Simulation of CuO/ZnO heterojunction for photovoltaic applications

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Abstract. Inorganic semiconductors become one of the most gifted candidate for photovoltaic applications instead of high cost silicon devices and organics ones. Therefore, in this paper, inorganic CuO/ZnO heterojunction is simulated as thin layer solar cells employing SCAPS program. Both effect of CuO and ZnO layers thickness on basic parameters of solar cells is investigated deeply. Simulated results of this solar cell device indicate that the absorber layer is responsible for separation process of generated carriers. Higher efficiency of about 23 % could be achieved with 2 μm of CuO thickness and 100 nm of ZnO layer for devices. Generally, the main aspects that controlling the solar cell performance are depletion region width, built-in potential, the charge carrier collection length and generation and recombination rates.

1. Introduction

Although Popular photovoltaics such crystalline silicon (c-Si), cadmium telluride (CdTe), and copper indium gallium diselenide (CIGS) have higher efficiencies, but there are some disadvantages of them [1]. For example, the fabrication of c-Si
needs high temperature and ultra-high vacuum, which make such process, is very expensive. CIGS and CdTe photovoltaics are based on non-earth abundant materials [1, 2]. Therefore, the wide spread of solar cells requires some aspects such as the used materials for fabrication should be abundant, inexpensive and non-toxic. In addition, the solar cells should easily fabricated at low temperature and cost-effective techniques [1-4].

For such purpose, inorganic metal oxide semiconductors are the most promising candidates which nearly imply these requests and considered as an alternative to the high cost silicon devices and organics ones [1, 2, 5-7].

Zinc oxide (ZnO) is a promising applicant for solar cell applications [1-3, 5, 8-12]. ZnO is a wide band gap semiconductor (3.37 eV) with negative conductivity [11, 13]. Moreover, ZnO has various application in many fields such light-emitting diodes [5, 6] catalysts [14], antioxidants [15], photodetectors [16] and water treatment [15]. There are different techniques could be employed to have several shapes of ZnO nanostructures such as chemical vapor deposition [17], pulsed laser deposition [18], molecular beam epitaxy [19], sputtering [1, 2], chemical bath deposition [20], electrodeposition [21], and hydrothermal [5, 6, 11].

Combination of ZnO nanostructures with another p-type semiconductor is a key to have higher efficiency heterojunction solar cells. Copper oxide (CuO) considered one of these semiconductors to fabricate solar cells since it has property band gap (1.2 eV) for such applications [22]. CuO has higher light coefficient with lower thermal emittance. Moreover, less mismatch between lattices will be achieved through ZnO/CuO heterojunction [22]. Consequently, alignment of energy level will develop the separation process of charge carriers and therefore increase the solar cells performances [23].

Numerical study of nanomaterials have become powerful methods for scientists and engineers to predicate the efficiency and performance of such materials on
optoelectronic applications like solar cells, and light emitting diodes. Here, we deeply investigated numerical simulation of ZnO/CuO heterojunction as solar cells. The effect of active layer and window layer thickness on the solar cell basic parameters was calculated employing Solar Cell Capacitance Simulator Structures (SCAPS) program in order to know the optimal thickness to obtain higher performances [24, 25].

2. Materials and Methods

2.1 Solar Cell Structure:

The structure of simulated solar is presented in figure 1. In this case, CuO film was employed as an active layer and ZnO was used as window layer in the presented heterojunction solar cell. Gold (Au) and Florin doped tin oxide (FTO) were employed as back and front contacts, respectively.

![Diagram structure of CuO/ZnO heterojunction thin film solar cell.](image)

Figure 1. Diagram structure of CuO/ZnO heterojunction thin film solar cell.

2.2 Materials Properties and Simulation process:

The properties of layers, which are used in numerical simulation, are obtained from previous literature [22, 26] are listed table 1.
Table 1. Properties of Materials used in our simulation

| Material properties                              | p-CuO  | n-ZnO  |
|--------------------------------------------------|--------|--------|
| Relative permittivity                            | 18.1   | 86     |
| Bandgap (eV)                                     | 1.2    | 3.37   |
| Electron affinity (eV)                            | 4.07   | 3.9    |
| Effective density of states of valence band max. (cm\(^{-3}\)) | 5.5E+20 | 1.50E+21 |
| Effective density of states of conduction band min. (cm\(^{-3}\)) | 3E+19   | 1.32E+20 |
| Acceptor concentration(cm\(^{-3}\))              | 1.00E+16 | 0      |
| Donor concentration(cm\(^{-3}\))                 | 0      | 1.00E+19 |
| Mobility of Hole (cm\(^{2}\)/V s)               | 10     | 20     |
| Mobility of Electron (cm\(^{2}\)/V s)           | 0.1    | 10     |

In this paper, Solar Cell Capacitance Simulator structures (SCAPS-1D) software program was used to simulate and explore devices [27-29] as shown in figure 2 as screenshot from the program. The impact of thickness of window layer as well as active layer on solar cell basic parameters was examined deeply. One sun illumination (AM 1.5 spectrum illumination -100 mW/cm\(^2\)) was used for all numerical simulations calculations while keeping temperature constant at 300 K. Both Poisson and continuity equations of holes and electrons were employed for the simulations [23]:

\[
\frac{d^2 \psi(x)}{dx^2} = \frac{e}{\varepsilon_0 \varepsilon_r} \left( p(x) - n(x) + N_D - N_A + \rho_p - \rho_n \right) \tag{1}
\]
\[
\frac{dJ_n}{dx} = G - R \quad \text{and} \quad \frac{dJ_p}{dx} = G - R
\]  

(2)

Figure 2. Screenshot from SCAPS program for simulated CuO/ZnO solar cell.

