Influence of band gap and carrier concentration on ZnO/CuO solar cells performance

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Here Solar Cell Capacitance Simulator (SCAPS) program is employed to simulate effect of band gap and carrier concentration on the basic parameters of CuO/ZnO solar cells including short circuit current density (Jsc), open circuit voltage (Voc), fill factor (FF), and the efficiency (η). In such argument, CuO thin film was used as active material while ZnO thin film as window layer for simulated devices. The results of simulated solar cells reveal that carrier concentrations of ZnO and CuO thin films should be around 4×10^{20} and 1×10^{16} cm^{-3} to have performance higher than of 24.5 %. Moreover, the value of band gaps for such window and absorber layers should be of about 3.25 and 1.35 eV to have higher efficiencies. The principal factors that controlling such performances of devices are built-in potential, light absorbing, generation rate and recombination rate of charge carriers. Such results are promising as step forward to fabricate high efficiency photovoltaics based on inorganic nanomaterials.

Keywords: Band gap, Carrier concentration, ZnO/CuO solar cells, SCAPS program

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1. Introduction

The combination of nanomaterials particularly metal oxides as n-type and p-type are outstanding key for fabrication of photonic devices involving solar cells and light emitting diodes (LEDs) [1, 2]. Among such oxides, copper oxide (CuO) is promising candidate as it has unique properties like stability, high absorption coefficient in the region of visible light [3], CuO is a p-type direct bandgap semiconductor with energy of about 1.4 eV [4].

Various methods and techniques could be utilized to growth different morphologies and shapes of nanostructures CuO like hydrothermal [5], microwave-assisted [6], precipitation [7], and biosynthesis [8]. Therefore, CuO nanomaterial could be easily employed for fabrication of wide variety of applications such as antimicrobial [9], photocatalysis [7], batteries [5], solar cells [10], light emitting diode [1], and gas sensors [11].

Through combination with another wide band gap n- type semiconductor such ZnO (3.2 eV) [12, 13], more light could be easily absorbed which enhance the performance of such heterojunction in solar cells. Moreover, the lattice mismatch will be reduced gradually producing more generation as well as separation of charge carriers through CuO/ZnO heterojunction interface and reducing recombination rate of electron-hole pairs [14, 15].

Many pervious work were published in the direction of solar cells based on CuO/ZnO heterojunction where the efficiency of 0.08 % [16], 0.25 % [17], 1.15 % [18], 1.69 [19] were obtained experimentally.

To have higher performance more theoretical investigations are required. Therefore here, the band gap and carrier concentration of nanomaterials are considered from the most important factors that affected on fundamental parameters of solar cells since they are controlling optical, structural, and electrical properties of nanomaterials. Consequently, we employ here Solar Cell Capacitance Simulator (SCAPS) program to investigate performing of CuO/ZnO solar cells based on the variation of the values of such two factors to obtain higher efficiencies [20].

2. Materials and Methods

2. 1 Solar Cell Structure:

Figure 1 presents the simulated solar cell where CuO thin film is applied as an absorber material and ZnO thin film as window in the photovoltaics. Back and front contacts are constructed from Gold (Au) and transparent conductive oxide (TCO).

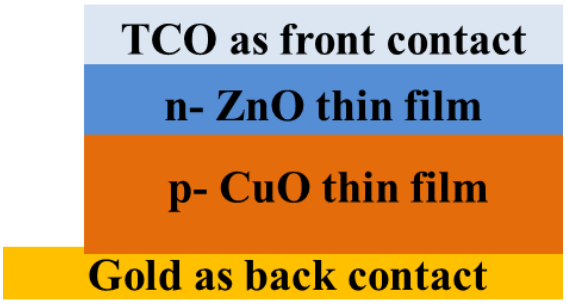

Fig 1: *Diagram for the structure of simulated solar cell based on CuO/ZnO.*

2.2 Properties of Materials:

The properties of materials that employed in our simulation are presented in Table 1 where they collected from previous literature [14, 21, 22].

