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## Optimization of defected ZnO/Si/Cu<sub>2</sub>O heterostructure solar cell

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#### ARTICLE INFO

#### ABSTRACT

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In the present work, we review the optimization of the performance of a newly defected ZnO/Si/Cu<sub>2</sub>O heterojunction solar cell using the Analysis of Microelectronic and Photonic Structures (AMPS-1D) computer simulator under the AM1.5G illumination and the operating temperature of 300 K. The light J-V characteristics were investigated by varying the input parameters and the temperature. The use of p-type Cu<sub>2</sub>O-back layer in the structure is to enhance the open-circuit voltage ( $V_{OC}$ ). The performance of ZnO/Si/Cu<sub>2</sub>O heterojunction solar cell is studied in order to optimize the layers parameters, such as the thickness of p-Si absorber layer, the doping and the defects concentrations of the p-Si absorber layer and to obtain an efficient proposed structure. The defects concentration of p-Si absorber layer was fixed in the first step at  $N_{def}(p-Si) = 10^{14}/cm^3$ . With the optimized p-Si layer parameters, an efficiency of 16.23% was obtained with  $J_{SC} \sim 26.25$  mA/cm<sup>2</sup>,  $V_{OC} \sim 0.72$  V and *FF*~0.85 for n-ZnO window (0.1 µm)/p-Si Absorber (10 µm)/p-Cu<sub>2</sub>O (0.1 µm) heterostructure. For  $N_{def}(p-Si) = 10^{11}/cm^3$  we estimate best characteristics of about:  $J_{SC} \sim 27.57$  mA/cm<sup>2</sup>,  $V_{OC} \sim 0.78$  V, *FF*~0.90 and Eff ~ 21.78%.

#### 1. Introduction

Intrinsic or doped, either by oxygen vacancies or by substitution of some of the atoms, zinc oxide (ZnO) and cuprous oxide (Cu<sub>2</sub>O) based semiconductors have received increasing concern because of their strong points of earth-abundance, non-toxicity, tunable optical band gap, low-cost in resources and ease of processing by versatile technology routes. Such pulse laser deposition [1], sol gel [2], electrodeposition [3], spray [4,5], sputtering [6,7] and other methods [8,9] are potential technologies offers a range of versatile new features and enhancements that meet the needs of ZnO and Cu<sub>2</sub>O based applications. So far a large number of studies have been widely conducted to apply ZnO and Cu<sub>2</sub>O semiconductors in broad applications such as gas sensors [10,11], glucose sensors [12,13], photocatalyst [14–16], photodegradation sensors [17,22,23], conductive switching [24] and photovoltaic (PV) devices [25–29].

ZnO thin films are electrically a high n-type conductive and optically an excellent transparent (85%) in the visible range. Furthermore, they have wide energy band gap of around  $\sim$ 3.37 eV at room temperature with high carrier concentration, where they act extensively as most suitable n-type partner with common p-type thin films such as Cu<sub>2</sub>O [25, 29], CIGS [30], CdTe [31] and silicon [32]. In addition, Cu<sub>2</sub>O thin films are non-stoichiometric, electrically natural p-type conductive and optically absorbing in the short-wavelength considered amount ( $\sim 10^4$ /cm) of the luminous spectrum as they have direct energy band gap of 1.9–2.1 eV [18,26,33] with low carrier concentrations of  $\sim 10^{-16} \, \text{cm}^{-3}$  at room temperature [9]. However, the low photovoltaic efficiency of metal oxide-based photovoltaics is still challenging. In other words, ZnO and Cu2O based semiconductors are still under further development in order to become suitable candidates for new photovoltaic heterostructures. Up till now, the achieved practical power conversion efficiencies of the most common ZnO/Cu<sub>2</sub>O heterojunction solar cells are remained significantly at lower percentages of ~6% because of some drawbacks, such as the non-ideal band alignment between the two heterojunction-sides and the defects within the layers [34-37]. Nevertheless, the sufficient electrical and optical properties of Cu<sub>2</sub>O thin films strongly nominate them to other PV-uses. In particular, to enhance the open-circuit voltage (Voc) by adding Cu2O back-layer in CuO based solar cells, the one dimensional simulation of Zhu et al. [38] has shown that the conversion efficiency increased from 19% for a non-defected TiO<sub>2</sub>/CuO two-layer structure to 28.5% for a non-defected TiO<sub>2</sub>/-CuO/Cu2O three-layers structure. Considering the enormous use of the robust and expensive crystalline silicon materials in advanced photonics