3. Results and discussion

To investigate the influence of absorber layer thickness on solar cell basic parameters (open circuit voltage \(V_{oc}\), short circuit current density \(J_{sc}\), fill factor \(FF\), as well as cell efficiency \(\eta\)). The CuO layer thickness was varied from 0.01 to 5 μm while the window layer was fixed at 100 nm. Figure 3 shows the outline of the \(J_{sc}\), \(V_{oc}\), \(FF\), and \(\eta\) versus p-CuO film thickness. It is obvious that \(V_{oc}\) rises sharply from 0.715 to 0.785 V with increasing of the absorber layer as illustrated in figure 3a. This behavior could be attributed to the enhancement of built-in potential which produced by diffusion of holes from active layer to window layer of the solar cell [1]. This outcome is the same as that reported for Cu\(_2\)O solar cells in which increasing thickness creates a built-in potential with maximum value of about 0.7 V[1, 30]. Also, the increasing of \(V_{oc}\) could be explained by increasing the charge carriers generation rate as well as
reducing leakage current in interface of heterojunction which supported by the equation\[1].

\[
V_{oc} = \frac{k_B T}{q} \ln \left(1 + \frac{I_{ph}}{I_0}\right)
\]  \tag{3}

Figure 3b clarifies $J_{sc}$ of simulated heterojunction solar cells. It is clear that the current increase from about 36.4 mA/cm$^2$ to 38.7 mA/cm$^2$ with thickness growing from 100 nm to 500 nm. With further increase in layer thickness, the current become constant at about 38.7 mA/cm$^2$. The length of charge collection could recognize improvement of $J_{sc}$ with thickness increasing of CuO layer from 100 to 500 nm where photogenerated carriers will recombine together before collecting with lower thickness while with higher thickness; they will be separated and gathered easily. So generation rate of hole electron pairs will be improved with thickness increasing up to that determined from the absorption coefficient of CuO layer [30] achieving constant value of $J_{sc}$.

Figure 3c displays the FF behavior where a partial increase with thickness from 100 nm to 500 nm followed by monotonically decrease with thickness increase. Such change could be deduced from FF equation, which shows that FF is inverse proportional with $V_{oc}$ and $J_{sc}$ values as following.

\[
FF = \frac{V_m J_m}{V_{oc} J_{sc}}
\]  \tag{4}
Figure 3. Simulated (a) $V_{oc}$, (b) $J_{sc}$, (c) FF, and (d) η of ZnO/CuO heterojunction devices with absorber layer thickness.

Figure 3d shows the change in η of simulated devices with thickness of CuO layer. It is obvious that η displays significant improvement with thickness increasing from 100 nm to 500 nm followed by slight increase from about 21.25 % to about 23 % with increasing thickness up to 5 μm. Such trend of the η could be explained by its dependence on the $V_{oc}$, $J_{sc}$, and the FF values as presented by the following equation [31]:

\[
\eta = \frac{V_{oc} \cdot J_{sc} \cdot FF}{P_{in}}
\]
\[
\eta = \frac{FF \, V_{oc} \, J_{sc}}{P_{in}}
\]  

From that, it could be assume that 2-μm thickness for CuO film is the optimum one to have higher performance of the simulated photovoltaic solar cell here.

Figure 4 display a brief for the simulated results of basic parameters for the heterojunctions with different window layer thicknesses keeping the absorber layer constant at 2 μm. It is clear from figure 4a that, \( V_{oc} \) decline with ZnO layer increasing. This case happen because of reducing of photogenerated current and increasing of the recombination rate of charge carries according to equation (3). In addition, increasing thickness of window layer blocks light to pass through the heterojunction interface. Moreover, this confirmed that the built-in potential which is responsible for the formation of \( V_{oc} \), is formed in active layer side (CuO) [1]. Figure 4b presents the \( J_{sc} \) where it has the same behavior the \( V_{oc} \). This style could be explained by increasing the leakage current, which affect negatively on the generated current as well as length of charge collection reached maximum value. Inserting of buffer layers at the interface of the heterojunction could paly important factor to reduce the leakage current through reducing layer mismatch and increasing band gaps alignment.

The behavior of FF as illustrated in figure 4c have inverse shapes of the \( J_{sc} \) and the \( V_{oc} \) where it is inverse proportional to their values as previously discussed according to equation (4). Figure 4d reflects the dependence of the \( \eta \) on values of the \( V_{oc} \), the \( J_{sc} \), and the FF as shown in equation (5). In this situation, then firstly increase from 22.9 to 23.3 % by increasing thickness from 10 nm to 100 nm. Then, with further thickness increasing, it falls down to about 23.1% and become constant. It can conclude that the higher performance of solar cells could be obtained with 100 nm thickness of ZnO as window layer.
Figure 4. The calculated (a) $V_{oc}$, (b) $J_{sc}$, (c) FF, and (d) $\eta$ of the heterojunction devices versus the window film thickness.

### 4. Conclusion

CuO/ZnO heterojunction solar cells were simulated employing SCAPS program. Impact of active layer and window layers on solar cell basic parameters was examined deeply. Results of simulated devices showed that the built-in potential was formed in CuO side and higher efficiency of 23 % was achieved with thickness of 2 μm of absorber layer. The thickness of 100 nm for ZnO as window...
layer should be applied to have higher efficiencies. The main factors directing the performance of heterojunction devices are the charge carrier collection length, generation and recombination rates, depletion region width and built-in potential. Application of our simulated results on the experimental area would support and improve the solar cell conversion efficiency.

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