Table 1. Materials properties of simulated solar cell.

Material properties	n-ZnO	p-CuO
Bandgap (eV)	3.37	1.2
Relative permittivity	86	18.1
Electron affinity (eV)	3.9	4.07
Effective density of states of valence band maximum (cm^{-3})	1.5×10^{21}	5.5×10^{20}
Effective density of states of conduction band minimum (cm^{-3})	1.32×10^{20}	3×10^{19}
Mobility of Hole ($cm^2/V\ s$)	10	0.1
Mobility of Electron ($cm^2/V\ s$)	20	10
Acceptor concentration (cm^{-3})	0	1×10^{16}
Donor concentration (cm^{-3})	1×10^{19}	0
Thickness (µm)	0.1	2

Solar Cell Capacitance Simulator (SCAPS-1D) program is applied to simulate and investigate the basics parameters of solar cells [23-25]. Effect of carrier concentration and band gap on the fundamental parameters of ZnO/CuO solar cells (including short circuit current density (J_{sc}), open circuit voltage (V_{oc}), fill factor (FF), and cell efficiency (η)) will be examined intensely. All of simulations will be investigated under one sun radiance (AM 1.5 /100 mW/cm^2) and at constant temperature of 300 K. Holes and electrons Continuity and Poisson equations were utilized for the simulations as following [22, 26]:

$$\frac{d^2}{dx^2}\Psi(x) = \frac{e}{\varepsilon_0 \varepsilon_r}\left(p(x) - \mathrm{n(x)} + N_D - N_A + \rho_p - \rho_n\right) \qquad (1)$$

$$\frac{dJ_n}{dx} = \mathrm{G - R} \qquad \text{and} \qquad \frac{dJ_p}{dx} = \mathrm{G - R} \qquad (2)$$

3. Results and discussion

Figure 2 shows the change of the solar cells' basic parameters with different carrier concentrations of ZnO thin films. The values of the J_{sc} and the V_{oc} decrease from about 38.1 mA/cm^2 and 0.802 V to about 37.9 mA/cm^2 and 0.801 V, respectively with carrier concentration increasing and remaining constant with concentration above 10 ^{20} cm^{-3}. The action of J_{sc} and V_{oc} values may be attributed

to built-in potential which is full completed and therefore the collection rate of the charge carrier become constant resulting stability of such values [26, 27].

On contrast, both FF and η values increasing dramatically with carriers' concentrations increasing from about 76 % and 23.2 % to about 81.5% and 24.7%, respectively and then become stable with further concentrations increasing. Such behavior of FF could be explained from its equation where their values are inverse proportional to the values of J_{sc} and V_{oc} as following [26]:

$$FF = \frac{V_m J_m}{V_{oc} J_{sc}} \qquad (3)$$

The shape of η values could be clarified from the relation among the basic parameters of solar cell devices as exhibited in the following equation [26]:

