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Research Article

THE EFFECT OF SEVERAL PARAMETERS ON THE PERFORMANCE OF $CuInS_2$-BASED SOLAR CELLS USING THE SCAPS-1D SOFTWARE

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ABSTRACT

In this work, we have used one dimensional solar cells simulator SCAPS-1D (Solar Cell Capacitance Simulator) to design solar cells based on $CuInS_2$ as the absorber material and study their device performances. Solar cells having a typical structure Al/ZnO:Al/CdS/$CuInS_2$/Mo have been modeled. We focus on studying effects of varying band gap and thickness of $CuInS_2$ absorber layer on the performance of the $CuInS_2$ based solar cells. And also, various replacements for conventional cadmium sulphide (CdS) buffer layer, such as ZnSe and In_2S_3 based buffer layers have been studied to find out the optimum choice. The photovoltaic parameters (short-circuit current density (Jsc), open-circuit voltage (Vco), fill factor (FF) and effciency (η)) have been calculated from the current density-voltage curves. In this study, a simulated effciency of 21.93 % has been obtained with Vco of 0.94 V, Jsc of 27.64 mA/cm_2 and FF of 84.25 % for the $CuInS_2$ solar cell with an absorber layer band gap of 1.40 eV, absorber thickness of 2µm and In_2S_3 buffer layer. The analysis made from this numerical simulation has revealed the good structure Al/ZnO:Al/In_2S_3/$CuInS_2$/Mo solar cell.

Keywords: $CuInS_2$; solar cell; SCAPS-1D; photovoltaic; efficiency.

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1. INTRODUCTION

The ternary and quaternary chalcopyrite semiconductors $CuInX_2$ and $CuInGaX_2$ (X = S, Se) of the family I-III-VI_2 aroused great interest because of their characteristics, especially their very high absorption coefficient in the range of the solar spectrum [1]. These materials are important for many applications because of their optoelectronic characteristics, such as the appropriate band gap, high absorption coeffcient, low cost production, long-term stable performance and good thermal, chemical and radiant stabilities etc. [2]-[3]. Additionally, the $CuInS_2$ does not contain toxic elements such as Cd and Se. Therefore, $CuInS_2$ is not dangerous for the environment and suitable for solar cell applications [3]. It is also possible to produce large-area solar cells using $CuInS_2$ as an absorbing layer [4]. For these reasons, $CuInS_2$ needs optimizations to increase its effciency. Theoretically, the conversion effciencies of $CuInS_2$ thin film solar cells have been calculated to be 27-32% [5]. The best conversion effciency for polycrystalline $CuInS_2$ solar cells achieved to date is 13.2% [6]. Solar cells based on an absorbing layer $CuInS_2$ with a conversion effciency of 11.4% were prepared by a rapid thermal process (RTP) [7]. Solar cells based on CIGS, CdS and CZTS thin films have already reached effciencies of 22.9%, 21% and 10% respectively [8]. A conversion effciency of 21.7% is obtained by solar cells based on $CuIn_xGa_{1-x}Se_2$ fabricated by vacuum co-evaporation method at high temperature [9]. Other semiconductors such as $CuInS_2$, Cu_2SnS_3 and $Cu_2ZnSn(S,Se)$ have also been considered as thin absorbing layers in next generation high effciency solar cells [10].

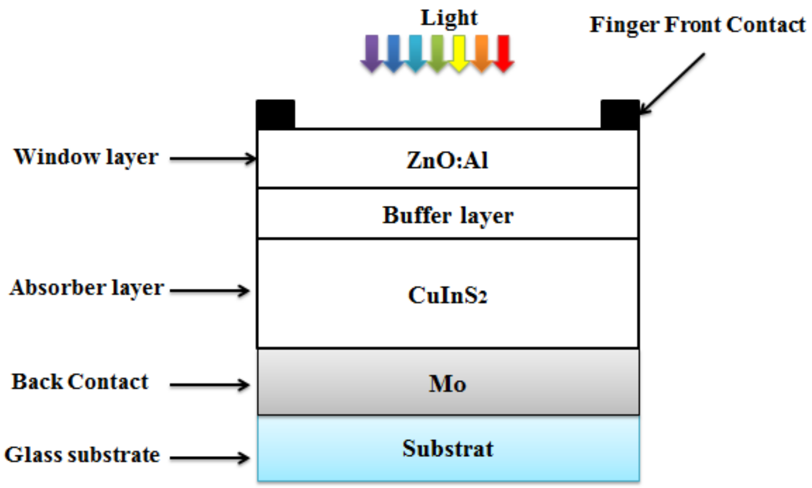
The simulation has become an important step in the design of solar cells prior to the experimental process due to the high cost of chemical products and processing equipment. The simulation minimizes the time and raw material used in the preparation of solar cells. In addition, the simulation allowed us to identify the physical parameters that affect the performance of our solar cells [11]-[12]. In this paper, we present a numerical study of $CuInS_2$ thin film solar cells with SCAPS-1D (Solar Cell Capacitance Simulator one Dimension) [13]. This software was used to calculate the photovoltaic parameters (short circuit current density (Jsc) open-circuit voltage (Vco), fill factor (FF) and effciency (η)) with standard lighting (AM1.5G, 1000 W/m^2, 300K). This work examines the influence of the band gap energy, the thickness of the absorbent layer and the choice of the buffer layer on the performance of solar cells based on $CuInS_2$.