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Fig. 1. Schematic of the newly ZnO/Si/Cu<sub>2</sub>O heterostructure solar cell.

and electronics, it should be advisable to motivate the present-day extensively studied materials such as the TCOs and chalcopyrite thin films by using them as partners or supporters, side by side with thin films of crystalline silicon. Recently, based on one-dimensional simulator

(SCAPS) and using an absorber of 1 µm of CIGS backed by 1 µm of crystalline silicon (c-Si) thin film in order to minimize the indium and gallium constituents, Heriche et al. [30] have reported conversion efficiency of 21.3%. In addition, because of its transparency and excellent electrical properties, ZnO has been integrated as n-type partner with p-type silicon to fabricate low cost thin film solar cells. Currently, the achieved practical power conversion efficiencies of the ZnO/Si heterojunction solar cells are also remained at modest percentages, under 8.5% [39,40]. This modesty is likely due to the strong dependence of the common ZnO/Si heterojunction performance on the properties of deposited ZnO films. Here, ZnO/Si/Cu<sub>2</sub>O heterojunction has high harvest of photons because of its double distinct p-type band gaps. The incident photons having energies smaller than the band gap of ZnO and greater than the band gap energy of Si will be absorbed near the depletion region as they competently transmit through the ZnO window. Those photons who have absorption length longer than the absorber

## Table 1 Settings for ZnO, Si and Cu<sub>2</sub>O layers used in the simulation.

Parameters	n-ZnO	p-Si	p-Cu <sub>2</sub> O
w (µm)	0.1	10	0.1
$\varepsilon/\varepsilon_0$	9.0	11.9	9.0
$E_g(eV)$	3.37	1.12	2.1
$N_{a,d}$ (cm <sup>-3</sup> )	$N_d$ : $1 \times 10^{19}$	$N_a$ : $1 imes 10^{19}$	$N_a:1 imes10^{16}$
$\chi_e(eV)$	4.5	4.05	3.2
$\mu_n(\text{cm}^2\text{V}^{-1}\text{s}^{-1})$	100.0	1450	20.0
$\mu_p (\text{cm}^2 \text{V}^{-1} \text{s}^{-1})$	25.0	500	40.0
$N_{c}(cm^{-3})$	$2.22\times 10^{18}$	$2.80\times10^{19}$	$2.20\times10^{18}$
$N_{\nu}({\rm cm}^{-3})$	$1.8\times10^{19}$	$2.65\times 10^{19}$	$1.11\times 10^{19}$
$N_{def}(\text{cm}^{-3})$	$1\times 10^{14}$	$1\times 10^{14}$	$1\times 10^{14}$



Fig. 2. Typical data input panels of the AMPS-1D graphical user interface, allowing to set the solar cell device and its settings.



Fig. 3. Separated layers-energy level diagram of ZnO/Si/Cu<sub>2</sub>O solar cell heterostructure.



Fig. 4. Light J-V curve of the  $0.1\,\mu\text{m-ZnO}/10\,\mu\text{m-Si}/0.1\,\mu\text{m-Cu}_2\text{O}$  solar cell.

interlayer thickness and successfully traveled in the thin film Si interlayer will be absorbed into Cu<sub>2</sub>O back layer. The Cu<sub>2</sub>O back layer itself will be also acting as barrier layer between p-Si material and the back contact to enhance the open circuit voltage  $V_{\rm OC}$  [38] of the ZnO/Si heterojunction.

To avoid wasting resources, effort and time, solar cell community need to understand, explain and solve the physic and technology interferences of solar cell devices by using numerical simulators [30,31, 40,41]. These requirements have been reflected on the development of solar cells in which diverse abundant/non-abundant and low/high-cost materials, as well as their large influencing parameters, have been explored to renovate solar cell devices. The freely available Analysis of Microelectronic and Photonic Structures (AMPS-1D) one dimensional program was developed in 1990's by professor Fonash's team at the Pennsylvania State University [42].