$$\eta = \frac{FF\, V_{oc}\, J_{sc}}{P_{in}} \qquad (4)$$

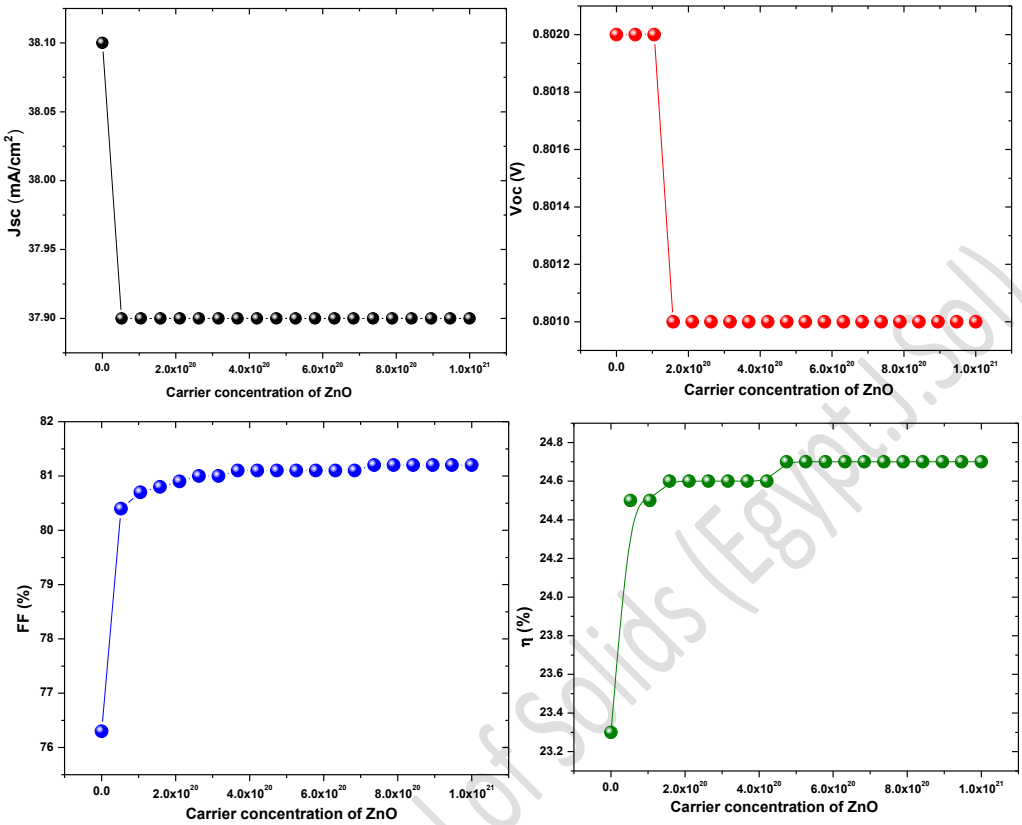

Fig 2: *Variance of the basic parameters of solar cells with carrier concentrations of ZnO nanostructures.*

Figure 3. presents the basic parameters of simulated photovoltaics according to the variation of *window* layer band gaps. The J_{sc} values increase from zero to about 38 mA/cm^2 with increasing of band gap from about 3.1 eV to 3.15 and then become constant at the same value with further band gap enhancement. This result could be described as the increasing of band gap value resulting in more light will successfully path through the device junction and therefore more photogenerated electron- hole pairs will be produced [26].