2. RESULTS AND DISCUSSION

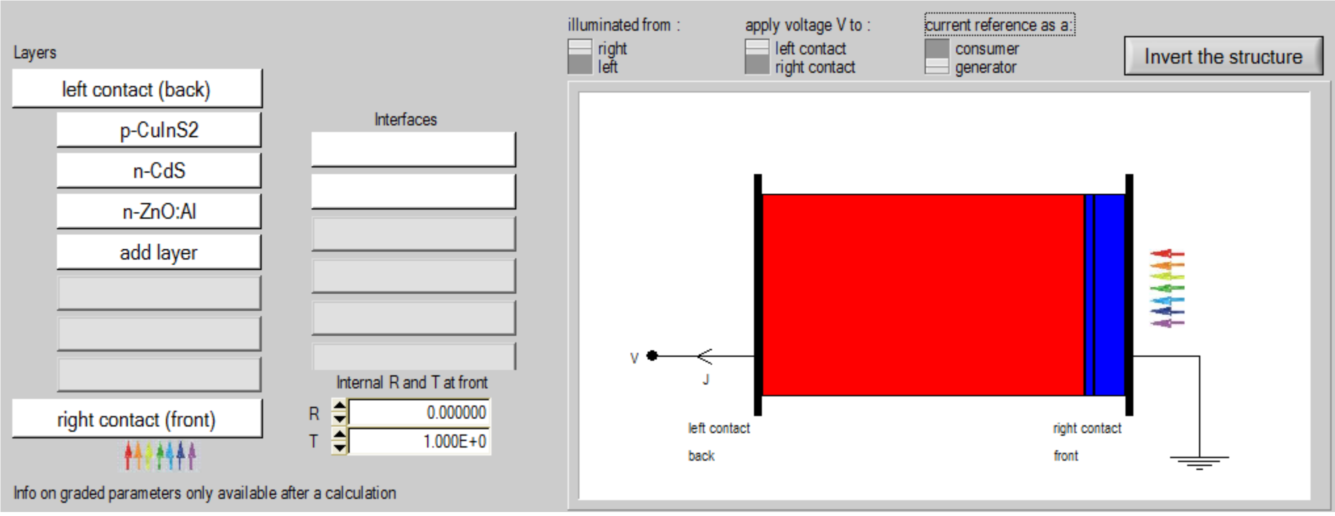
2.1. Studied Structure

In this work, we used One Dimension of Solar Cell Capacitance Simulator (SCAPS-1D) to analyze solar cells based on $CuInS_2$. SCAPS-1D is powerful computing software and a numerical modeling tool designed to simulate the characteristics of solar cells [14]. SCAPS-1D is able to solve basic equations of semiconductors (Poisson equation and continuity equations for electrons and holes) [15]-[17]. It was designed and developed by the University of Gent, which is available for free to the photovoltaic research community [18]-[19]. In this paper, we designed three solar cells based on an absorbing layer $CuInS_2$, a buffer layer (Either CdS, ZnSe or In_2S_3) and a window layer (ZnO:Al) with Molybdenum (Mo) as contact back. The design of our solar cell is illustrated in Fig. 1(a). Figure 1(b) shows the solar cell with the CdS buffer layer in the SCAPS 3.3.03 interface (Similarly we have designated solar cells based on ZnSe and In_2S_3). For each film, the properties of the material must be assigned to the software as input parameters. Before starting the calculation, the test conditions, such as temperature, polarization voltage and illumination, must be introduced in the program. The parameters used for the simulation of solar cells based on $CuInS_2$ are summarized in Tab. 1 [20].

(a)



(b)



Internal R and T at front

R 0.000000

T 1.000E+0

Info on graded parameters only available after a calculation

Fig.1. (a) Schematic representation of $CuInS_2$ solar cell and (b) the structure of the $CuInS_2$ solar cell used for simulation in SCAPS-1D program.)

Table 1. Material parameters used in this simulation.

Layer properties	**$CuInS_2$**	**ZnO:Al**	**CdS**	**ZnSe**	**In_2S_3**
Thickness (µm)	2.0	0.2	0.05	0.08	0.05
Band gap (eV)	1.40	3.3	2.4	2.9	2.8
Electron affinity (eV)	4.5	4.6	4.4	4.2	4.7
Dielectric permittivity (relative)	13.6	9	10	10	13.5
N_c effective density of states (1/cm^3)	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	1.5×10^{18}	4×10^{13}
N_v effective density of states (1/cm^3)	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Electron thermal velocity (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Hole thermal velocity (cm/s)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Electron mobility (cm^2/Vs)	100	100	100	50	400
Hole mobility (cm^2/Vs)	25	25	25	20	210
Donor concentration N_D (1/cm^3)	10	1×10^{18}	1×10^{17}	1×10^{17}	1×10^{18}
Acceptor concentration N_A (1/cm^3)	2×10^{17}	1	1	1	10
Front surface recombination velocity (cm/s)	10^7				
Back surface recombination velocity (cm/s)	10^7				
Front reflectivity	0.05				
Back reflectivity	0.8				

In this study, we used SCAPS-1D to study solar cells based on $CuInS_2$ with the typical structure of Al/ZnO:Al/CdS/$CuInS_2$/Mo. The curve of the characteristic (J-V) results from the simulation using the values of table (1) is illustrated in FIG. (2). Table (2) contains short-circuit current density (Jsc), open-circuit voltage (Vco), fill factor (FF) and effciency (η) of the solar cell based $CuInS_2$ with a CdS buffer layer. The effciency of this solar cell is 20.48%; This is not very different from that of a solar cell based on $CuInS_2$ obtained by the AMPS-1D software [20] (Analysis of microelectronic and photonic structures one dimension) (Tab.2). This confirms the mastery of the software and the validated model can be used to study the effects of different parameters on the overall performance of the solar cell.