In this paper, AMPS-1D simulator was considered to optimize a newly proposed defected ZnO/Si/Cu<sub>2</sub>O heterojunction solar cell. The structure is analyzed numerically by changing different input

parameters of the device such as thickness, doping and defect densities, and temperature. We examine the structural templates  $\text{ZnO/Si/Cu}_2\text{O}$  by light J-V characteristics and their electrical parameters: the short circuit current ( $J_{\text{SC}}$ ), the open circuit voltage ( $V_{\text{OC}}$ ), the fill factor (*FF*) and the efficiency ( $\eta$ ).

#### 2. Device settings and simulation process

Fig. 1 shows schematic of the newly proposed n-ZnO/p-Si/p-Cu<sub>2</sub>O heterostructure solar cell. In order to analyze the transport physics in this structure, AMPS-1D solves the dipolar problems of device according to the Poisson equation and the continuity equations for electrons and holes. AMPS-1D simulator is a software environment, which is used to emulate a real solar cell behavior. In general, the simulation process would have to go through the following steps described by the screenshots in Fig. 2. The screenshot (a) shows the typical information input panel of the AMPS-1D graphical user interface for simulation process of solar cell. The input buttons in this panel allow to specify the model of simulation and to access to the device operating conditions and the device structure and material parameters panels. The DOS mode is chosen for the device simulation. The screenshot (b) demonstrates the structure and the set of the material parameters of one particular layer as well as the input buttons of optical properties and defects. The screenshot (c) shows the results of light J-V characteristics visualized in the form of curve and axes. During simulation handling, the AM1.5 illumination spectrum with incident power of 100 mW/cm<sup>2</sup> is considered. The input parameters of each layer of the proposed structure have been summarized in Table 1. These parameters were the thickness, t, permittivity constant  $\varepsilon/\varepsilon_0$ , band gap  $E_g$ , electron affinity  $\chi_e$ , electron/ hole mobility  $\mu_n/\mu_n$ , effective density of states in conduction/valence band  $N_c/N_{\nu}$ , donor/acceptor concentration  $N_D/N_A$ , defect concentration  $N_{def}$  and the absorption coefficient in the range wavelength of 320-1100 nm. At the front contact, the reflection was neglected. The thermal velocity recombinations for holes/electrons  $S_n/S_p$  at front and back contacts were  $1.0 \times 10^7$  cm/s. In Addition, the barrier height potentials PHIBO and PHIBL were considered Ohmic or slight Schottky barrier. As shown in Fig. 3, PHIBO (PHIBL) is the difference between the work function of the metal front-contact (back-contact) and the electron affinity of the semiconductor in contact [E<sub>C</sub>-E<sub>F</sub>] with the unit of eV at front (back) contact.



Fig. 5. Photovoltaic parameters of defected ZnO/Si/Cu<sub>2</sub>O solar cell as a function of ZnO window layer thickness.



Fig. 6. Photovoltaic parameters of defected ZnO/Si/Cu<sub>2</sub>O solar cell as a function of p-Si absorber layer thickness.



Fig. 7. Photovoltaic parameters of defected ZnO/Si/Cu<sub>2</sub>O solar cell as a function of p-Cu<sub>2</sub>O back layer thickness.

#### 3. Results and discussion

In this section, we will examine the performance of the ZnO/Si/Cu<sub>2</sub>O solar cell based on the settings summarized inTable 1. Fig. 3 shows the separated energy levels diagram for the ZnO, Si, Cu<sub>2</sub>O layers. The conduction band offset ( $\Delta E_{\rm C}$ ) at the ZnO/Si junction is the difference between the electron affinities of the ZnO and Si semiconductors:  $\Delta \chi = \chi_{\rm Si} \cdot \chi_{\rm ZnO} = -0.45$  eV. The obtained cliff will allow the transport of photogenerated electrons to get form p-Si absorber layer to ZnO emitter layer before they recombine. On the other hand, the small valence band offset ( $\Delta E_{\rm V}$ ) for Si/Cu<sub>2</sub>O is found to be about -0.07 eV [( $\chi_{\rm Cu<sub>2</sub>O} + E_{\rm gCu<sub>2</sub>O}) - (\chi_{\rm Si} + E_{\rm gSi}) = -0.07$ eV]. Therefore, this established semi-alignment will allow the holes flowing through the rear contact. Thus, there is a good alignment between ZnO and Si and between Si and Cu<sub>2</sub>O.