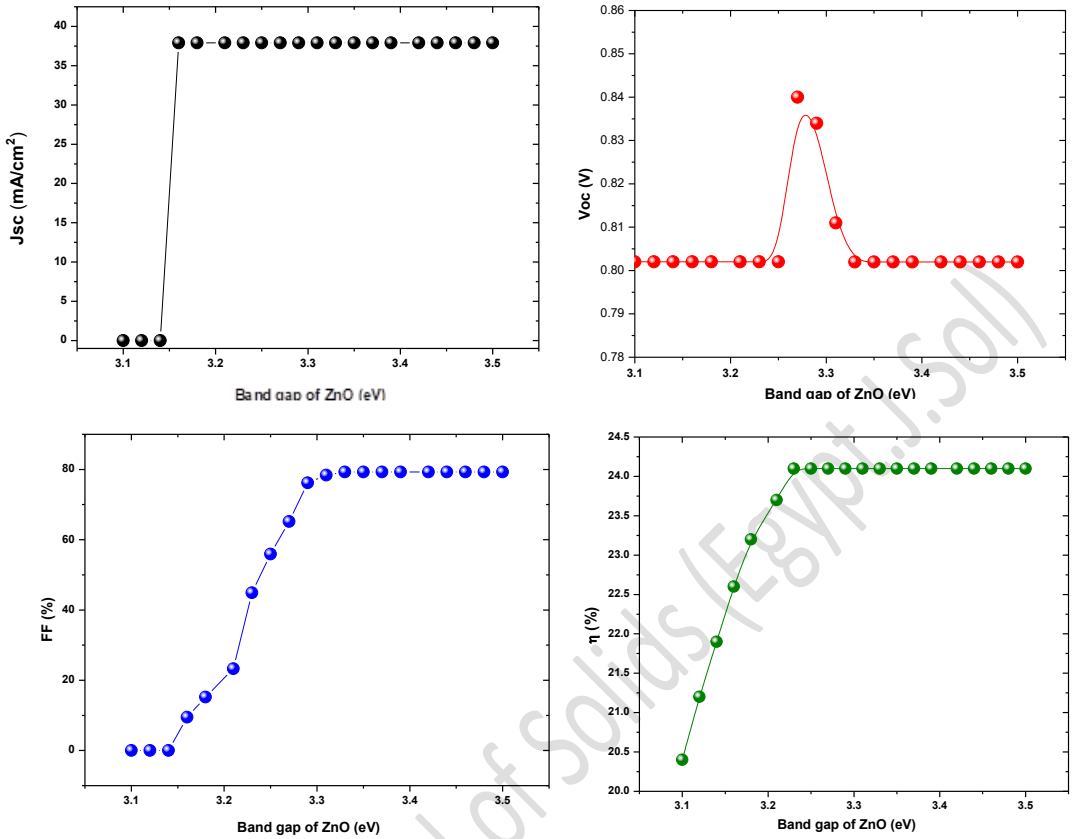

Fig 3: *Variance of the basic parameters of solar cells with band gap of ZnO nanostructures.*

The V_{oc} of simulated devices have a Gaussian curve with value of 0.84 V as a maximum at about 3.28 eV of band gap of window layer. Such behavior could be attributed to the ratio of light absorbed and passing through the window layer. FF values show improvement with band gap increasing which precious by both J_{sc} and V_{oc} values. The performance of the simulated devices shows dramatically improving from about 20% to 24% with bang gap increasing from 3.1 to 3.25 eV

then have stability with further band gap value increasing. This behaviour is resultant from other solar basic parameters [26].

Figure 4. illustrates the simulated device basic parameters with the change of CuO thin film carrier concentration. The values of J_{sc} declines from about 38.1 to about 37.9 mA/cm^2 with growing of carrier concentration may be attributed to increase of the recombination rate than the generation rate of electron - hole pairs. On the other hand, the V_{oc} values of simulated solar cells devices enhancement with growing with carrier concentration of active layer [27]. This could be recognized by rising built-in potential that formed mainly in absorber layer side. Both FF and η values progress with upward the carrier concentration which subsequent from the shape behavior of Jsc and Voc values as presented in equations 1 and 2.