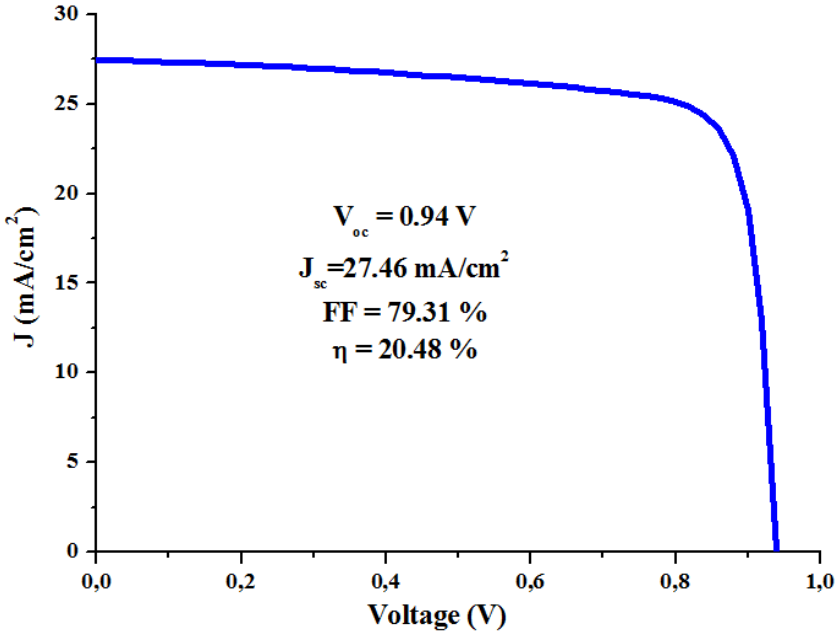


Fig.2. J-V characteristic of $CuInS_2$ solar cell simulated

Table 2. SCAPS-1D simulation results of $CuInS_2$ solar cell with AMPS-1D simulation results.

Parameters	**Voc (V)**	**Jsc (mA/cm^2)**	**FF (%)**	**η(%)**
$CuInS_2$ SCAPS-1D simulation	0.94	27.46	79.31	20.48
$CuInS_2$ AMPS-1D simulation [20]	0.94	26.2	84	20.4

2.2. The effect of absorber layer thickness on $CuInS_2$ cell performance

In this section, the thickness of the $CuInS_2$ absorber was varied to determine the optimum thickness for the $CuInS_2$ structure with CdS as a buffer layer. We have varied the thickness of the p-$CuInS_2$ region from 1 µ*m* to 5 µ*m*. The results of the simulation show that the effciency of the solar cell increases with the thickness of the $CuInS_2$ absorbent layer. Figure (3) shows the variation of the photovoltaic parameters (Jsc, Voc, η, FF) as a function of the thickness of the absorber. It is observed in Figure (3) that Jsc and Voc increase substantially with increasing thickness of the absorbent film. When the thickness of the absorbent layer increases, more photons are absorbed, particularly the long wavelengths of the illumination [21]. Therefore, a significant amount of electron-hole pairs would be produced. This will lead to an improvement in the effciency of our solar cell. Moreover, the quantum effciency of the cells will improve by increasing the thickness since there will be more charge carriers collected before recombination. Figure (4) shows the variation of the quantum effciency of the solar cells as a function of the increase in the thickness of the absorbent layer. The reduction in the thickness of our absorbent layer will be influenced by an easy capture of electrons by the back contact which is located near the depletion region [21]. This causes a substantial increase in the recombination of back contact. Figure (5) shows the recombination current density at the back contact as a function of the voltage for the solar cells with different thicknesses of the $CuInS_2$ absorbent layer. From this result, we found that when increasing the thickness of the absorbing layer, the recombination of the electrons at the back contact will decrease. Therefore, more electrons contribute to improving the effciency of solar cells. A similar study on CdTe-based solar cells using SCAPS-1D simulation also showed that overall conversion effciency was increased as a function of thickness [22].

As stated above, an increase in the thickness of the absorber layer can improve the performance of the solar cell, but this requires optimization. Figure 3 shows, for thicknesses greater than 2µm, the open-circuit voltage (Vco), the short-circuit current density (Jsc), the fill factor (FF) and the effciency (η) increase only slightly and we may assume it to be almost constant. This is because photons (hν) with higher wavelengths have been absorbed deep into the CuInS2 absorbing film, far from the depletion region [23]. If the thickness of the absorbent film is increased, the resulting charge carriers recombine in the rear portion of the absorber before reaching the depletion region. The probability of quasi-neutral recombination may be due to the increase in thickness. Certainly, increasing the thickness of the absorber causes photon absorption, especially those that have a high wavelength, but the resulting charge carriers can not be used to improve solar cell yields and recombine before reaching the depletion region [23]. The variation of the quasi-neutral recombination current density of the CuInS2-based solar cells as a function of the thickness of the absorber film has been presented in FIG. (6). Therefore, we found and justified that the optimum value for the thickness of the absorbent layer is 2 µm. Thus, it is not necessary to produce solar cells based $CuInS_2$ with a large thickness, as there must be a compromise between the effciency of the solar cell and cost of production. To obtain a high effciency solar cell at low cost, it is necessary to control the thickness of the photovoltaic devices [24].

