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Theoretical Investigation on Improvement of CIGS-based Solar Cells

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As the energy demand continues to increase, the need for various energy sources is evident. The renewable energy sources provide sustainable and environmentally friendly energy, which can be alternative to traditional energy. Solar cells are the widespread forms of renewable energy. Many materials have been developed to produce thin-film solar cells. The Cu(In, Ga)Se_2 (CIGS)-based solar cell is considered as one of the most promising thin-film solar cells due to its many attractive features. In this paper, numerical simulations of thin-film CIGS solar cells using two-dimensional device simulator called Silvaco-Atlas are presented. Several studies of CIGS solar cell structures have been examined by employing CdS as a buffer layer. In this scenario, we first investigate CIGS solar cell based on CdS as a buffer layer. The simulation results are compared with those of previous related experimental and theoretical studies. In addition, the photovoltaic parameters are in good agreement with the experimental ones, which validate our simulation model. Secondly, we examine CIGS solar cell based on ZnS as a buffer layer in order to enhance the power conversion efficiency of CIGS solar cells. Therefore, the photovoltaic parameters of CdS-CIGS solar cell design are compared with those of ZnS-CIGS solar cell design showing a significant improvement of efficiency by including ZnS buffer layer. In particular, the efficiency increases from 22.92 % to 24.4 %. Moreover, an optimization process is applied to ZnS-CIGS solar cell design, which gives an efficiency of 25.1 %. The proposed CIGS solar cell design may significantly enhance the solar cell performances. Thus, ZnS can be considered as a promising alternative buffer layer for improving thin-film CIGS solar cell efficiency.

Keywords: CIGS solar cell, ZnS, Efficiency, Buffer layer, Optimization.

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1. INTRODUCTION

The increasing demand for energy and the environmental effects of fossil fuels lead to need for variable sources of sustainable and clean energy that can be an alternative to traditional energy. The Sun is the most important source of renewable and clean energy. The solar cells are devices that convert directly the solar light energy into electricity. Many materials have been developed to produce thin-film solar cells such as CIGS, CdTe and amorphous silicon (a-Si).

Copper-Indium-Gallium-diSelenide (CIGS) solar cell is the best candidate for thin-film solar cells because of many advantages such as higher efficiency on both the module and the cell levels [1], simple processes of manufacture [2], low cost production [2], excellent durability and stability [3] and radiation resistance [4]. CIGS solar cells have other attractive options for consumers such as flexibility and lightweight [5]. In addition, CIGS material has a direct adjustable band gap [6] and a very high absorption coefficient [2, 7].

The *p-n* junction is the main component of the solar cell, which is formed by the *n*-doped buffer layer with the *p*-doped CIGS absorber layer. Therefore, the buffer layer is an important film in CIGS solar cell. Usually, CdS is one of conventional and traditional materials, which is employed as a buffer layer in CIGS cells. With CdS-CIGS solar cell structures, different efficiency values are reported by several groups such as the Center of Solar Energy and Hydrogen Research (ZSW) which reach a value of 22.6 % [8] and the current world record-efficiency of 22.9 % by Solar Frontier K.K. (SF) [1, 9]. However, due to cadmium (Cd) toxicity, different non-cadmium and non-toxic materials such as ZnS, ZnSe, ZnS (O, OH) and In_2S are investigated and tested as buffer layers which replace CdS [10-13]. The idea of this work is to replace CdS buffer layer by non-toxic one called ZnS. The latter has wider band gap and smaller light absorption in comparison with CdS. In this context, numerical simulations of CIGS solar cells using both CdS and ZnS buffer layers are performed. By introducing ZnS buffer layer in CIGS solar cell, photovoltaic parameters are compared to those of CdS-CIGS solar cell structure and the results are reported. Therefore, the work is extended by optimizing ZnS-CIGS solar cell design. The obtained results illustrate that the proposed structure may notably enhance the CIGS solar cell performances.

2. NUMERICAL MODEL DESCRIPTION

In this study, Atlas-Silvaco [14] is used for modeling and optimization of both single junction CdS-CIGS solar cell and ZnS-CIGS solar cell designs, which are conducted by solving coupled system of the basic semiconductor equations. The main basic semiconductor equations are the Poisson and the continuity equations for both holes and electrons.