The light current density-voltage (J-V) characteristics are the fitting of current density versus the voltage. Based on the settings mentioned in Table 1, the light J-V curve and its characteristics, are shown in Fig. 4. The defect concentration of p-Si absorber layer was fixed at  $N_{def}(p-Si) = 10^{14}/cm^3$ . It has been demonstrated a good performance:  $\eta \sim 16.234\%$  with  $J_{SC} \sim 26.251 \text{ mA/cm}^2$ ,  $V_{OC} \sim 0.727 \text{ V}$  and  $FF \sim 0.85$ .

#### 3.1. Effect of the ZnO layer thickness on the cell performance

Fig. 5 summarizes the effect of the ZnO window layer thickness on the performance of the ZnO/Si/Cu<sub>2</sub>O solar cell from 100 nm to 500 nm. As shown in Fig. 5, all J-V characteristics remain unchanged and a fixed efficiency of about 16.2% was obtained, with  $J_{SC} \sim 26.2 \text{ mA/cm}^2$ ,  $V_{OC}$ 

 ${\sim}0.72$  V and FF  ${\sim}0.85$ . This behavior is a result of the deficient carrier generation in the ZnO layer due to its wide band-gap energy of 3.37 eV.

#### 3.2. Thickness optimization of p-Si absorber layer

Fig. 6 shows the evolution patterns of  $V_{\text{OC}}$ ,  $J_{\text{SC}}$ , *FF* and  $\eta$  of ZnO/Si/ Cu<sub>2</sub>O solar cell as a function of p-Si absorber layer thickness from 0.5 µm to 50  $\mu$ m. Particularly, J<sub>SC</sub> and  $\eta$  increase rapidly from 14.37 to about  $26.25\,mA/cm^2$  (by  $\sim 45.23\%$ ) and from 9,71 to about 16.23% (by  $\sim$  40.17%), respectively, when the Si-layer thickness increases from 0.5 to 10  $\mu$ m. While, V<sub>OC</sub> (~0.7 V) and FF (~0.85) are almost unchanged. For a thick p-Si absorber layer (more than 10 µm), all photovoltaic parameters have almost unchanged values. This overall behavior is resulted from the increase of the photons absorption and even the increase of the electron-hole generation in the p-Si absorber layer. Therefore, the thickness of  $10 \, \mu m$  is chosen as an optimum thickness for p-Si absorber layer for efficient ZnO/Si/Cu2O solar cell. This is consistent with what has been found in previous research. It was reported that 10-50 µm thick c-Si based solar cells can have conversion efficiencies up to  $\sim$ 17%. Reuter et al. [43] reported that an efficiency of 17% is achieved on mono-crystalline silicon solar with thickness of approximately  $47 \,\mu\text{m}$ , which is fabricated by using transfer layer process. Yoon et al. [44] reported an efficiency of about 17.5% within 15  $\mu$ m thick crystalline Si solar cells. Cruz-Campa et al. [45] obtained an efficiency of 14.9% within 14 µm thick crystalline silicon solar cells. Li et al. [46] attempted to demonstrate that tandem ultra-thin a-Si/c-Si solar cells with a nanopyramid structure could obtain efficiencies as high as 13.3% within



Fig. 8. Photovoltaic parameters of defected  $ZnO/Si/Cu_2O$  solar cell as a function of doping concentration  $N_A(p-Si)$ .

only 8 µm thick silicon solar cells.