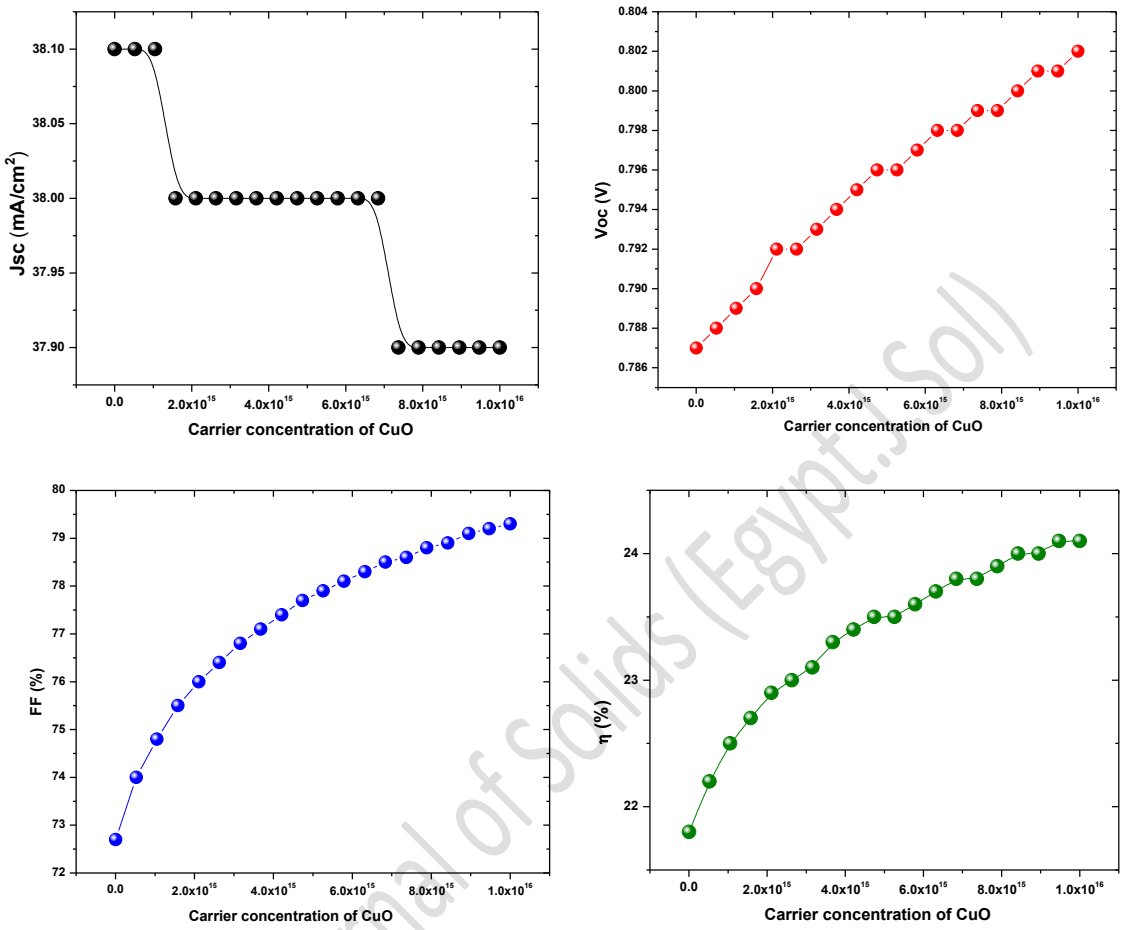

Fig 4: *Variance of the basic parameters of solar cells with carrier concentrations of CuO nanostructures.*

Figure 5 clears the main parameters of photovoltaic devices with variation of absorber layer band gaps. The J_{sc} values dropped dramatically from about 48 to about 32 mA/cm^2 with increasing of band gap from about 1 eV to 1.4. Such result may be attributed to light blocking with band gap increasing and therefore lowering photogenerated electron- hole pairs and increasing of recombination rate. On the other side, the Voc values of the devices grow with

multiplying of band gap values. This could be identified by the ability of charge length collection and rising built-in potential. FF values show small variation towards increasing then intensely falling over 1.3 eV which is a result of combination of the Jsc and Voc values. The values of η advance with increasing of band gap and having Gaussian shape with highest value of 25.5 % at about 1.3 eV. Such behaviour of performance of the solar cells could be explained by the summing of other basic parameters as presented in equation 2.