The following expressions that describe the main basic semiconductor equations and the performance

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parameters are obtained from literature [2, 14, 15].

The Poisson equation is given by:

$$\Delta V = -\frac{q}{\varepsilon}\left[p - n + N_D - N_A + N_t\right], \quad (1)$$

where V is the electrostatic potential, ε is the permittivity, q is the electron charge, N_D is the donor doping density, N_A is the acceptor doping density, p is the hole density, n is the electron density and N_t is the donor-type and acceptor-type defect density.

The continuity equation for electrons and holes is obtained respectively from the following expressions given as:

$$-\frac{1}{q}\frac{dJ_n}{dx} = G_{op}(x) - R_n , \quad (2)$$

$$\frac{1}{q}\frac{dJ_p}{dx} = G_{op}(x) - R_p , \quad (3)$$

where J_n is the electron current density, J_p is the hole current density, R_n and R_p are the recombination rates for electrons and holes, respectively, G_{op} is the optical generation rate.

The photogeneration rate G_{op} is given by:

$$G_{op}(x) = \frac{P_{in}(1-r)\alpha}{AE_{ph}} exp(-\alpha x) , \quad (4)$$

where α is the absorption coefficient, A is the illuminated device area, E_{ph} is the photon energy, r is the surface reflection and P_{in} is the incident optical power.

The recombination rates calculated by Shockley-Read-Hall (SRH) model can be expressed as:

$$R_{n,p} = \frac{\sigma_n \sigma_p v_{th} N_t\left(np - n_i^2\right)}{\sigma_n\left[n + n_i\, exp\left(\frac{E_t - E_i}{kT}\right)\right] + \sigma_p\left[p + n_i\, exp\left(\frac{E_t - E_i}{kT}\right)\right]} , \quad (5)$$

where σ_n and σ_p are the capture cross sections for electrons and holes, respectively, n_i is the intrinsic carrier density, v_{th} is the thermal velocity, E_i is the intrinsic Fermi energy level and E_t is the trap energy level.

The current-voltage (J-V) characteristic of the solar cell is a summation of the dark current and the photocurrent I_{ph}, and it is obtained by the celebrated Shockley equation:

$$I = I_{ph} - I_0\left(exp\left(\frac{qV}{akT}\right) - 1\right). \quad (6)$$

The main performance parameters of the solar cell are defined as follows.

The short-circuit current is given by:

$$I_{sc} = I_{ph} , \quad (7)$$

The open-circuit voltage is expressed as:

$$V_{oc} = \frac{akT}{q} ln\left(\frac{I_{ph}}{I_0}\right). \quad (8)$$

The fill factor FF is calculated by:

$$FF = \frac{P_{max}}{V_{oc} I_{sc}} . \quad (9)$$

The cell efficiency η is given as:

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{oc} I_{sc} FF}{P_{in}} , \quad (10)$$

where a represents the ideality factor, P_{max} is the maximum power and I_0 is the reverse saturation current.

The approximate expression of the reverse saturation current I_0 is given as:

$$I_0 = q\left(\frac{D_n n_{i,p}^{\ 2}}{L_n N_A} + \frac{D_p n_{i,n}^{\ 2}}{L_p N_D}\right), \quad (11)$$

where $n_{i,n}$ and $n_{i,p}$ are the intrinsic carrier densities of n-doped and p-doped layers, respectively, and D_n and D_p are the electron and hole diffusion coefficients, respectively, L_n and L_p are the electron and hole diffusion lengths, respectively.

3. SOLAR CELL CONFIGURATION

Both solar cell structures were analyzed. The first one is CIGS solar cell with CdS as a buffer layer and is presented in Fig. 1. The latter is similar to those experimentally performed and reported in [8, 9]. The second structure is CIGS solar cell with ZnS as a buffer layer.