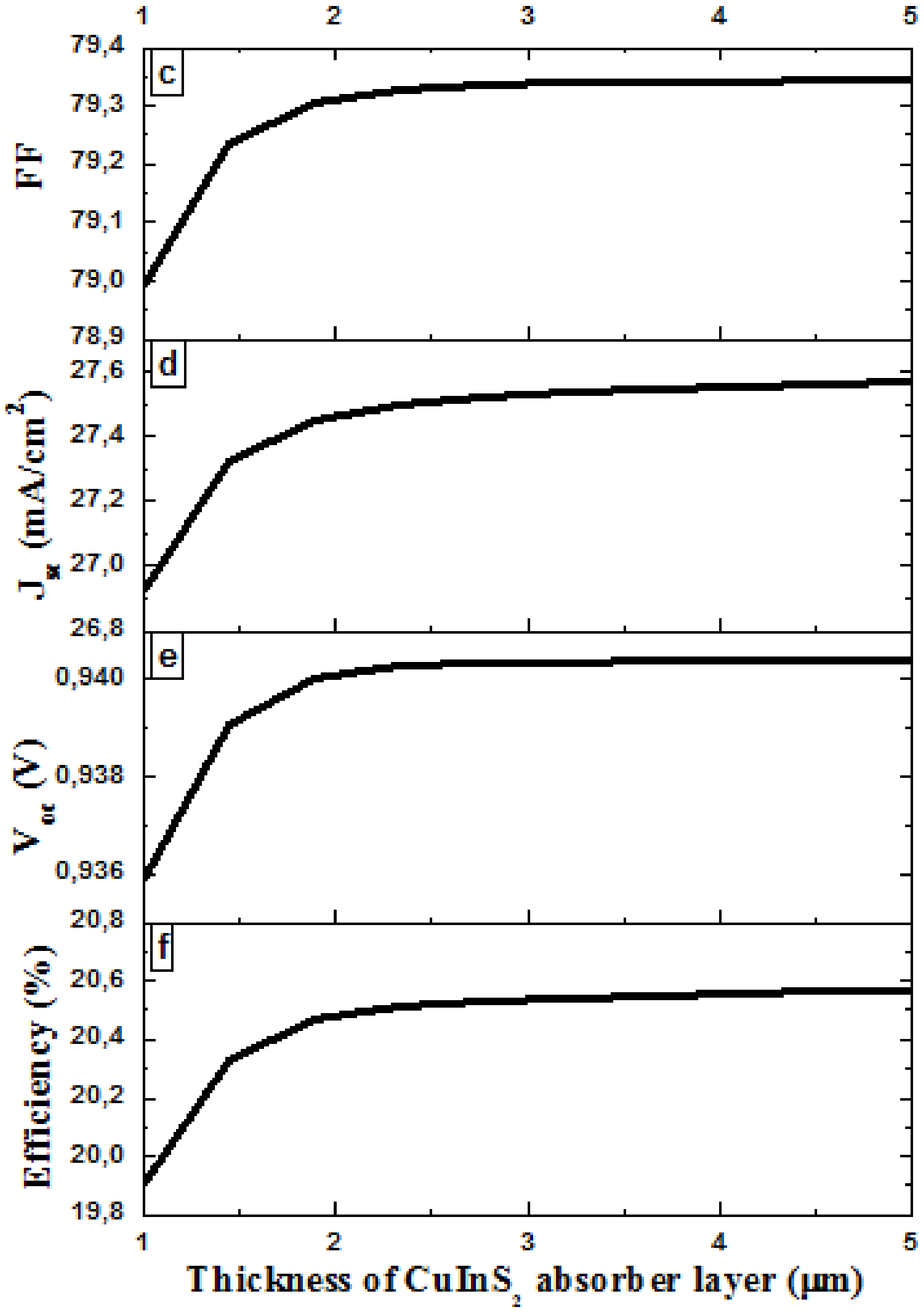


Fig.3. Simulated performance of cells with various $CuInS_2$ thicknesses

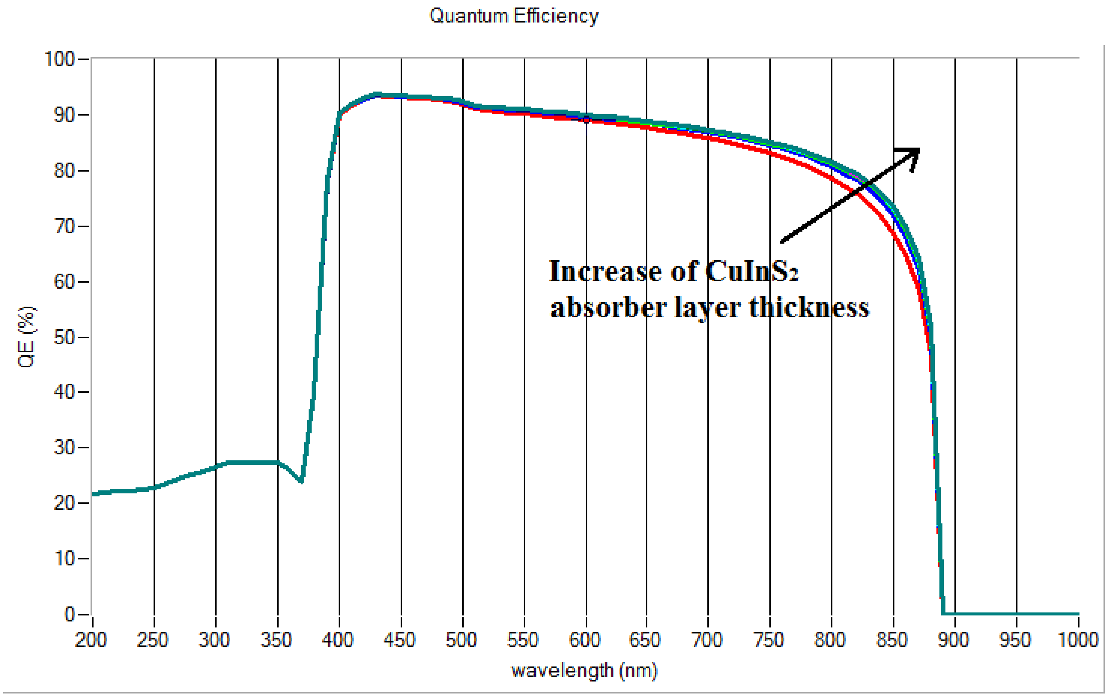


Fig.4. The enhancement of the quantum effciency