper, in order to investigate the effects of cell composed layers thickness on the performance of the cell, a typical CIGS structure which composed of five layers grille/graded Zn(O,S) / CdS / graded CIGSe / Metalas is shown in Figure 1.

The aim of this article is to illustrate the effects of band gap grading in Cu(In,Ga)Se\textsubscript{2} absorber or CIGSe and in Zn(O,S) the purpose is to demonstrate that solar capacitance simulator (SCAPS) can handle such complicated structure.

**NUMERICAL SIMULATION METHODOLOGY**

In this study, numerical modeling of CIGS thin films solar cell has been carried out by SCAPS-1D, version 3.2.01 computer software to investigate the effects on absorber band gap grading on the overall CIGS solar cell device performance. SCAPS is a one-dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent.

Several researchers have contributed to its development (Burgelman et al., 2000; Decock et al., 2011). This version has several features such as almost all parameters can be graded (that is, dependent on the local composition or on the depth in the cell) : E.g. \( \chi, \varepsilon, \beta, \beta_c, N_c, N_v, V_m, V_n, \mu_n, \mu_p, N_{A}, N_{D}, N_{i}, \) all traps (defects)\( N_t \).

Poisson equation used for semiconductor device:

\[
\frac{\partial}{\partial x} \left( \varepsilon(x) \frac{\partial \psi(x)}{\partial x} \right) = q \left( n(x) - p(x) - N_D + N_A - \rho_{\text{def}} \right) 
\]  

Where \( \psi \) is electrostatic potential, \( q \) is charge of electron, \( \varepsilon \) and \( \varepsilon_0 \) are the relative and the vacuum permittivity, respectively, \( p \) and \( n \) are hole and electrons concentrations, \( N_D \) is charge impurities of donor and \( N_A \) is acceptor type, \( \rho_{\text{def}} \) is the defect distribution.

The continuity equations for electrons and holes are:

\[
-\frac{\partial}{\partial x} J_n(x) + G(x) - R(x) = \frac{\partial n}{\partial t} 
\]

\[
-\frac{\partial}{\partial x} J_p(x) + G(x) - R(x) = \frac{\partial p}{\partial t} 
\]

Where

\[
J_n = -\frac{\mu_n}{q} n \frac{\partial E_F}{\partial x}
\]

\[
J_p = \frac{\mu_p}{q} p \frac{\partial E_F}{\partial x}
\]

Where \( J_n \) and \( J_p \) are electron and hole current densities, \( E_{Fp} \) and \( E_{Fn} \) are Quasi-Fermi level for electrons and holes, \( G(x) \) and \( R(x) \) are charge generation and recombination rates. The system of equations described that Equations 1, 2 and 3 are solved numerically, using a Gummel iteration scheme with Newton Raphson substeps (Niemegeers et al., 1998; Selberherr, 1984).

SCAPS calculates solution of the basic semiconductor equations in one-dimensional and in steady state conditions.

Recombination in deep bulk levels and their occupation is described by the Shockley Read Hall (SRH) formalism. The current transport mechanism of our model can be explained in general terms by considering the effect of light on the band diagram.

Since the calculations require the input of device parameters, the surface recombination velocities of both electrons and holes were set at \( 10^7 \) cm/s. The solar AM 1.5 radiation was adopted as the illuminating source with power density of 100 mW/cm\(^2\). The light refection of the front and back contacts was set at 0.1 and 1, respectively. The light absorption coefficient for CIGS layer was taken from absorption file. The other simulating parameters are given in Table 1.