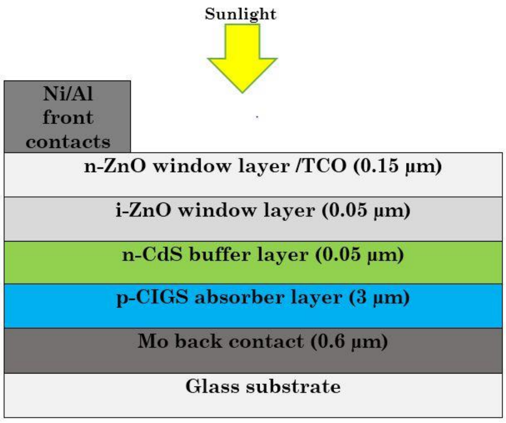

Fig. 1 – CIGS solar cell based on CdS buffer layer

The two structures are composed by stack of layers deposited on a glass substrate. Layers from bottom to top are as follows: the molybdenum back contact (0.6 µm), the 3 µm thickness of p-type doped CIGS ($CuIn_{1-x}Ga_xSe_2$) with $x = 0.3$ used as an absorber layer, the n-doped CdS (first structure) or ZnS (second structure) with 0.05 µm as buffer layers, and the intrinsic i-ZnO (0.05 µm) and the n-doped ZnO (0.15 µm) as a window layer and transparent conducting oxide (TCO).

The diverse simulation parameters of each material used in CIGS solar cell are defined in Table 1 [11, 14, 19, 20]. It is to note that the operating temperature is set at room temperature (25 °C). In addition, CIGS solar cell has been illuminated under the standard solar spectrum at the earth's surface AM 1.5 G with incident power density of 100 mW/cm^2. The optical parameters of different materials are obtained from experimental studies taken from literature [16-18].

Table 1 – Different parameters of CIGS solar cell layers

Parameters	*p*-CIGS	*n*-CdS	*n*-ZnS	*n*-ZnO
Thickness w (μm)	3	0.05	0.05	0.15
Doping density (cm^{-3})	$N_A = 10^{16}$	$N_D = 10^{18}$	$N_D = 10^{18}$	$N_D = 10^{18}$
Relative permittivity ε_r (F.cm^{-1})	13.6	10	8.28	9
Band gap energy E_g (eV)	1.2	2.48	3.8	3.3
Electron affinity χ_e (eV)	4.58	4.18	4.13	4.5
Conduction band effective density of states N_c (cm^{-3})	2.2×10^{18}	2.41×10^{18}	1.7×10^{18}	2.2×10^{18}
Valence band effective density of states N_v (cm^{-3})	1.8×10^{19}	2.57×10^{19}	2.4×10^{19}	1.8×10^{19}
Electron mobility μ_n (cm^2/V s)	100	100	250	100
Hole mobility μ_p (cm^2/V s)	25	25	70	25
Defect density N_t (cm^{-3})	2×10^{14}	10^{18}	10^{17}	10^{17}
Defect energy position E_t (eV)	mid-gap	mid-gap	mid-gap	mid-gap
Electron capture cross section σ_n (cm^2)	10^{-13}	10^{-17}	10^{-12}	10^{-12}
Hole capture cross section σ_p (cm^2)	10^{-15}	10^{-12}	10^{-15}	10^{-15}

4. RESULTS AND DISCUSSION

4.1 Simulation of CdS-CIGS Solar Cell Structure

The *J-V* characteristic resulting from the simulation of CIGS solar cell based on CdS as a buffer layer is shown in Fig. 2. The various electrical parameters are 38.7 mA/cm^2, 748.12 mV, 79.18 % and 22.92 % for *Jsc*, *Voc*, FF and η, respectively.

In order to validate our used simulation model, the obtained parameters are compared with the experimental ones reported in [9] and other results found in literature [7]. All results are listed in Table 2. As seen from the table, it is evident that the electrical parameters of our simulation results are very close to that of the experimental ones, and they are better than the simulated results taken from literature [7]. This can effectively validate our model and parameters used in this simulation, and thus support the next simulation results.