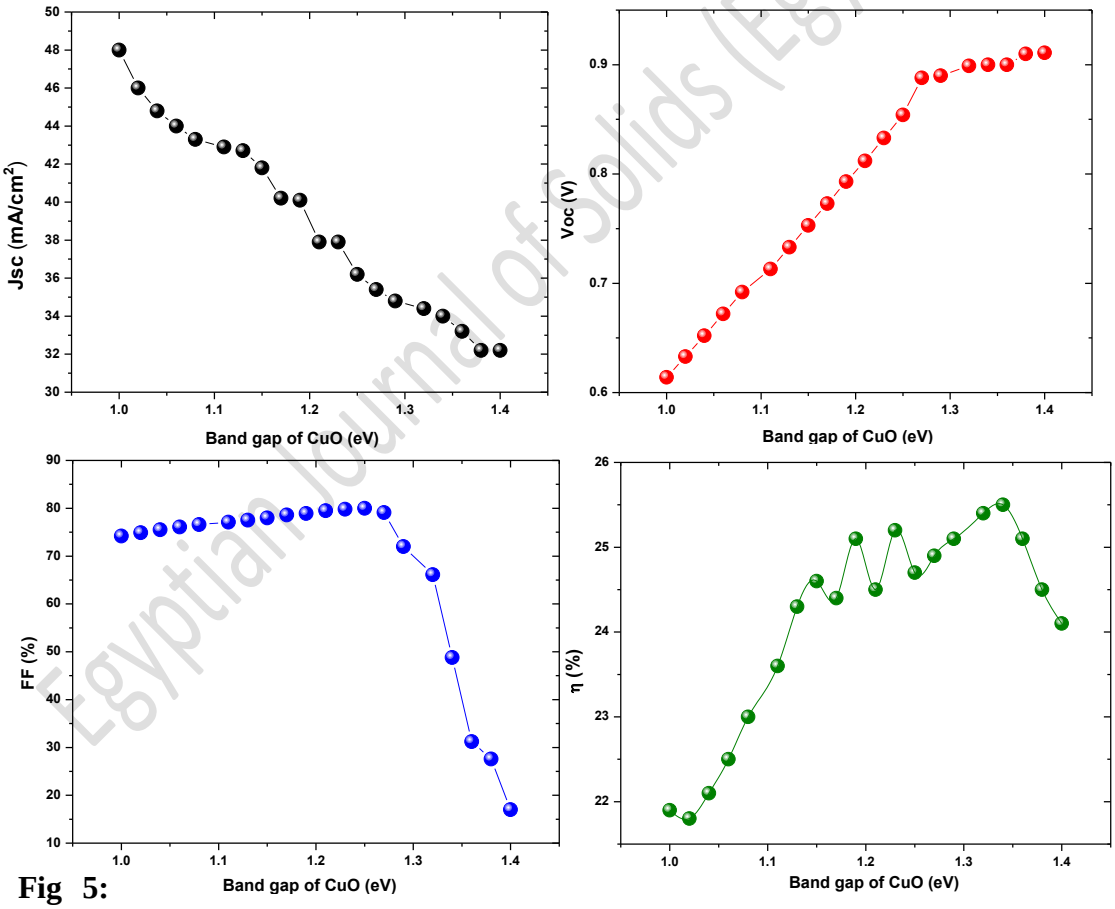

Fig 5:

Variance of the basic parameters of solar cells with band gap of CuO nanostructures.

Such explanations for effect of carrier concentration and band gap on the basic parameters of ZnO/CuO solar cells based mainly on the energy level and charge transfer in the ZnO/CuO junction as presented in **Figure 6**.

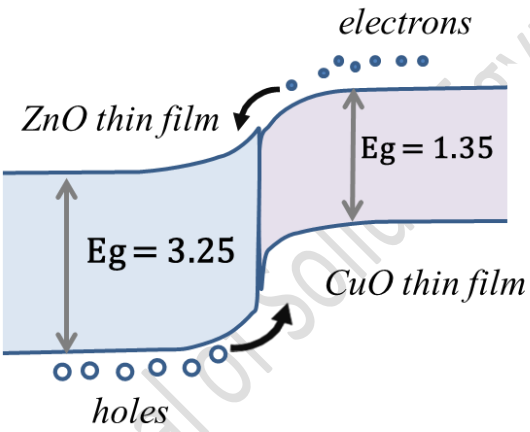

Fig 6: *The schematic for the energy level and charge transfer in the ZnO/CuO junction.*

4. Conclusion

SCAPS program was employed to simulate solar cells based on ZnO /CuO inorganic heterojunction. Effect of carrier concentrations and band gaps of both window layer and active layer were investigated deeply. Simulated results indicate that to have higher performance ZnO and CuO thin films should have carrier concentrations of around 4×10^{20} and 1×10^{16} cm^{-3} and band gaps of about

3.25 and 1.35 eV, respectively. Built-in potential, generation rate, recombination rate, and light absorbing are the major reasons that influencing the implementations of the devices. Link of such theoretical investigation with experimental one will be led to fabricate higher efficiency photovoltaics.

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