#### 3.3. Thickness optimization of Cu<sub>2</sub>O back layer

To clarify the effect of the Cu<sub>2</sub>O back layer thickness (from 0 nm to 500 nm) on the cell performance, the ZnO/Si/Cu<sub>2</sub>O heterostructure was simulated and the results are summarized in Fig. 7. At 0 nm thick (without Cu<sub>2</sub>O layer), the photovoltaic parameters are initially low with  $J_{SC} \sim 20.42 \text{ mA/cm}^2$ ,  $V_{OC} \sim 0.68 \text{ V}$ ,  $FF \sim 0.84$  and an efficiency of about 11.77%. In the presence of a Cu<sub>2</sub>O layer with an increased thickness, all J-V characteristics remain unchanged at a good efficiency  $\eta$  of about 16.2%, with  $J_{SC} \sim 26.2 \text{ mA/cm}^2$ ,  $V_{OC} \sim 0.72 \text{ V}$  and  $FF \sim 0.85$ . Therefore, a few µm of Si layer give more chances to a few nm of Cu<sub>2</sub>O back layer (several hundred nm to few µm for most experimental Cu<sub>2</sub>O based solar cells [47,48]) to absorb the photons who have absorption length longer than the p-Si interlayer thickness. Thus, a high efficiency of about 16.2% has been expected.

#### 3.4. Optimization of acceptor density of p-Si absorber layer

Fig. 8 shows the evolution patterns of  $J_{\rm SC}$ ,  $V_{\rm OC}$ , FF and  $\eta$  of ZnO/Si/ Cu<sub>2</sub>O solar cell versus different acceptor concentrations of p-Si absorber layer,  $N_{\rm A}$ (p-Si). For lowest and/or highest doping concentrations ( $N_{\rm A}$ (p-Si) < 10<sup>14</sup>/cm<sup>3</sup> and/or  $N_{\rm A}$ (p-Si) > 10<sup>19</sup>/cm<sup>3</sup>),  $N_{\rm A}$ (p-Si) have a large impact on the electronic properties (mobility, conductivity/resistivity and related parameters) of crystalline silicon. Consequently,  $N_{\rm A}$ (p-Si) was varied in a moderate range from  $1 \times 10^{14}/\text{cm}^3$  to  $1 \times 10^{19}/\text{cm}^3$  [49]. When  $N_A(\text{p-Si})$  exceed the effective density of states  $N_\nu$ (p-Si) (~10<sup>19</sup>/cm<sup>3</sup>), the crystalline silicon becomes degenerate semiconductor, thus the energy band-gag narrowing will be [50].

At the beginning, for  $N_A(p-Si) = 1 \times 10^{14}/\text{cm}^3$  the efficiency  $\eta$  and FF were achieved small values of about 8.67% and 0.67, respectively. For  $N_A(p-Si) > 1 \times 10^{14}/\text{cm}^3$ , we observe that  $J_{SC}$  shows slight decrease from 27.41 mA/cm<sup>2</sup> at the concentration  $1 \times 10^{14}/\text{cm}^3$  to 26.25 mA/cm<sup>2</sup> at the concentration  $1 \times 10^{19}/\text{cm}^3$ . In contrast, the open circuit voltage,  $V_{OC}$ , shows a considered increase from 0.47 V at the concentration  $1 \times 10^{14}/\text{cm}^3$  to 0.72 V at the concentration  $1 \times 10^{19}/\text{cm}^3$ . For  $N_A(p-Si) = 1 \times 10^{19}/\text{cm}^3$ , the efficiency  $\eta$  and FF were increased to about 16.23% and 0.85, respectively. The recommended acceptor density  $N_A(p-Si)$  should be higher than that of its defect density (in this case  $1 \times 10^{14}/\text{cm}^3$ ).

#### 3.5. Effect of Gaussian defects of ZnO/Si/Cu<sub>2</sub>O heterostructure

Simulation results for ZnO/Si/Cu<sub>2</sub>O heterostructure with different gaussian (both of acceptor-like and donor-like) defects located in the band gap of p-Si absorber layer are shown in Fig. 9. From this figure, the defect density,  $N_{def}$ (p-Si), shows harmful effects on the ovarall performance of the device. The highest possible values of J-V charactristics were obtained when  $N_{def}$ (p-Si) < 1 × 10<sup>14</sup>/cm<sup>3</sup>. At lower defects concentration  $N_{def}$ (p-Si) = 1 × 10<sup>11</sup>/cm<sup>3</sup> the corresponding characteristics were:  $J_{SC} \sim 27.57 \text{ mA/cm}^2$ ,  $V_{OC} \sim 0.78 \text{ V}$ ,  $FF \sim 0.90$  and  $\eta \sim 21.78\%$ .