Table 2 – Comparison of simulated and experimental results of CIGS solar cell

Electrical parameters	Our simulated results	Experimental results [9]	Other simulated results [7]
J_{SC} (mA/cm^2)	38.7	38.5	34.89
V_{OC} (mV)	748.12	746	646
FF (%)	79.18	79.7	78.03
η (%)	22.92	22.92	17.55

4.2 Simulation of ZnS-CIGS Solar Cell Structure

Substituting CdS by ZnS as a buffer layer in CIGS solar cell, Fig. 2 displays the *J-V* characteristics of both CdS and ZnS-CIGS solar cell designs. It is clearly that ZnS-CIGS solar cell design illustrates better performance in comparison with CdS-CIGS solar cell design. Accordingly, the corresponding photovoltaic parameters of both structures are summarized in Table 3.

As can be seen from Table 3, there is important increase in parameters by (case of ZnS-CIGS solar cell) 1.95 mA/cm^2, 4.48 mV and 1.48 % for short-circuit current J_{SC}, open circuit voltage V_{OC} and efficiency, respectively, and also a slight increase by 0.61 % for fill factor FF compared to CdS-CIGS solar cell. This is due to high band gap of ZnS compared to that of CdS, which lead to fewer photons absorbed by this layer and allow more photons to reach the CIGS absorber layer, which contribute to the photocurrent, and consequently increase the short-circuit current.

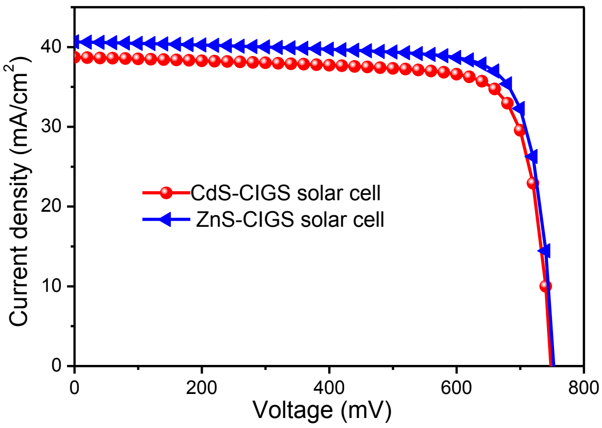

Fig. 2 – *J-V* characteristics of both CdS and ZnS-CIGS solar cell structures

Table 3 – The photovoltaic parameters of both CdS and ZnS-CIGS solar cell designs

Photovoltaic parameters	CdS-CIGS solar cell	ZnS-CIGS solar cell
J_{SC} (mA/cm^2)	38.7	40.65
V_{OC} (mV)	748.12	752.6
FF (%)	79.18	79.79
η (%)	22.92	24.4

4.3 Optimization of ZnS-CIGS Solar Cell

To obtain great performance of ZnS-CIGS solar cell, an optimization process is applied to the structure by varying its buffer layer doping density and keeping other parameter values constant. The ZnS buffer layer doping density is varied from 10^{18} to 10^{22} cm^{-3}. Fig. 3 plots the variation of different electrical parameters versus ZnS doping density. As illustrated in Fig. 3, all parameters (*Jsc*, *Voc*, FF and η) increase with increasing ZnS doping density (N_D) from 10^{18} to 10^{21} cm^{-3}. Particularly, the efficiency increases from 24.4 % to 25.1 %. However, beyond 10^{21} cm^{-3} doping density, the performance parameters become almost constant.