**RESULTS AND DISCUSSION**

This paper indicates a study to optimize the CIGS based solar cell by considering the effects of layer thickness on
Table 1. Summary of the input parameters of the SCAPS demonstration model. The contacts are ohmic (‘flat band’).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Graded p-CIGS</th>
<th>CdS</th>
<th>Graded n- Zn(O,S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\varepsilon_r)</td>
<td>13.6</td>
<td>10</td>
<td>9</td>
</tr>
<tr>
<td>(\chi) (eV)</td>
<td>4.5</td>
<td>4.2</td>
<td>4.45</td>
</tr>
<tr>
<td>(E_g) (eV)</td>
<td>1.04 - 1.68</td>
<td>2.4</td>
<td>3.6</td>
</tr>
<tr>
<td>(\mu_n) (cm(^2)/Vs)</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>(\mu_p) (cm(^2)/Vs)</td>
<td>100</td>
<td>25</td>
<td>25</td>
</tr>
<tr>
<td>(N_c) (cm(^{-3}))</td>
<td>(2.2 \times 10^{18})</td>
<td>(2.2 \times 10^{18})</td>
<td>(2.2 \times 10^{18})</td>
</tr>
<tr>
<td>(N_v) (cm(^{-3}))</td>
<td>(1.8 \times 10^{19})</td>
<td>(1.8 \times 10^{18})</td>
<td>(1.8 \times 10^{19})</td>
</tr>
<tr>
<td>(N_A) (cm(^{-3}))</td>
<td>(2 \times 10^{18})</td>
<td>1</td>
<td>(10^{17})</td>
</tr>
<tr>
<td>(N_D) (cm(^{-3}))</td>
<td>1</td>
<td>(10^{16})</td>
<td>1</td>
</tr>
<tr>
<td>(V_e) (cm/s)</td>
<td>(10^7)</td>
<td>(10^7)</td>
<td>(10^7)</td>
</tr>
<tr>
<td>(V_h) (cm/s)</td>
<td>(10^7)</td>
<td>(10^7)</td>
<td>(10^7)</td>
</tr>
</tbody>
</table>

Figure 2. Variation efficiency and FF as a function of graded Zn(O,S) thickness.

the performance of the cell and the graded structure of Zn(O,S). In this respect, the structure of CIGS based thin film solar cell is shown in Figure 1. Figure 2 shows variation of TCO thickness Zn(O,S) versus fill factor (FF) and efficiency. It is shown that by decreasing the thickness of graded n-Zn(O,S), cell efficiency increases. It is due to this fact that n-Zn(O,S) is not fully transparent for light and this layer absorbs and reflects the sunlight. As it is shown in Figure 2 by increasing the Zn(O,S) thickness, light absorption increases and leads to lower efficiency. By decreasing the Zn(O,S) layer from 100 nm to 10 nm, cell efficiency increases from about 19.60 to 20.44; also FF curve has the same increasing rate as it shown in \(\eta\). Calculation shows that variation of the Zn(O,S) thickness has no effect on the current density.

Figure 3 shows the variation of short circuit current \(J_{sc}\) and open circuit voltage \(V_{oc}\) in terms of the graded p-CIGS. It is shown that by increasing the thickness from 2 nm to 3 \(\mu\)m, \(J_{sc}\) increases and after about 1 \(\mu\)m is constant. Also, Figure 3 demonstrates that by increasing the thickness from 2 nm to 3 \(\mu\)m, \(V_{oc}\) decreases exponentially.

Figure 4 shows the variation of \(\eta\) efficiency and FF versus CIGS thickness. It is shown that by increasing the thickness from 10 nm to 0.5 \(\mu\)m, efficiency increases from 18.30 to 20.04; efficiency increases about 10% and after 0.5 \(\mu\)m falls down. From the simulation, results were found that the optimized value of the graded p-CIGS is 0.5 \(\mu\)m which leads to a thinner and cheaper solar cell. Simulation results shows optimized value of CIGS and graded n-Zn(O,S) thickness is 0.5 \(\mu\)m and 10 nm, respectively. By choosing the optimized value \(J_{sc}\), \(V_{oc}\) and \(\eta\) are 41.85 mA/cm\(^2\), 0.63 V and 20.44%, respectively. From Figure 5, it is clear that in optimized structure \(V_{oc}\) increased, \(J_{sc}\) decreases a little but cell efficiency increases from 18.35 to 20.04.
Figure 3. Variation of $J_{sc}$ and $V_{oc}$ as a function of graded CIGS thickness.

Figure 4. Variations of efficiency and FF as a function of graded CIGS thickness.

Figure 5. J-V characteristics of typical (red curve) and optimized (blue curve) graded CIGS.
Conclusion

This paper indicated a numerical investigation of graded CIGS based solar cells. Numerical optimizations have been done by adjusting parameters such as the combination of band gap, as well as the specific structure of the cell. From the simulation result, it was found that by optimization of the considered structure, optimized value of CIGS and TCO thickness is 0.6 um and 10 nm and an improvement of conversion efficiency has been observed in comparison to the conventional CIGS which cell efficiency increases from 18.04 to 20.04%.

Conflict of Interests

The author(s) have not declared any conflict of interests

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REFERENCES