Fig. 9. Photovoltaic parameters of defected ZnO/Si/Cu<sub>2</sub>O solar cell as a function of defects concentration N<sub>def</sub>(p-Si).

Increasing  $N_{\rm def}(p-Si)$  more than  $1 \times 10^{14}/{\rm cm}^3$ , the  $J_{\rm SC}$  and  $V_{\rm OC}$  were significantly affected. The defect concentration of  $1 \times 10^{17}/{\rm cm}^3$  caused a sharp fall in the J-V charactristics:  $J_{\rm SC} \sim 7.23 \,{\rm mA/cm}^2$ ,  $V_{\rm OC} \sim 0.58 \,{\rm V}$ , *FF*  $\sim 0.82$  and  $\eta \sim 3.46\%$ . This poor behavior of the ZnO/Si/Cu<sub>2</sub>O device at high bulk defects is resulted from recombination phenomena. Therefore, the current transport may severely affected by the bulk defect density of the layer. This effect is related to created trapping (recombination) in the bulk layer that limits the efficiency [51].

# 3.6. Operating temperature effect on $ZnO/Si/Cu_2O$ heterostructure performance

In the literature, the dependence of the  $V_{\rm OC}$  to the operating temperature is used as an indicator on the stability of solar cells [30]. To testify this vital dependence on the defected ZnO/Si/Cu<sub>2</sub>O hetero-structure solar cell, the operating temperature is stepped from 300 K to 600 K by 50 K. Fig. 10 shows the evolution pattern of the photovoltaic parameters as a function of the operating temperature. Generally, increasing the operating temperature conduct to a decrease of material band gap and eventually an increase to the leakage current and a decrease to the  $V_{\rm OC}$ . The current density  $J_{\rm SC}$  has almost unchanged pattern (~26.5 mA/cm<sup>2</sup>). From Fig. 10,  $V_{\rm OC}$  decreased from ~0.73 V (recorded at 300 K) to ~ 0.32 V (recorded at 600 K). A similar behavior is observed for *FF* and efficiency which decreased from ~0.85 to ~16, 234% (at 300 K) to 0.59 and 4.97% (at 600 K), respectively.

#### 4. Conclusion

In this contribution, a newly proposed ZnO/Si/Cu<sub>2</sub>O heterostructure solar cell was studied by computer simulation using AMPS-1D software. We studied firstly the influence of thicknesses of different layers in the proposed structure and the acceptor concentration of p-Si absorber layer on the light J-V characteristics, in order to optimize the input parameters of the ZnO/Si/Cu<sub>2</sub>O solar cell. The impact of defects density of p-Si absorber layer and the operating temperature on the proposed ZnO/Si/ Cu<sub>2</sub>O solar cell performance were also investigated. A 0.1 µm-ZnO/ 10  $\mu$ m-Si/0.1  $\mu$ m-Cu<sub>2</sub>O heterostructure with  $N_A$ (p-Si) = 10<sup>19</sup> cm<sup>-3</sup> showed a good characteristics:  $J_{SC} \sim 26.25 \text{ mA/cm}^2$ ,  $V_{OC} \sim 0.72 \text{ V}$ ,  $\textit{FF} \sim 0.85$  and  $\eta \sim 16.23\%$  . These considered values were attributed to a low defect density of  $1 \times 10^{14}$ /cm<sup>3</sup> in p-Si absorber layer. By optimization, we realized a record efficiency for  $N_{def}(p-Si)$  lower than  $10^{14}/$ cm<sup>3</sup>. For  $N_{\text{def}}(\text{p-Si}) = 10^{11}/\text{cm}^3$  best characteristics have been estimated of about:  $J_{\rm SC} \sim 27.57 \, {\rm mA/cm^2}, \quad V_{\rm OC} \sim 0.78 \, {\rm V}, \quad FF \sim 0.90$  and Eff  $\sim 21.78\%$ . These results are very promising for defected ZnO/Si/ Cu<sub>2</sub>O solar cells, and leave ample room in the future for further improvement.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.



Fig. 10. Photovoltaic parameters of defected ZnO/Si/Cu<sub>2</sub>O solar cell as a function of operating temperature.

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