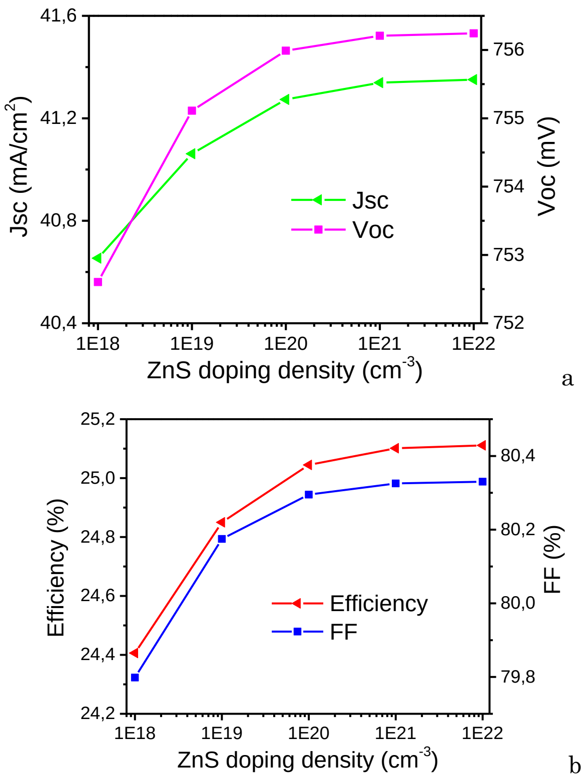

Fig. 3 – Different electrical parameters against ZnS buffer layer doping density: (a) short-circuit current and open circuit voltage; (b) fill factor and efficiency

Accordingly, the doping density value of 10^{21} cm^{-3} can be considered as an optimal value of the ZnS buffer layer, which gives higher efficiency of ZnS-CIGS solar cell. The obtained results can be explained according to equations (8) and (11), as the donor doping density N_D increases, the reverse saturation current I_0 decreases leading to the increase in the open circuit voltage V_{OC} and thus the device performance.

Using the optimal ZnS buffer layer doping density of 10^{21} cm^{-3}, the optimized ZnS-CIGS solar cell reaches an efficiency of 25.1 %.

5. CONCLUSIONS

In this study, numerical modelling of CIGS solar cell based on CdS as a buffer layer is carried out using Atlas-Silvaco program. The obtained simulation results are compared to the experimental ones where a good agreement was found between them, which potentially validates our model. In addition, an alternative buffer layer ZnS is introduced in CIGS solar cell. Then, the simulation results are compared with those of CdS-CIGS solar cell indicating an enhancement of performance of CIGS solar cell by including ZnS as a buffer layer. In particular, the efficiency increases from 22.92 % to 24.4 %. Therefore, an optimization process has been applied, and the power conversion efficiency reaches its maximum value of 25.1 %. The results of this simulation can be helpful for designers to fabricate high-performance CIGS solar cell.

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Теоретичне дослідження щодо вдосконалення сонячних елементів на основі CIGS

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Оскільки потреба в енергії продовжує зростати, необхідність в різних її джерелах є очевидною. Поновлювані джерела енергії забезпечують стійку та екологічно чисту енергію, яка може бути альтернативою традиційній енергії. Сонячні елементи – це поширена форма відновлюваної енергії. Для виробництва тонкоплівкових сонячних елементів було розроблено багато матеріалів. Сонячний елемент на основі $Cu(In, Ga)Se_2$ (CIGS) вважається одним з найбільш перспективних тонкоплівкових сонячних елементів завдяки безлічі привабливих особливостей. У роботі представлено чисельне моделювання тонкоплівкових сонячних елементів CIGS за допомогою двовимірного імітаційного пристрою під назвою Silvaco-Atlas. Було вивчено кілька структур сонячних елементів CIGS, використовуючи CdS як буферний шар. У роботі ми спочатку досліджуємо сонячний елемент CIGS на основі буферного шару CdS. Результати моделювання порівнюються з результатами попередніх пов'язаних експериментальних та теоретичних досліджень. Крім того, фотоелектричні параметри добре узгоджуються з експериментальними, що підтверджує нашу імітаційну модель. По-друге, ми розглядаємо сонячний елемент CIGS на основі ZnS як буферного шару з метою підвищення ефективності перетворення енергії сонячних елементів CIGS. Тому фотоелектричні параметри конструкції сонячних елементів CdS-CIGS порівнюються з параметрами конструкції сонячних елементів ZnS-CIGS, що демонструє значне підвищення ефективності при буферному шарі ZnS. Зокрема, ефективність збільшується з 22,92 % до 24,4 %. Крім того, для проектування сонячних елементів ZnS-CIGS застосовується процес оптимізації, що дає ефективність 25,1 %. Запропонована конструкція сонячних елементів CIGS може значно підвищити продуктивність сонячних елементів. Таким чином, ZnS можна розглядати як перспективний альтернативний буферний шар для підвищення ефективності тонкоплівкових сонячних елементів CIGS.

Ключові слова: Сонячний елемент CIGS, ZnS, Ефективність, Буферний шар, Оптимізація.