when the thickness of the absorber layer increase

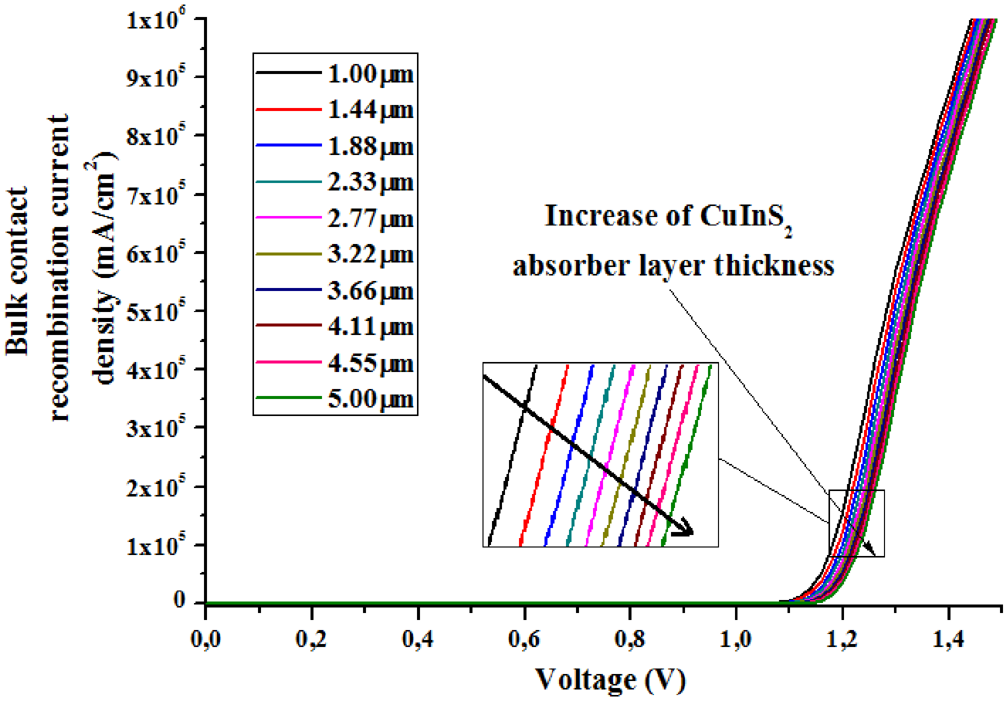


Fig.5. Back contact recombination current density decrease due to the increase of absorber layer thickness

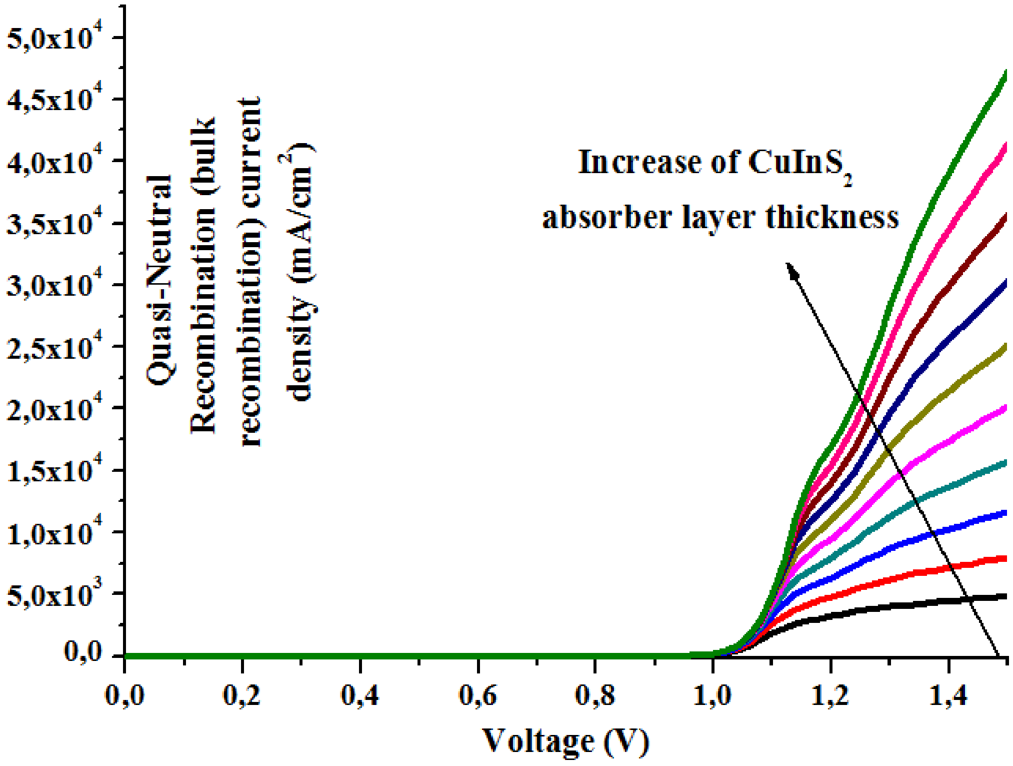


Fig.6. Quasi-Neutral recombination current density increase due to the increase of absorber layer thickness

2.3. Modeling with various $CuInS_2$ band gaps

In this regard, we studied the effect of gap energy on the performance of $CuInS_2$ solar cells. CuInS2 absorbing layers with gap energies between 1.0 eV and 1.6 eV were modeled in this work. Figure 7 illustrates the effect of the variation of the gap energy on the characteristics J(V) of the $CuInS_2$ solar cells. The effect of gap energy on the performance of $CuInS_2$ solar cells is shown in Figure 8. We have found from this figure that the optimum gap energy of the absorbent layer is 1.40 eV. It has also been observed that the short-circuit current density Jsc decreases while the open-circuit voltage Voc increases with the increase in gap energy. This decrease is due to the fact that the absorbers with large gap energy do not absorb the photons at low energy [20]. If we have an absorbent layer with a high energy gap is required to absorb photons with low wavelengths to release electrons from the valence band to the conduction band based on Einstein's equation [25]-[26]:

$$E_g=hc/\lambda_g \qquad (1)$$

where h, ν, c and λ_g are Planck's constant, frequency, velocity of light and the wavelengths corresponding to the optical band gap, respectively. Figure (9) shows the spectral responses of our solar cell by varying the band gap energy of the absorbing layer. We have demonstrated that increasing gap energy of $CuInS_2$ decreases the quantum effciency of the solar cell. As you know, if you have a narrow band gap, this will favor the movement of electrons from the valence band to the conduction band, but the voltage across the cell will be low [27]. On the other hand, if you have a higher band gap, the electrons will have trouble releasing from the valence band and no current will appear. Similarly, a study on CZTS-based solar cells showed that the effciency decreased for higher gap energies [28]. Therefore, a reasonable band gap of the absorber layer is the main one for improving the performance of solar cells based $CuInS_2$. From this study, we concluded that the remarkable reduction in conversion effciency and solar cell power is due to the degradation of the short-circuit current density of the cell. The simulation results were in good agreement with the theoretical estimate for achieving the best performance of photovoltaic devices with the optimum band energy in the range of 1.4 to 1.5 eV for solar spectrum of AM1.5G [29]-[30].

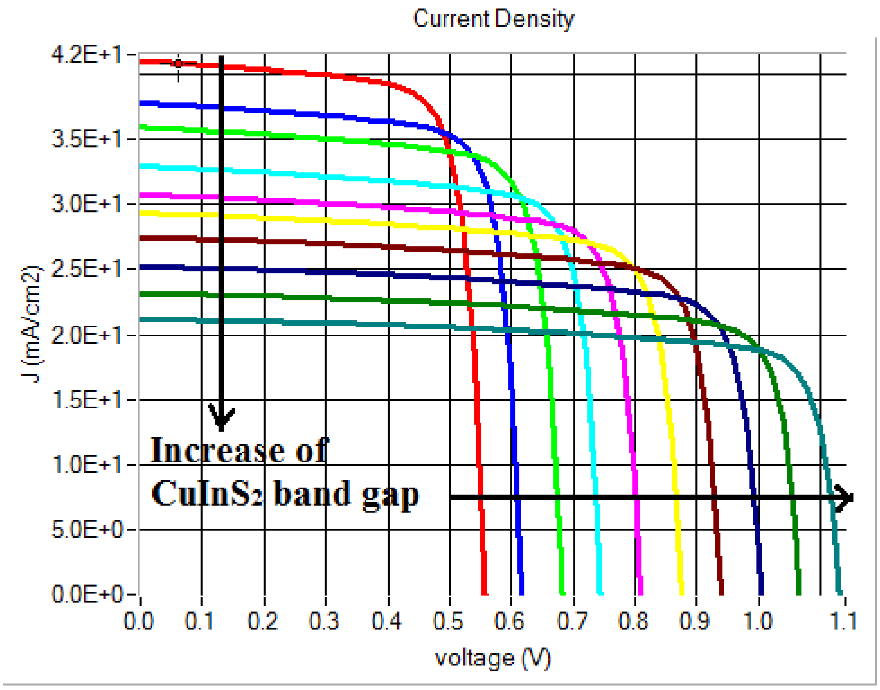


Fig.7. J-V characteristics of $CuInS_2$ solar cell with various $CuInS_2$ bandgaps.

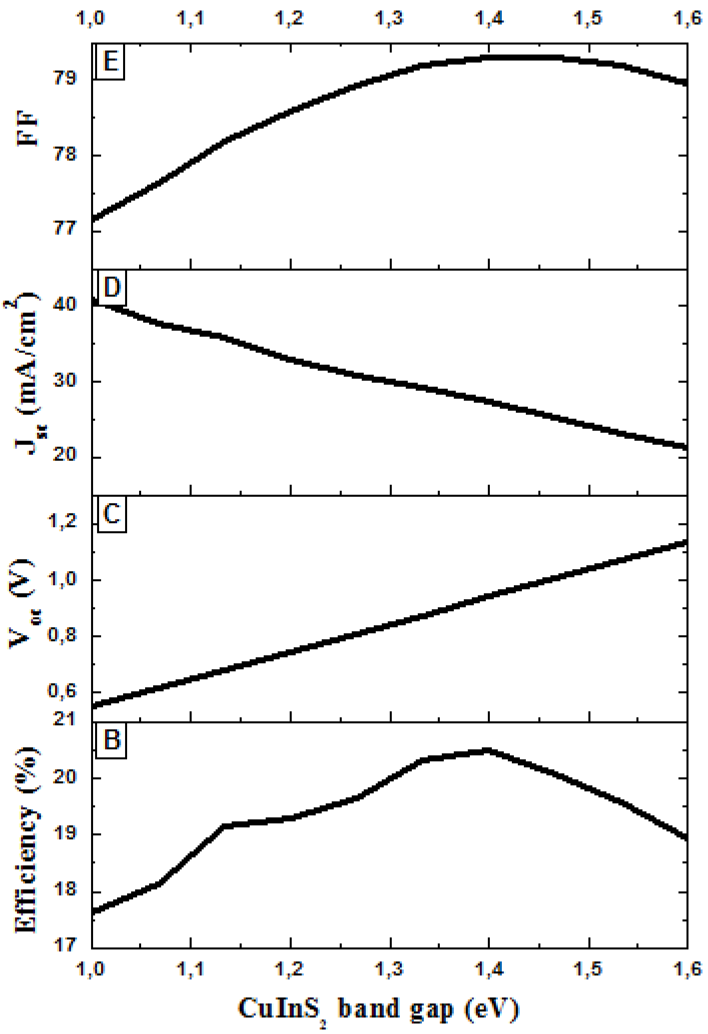


Fig.8. J-V Simulated performance of cells with various $CuInS_2$ bandgaps

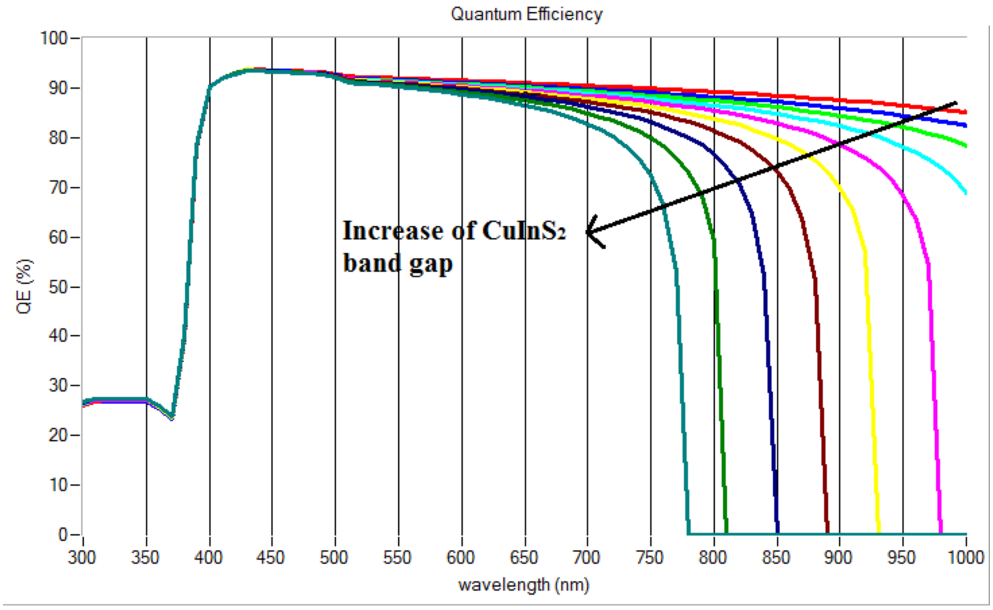


Fig.9. Spectral response of cells with various $CuInS_2$ band gaps

2.4. Effect of buffer layer on the J-V characteristics

In order to obtain a better stability and a high effciency of the solar cells, the buffer layers ZnSe and In_2S_3 have been studied outside the most used CdS. The figure (10) illustrates the calculated characteristics J-V for different buffer layer. The photovoltaic parameters of the solar cell with a different buffer layer have been summarized in Table (3). Figure (10) shows that solar cells with CdS and In_2S_3 as buffer layer have a high conversion effciency. The solar cell based on the In_2S_3 buffer layer has achieved a conversion effciency of 21.93%, con_rming that it to be a potential replacement for CdS. In addition, the two solar cells based on ZnSe and In_2S_3 as buffer layers reached the yields of 8.43% and 21.93% respectively. So, we can say that the material In_2S_3 is promising as a CdS replacement because of their important properties. Similar results were found by A. Bouloufa et al. using another calculation software the AMPS-1D [31]. Our study on the three buffer layers showed that the best photovoltaic parameters are obtained with the In_2S_3 or CdS buffer layers and, on the other hand, the solar cell with a layer ZnSe represents the least conversion effciency.

Table 3. SCAPS-1D simulation results of $CuInS_2$ solar cell with different buffer layer.

Parameters	**Voc (V)**	**Jsc (mA/cm^2)**	**FF (%)**	**η(%)**
CdS	0.94	27.46	79.31	20.48
In_2S_3	0.94	27.64	84.25	21.93
ZnSe	0.94	26.2	84	20.4

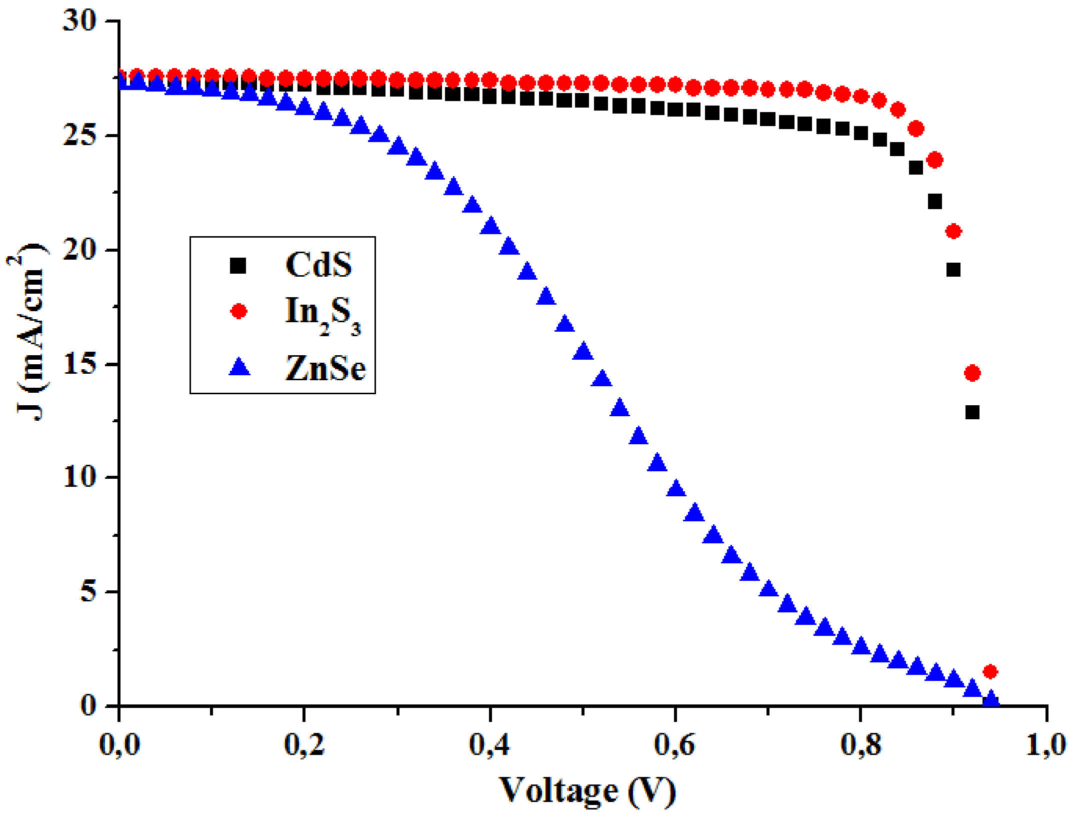


Fig.10. J-V characteristics of $CuInS_2$ solar cell with different buffer layer.

3. CONCLUSION

Numerical simulations have been done on $CuInS_2$-based solar cells by a simulation program called SCAPS-1D. Several parameters have been studied such as the thickness and band gap of the $CuInS_2$ absorber layer and various buffer layers, to see the inuence of each parameter on the overall performance of solar cells. The optimal thickness of the $CuInS_2$ absorbent layer with a CdS buffer layer is found to be 2 µm. The results of the simulation showed that it is not necessary to use a thicker absorber if one wants to make a compromise between the effciency of the cell and the cost of production. The effect of the band gap on the performance of the cell is revealed that the optimum band gap of the absorbing layer is 1.40 eV. Several buffer layers have replaced the CdS to improve the performance of solar cells. From the study with different types of buffer layers, cells with In_2S_3 buffer layer produce the best effciency of 21.93 % among others (with Voc of 0.94 V, Jsc of 27.64 mA/cm^2 and fill factor of 84.25 %). We concluded that In_2S_3 can be used as an alternative material to CdS.

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