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Numerical analysis of the effect graded Zn (O, S) on the performance of the graded CIGS based solar cells by SCAPS-1D

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Abstract

We used a one-dimensional simulation program solar cell Capacitance Simulator in 1 Dimension (SCAPS-1D) to investigate Copper-Indium-Gallium-Diselenide- (CIGS-) based solar cells properties. CIGS Solar cells, constituted by a pile of thin layers, contain in a particular fine layer called buffer layer cadmium sulfide (CdS) between the absorber (CIGS) and before the contact oxysulfure of zinc (Zn(O,S). The study will focus on the simulation of the characteristics of a photovoltaic module (the open circuit voltage, the short circuit current, the form factor and performance of the cell). The results obtained after optimization of the thickness and doping of the holders of the absorbent layer and the window layer are Voc = 0.92 V, Icc = 38.33 mA/cm², FF = 77.23% and the energy conversion efficiency is 27.51%.

Keywords: Thin film solar cells; Graded CIGS; Graded Zn (O, S); Thickness optimization; SCAPS 1-D.
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1. Introduction

Thin film solar cells offer a number of interesting advantages compared to the bulk silicon devices, which are fairly complicated and expensive to produce [1]. Chalcopyrite Cu (In,Ga)Se_2 (CIGS) is a very promising material for thin film photovoltaic's and also, chalcopyrite based solar modules uniquely combine advantages of thin film technology with the efficiency and stability of conventional crystalline silicon cells [2,3]. CIGS based thin film solar cells have up to now yielded efficiencies of up to 20% in lab scale fabrication [1], however, there is a large gap between the efficiency of lab scale fabricated cells and commercial modules. This can be narrowed by a concerted effort at the fundamental science of thin film materials and interfaces [4]. CIGS absorbers today have a typical thickness of about 1–2 µm, however, on the way toward low-cost mass production, it will be necessary to reduce the thickness even further [5]. The main reasons for this are the material costs, the fact that indium and gallium resources are limited, and the need to cut the process duration in order to achieve a higher production output. So far, absorbers down to a thickness of about 0.5 µm have already been achieved with no or only little reduction of the open circuit voltage and the fill factor [6]. But, the short-circuit current density is decreased significantly in those devices, as the absorber thickness is no longer much larger than the absorption and

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it should be necessary to optimize all cell structure. CIGS devices are typically fabricated in a substrate configuration by sequentially depositing metal and semiconductor layers on a suitable base substrate (*figure 1*).

In this paper, in order to investigate the effects of cell composed layers' thickness on the performance of the cell, a typical CIGS structure which composed of five layers, a layer of Mo deposited on a glass substratum with lime sodium as contact defers for the solar cells. Cu (In,Ga)Se2 is deposited on the back electrode of Mo as photovoltaic material absorber. The heterojunction is then achieved by the deposit of chemical bath (CBD) of CdS [8] and by deposit Sputtered deposited (PVD) of Zn (O, S), the structure is shown in figure 1.

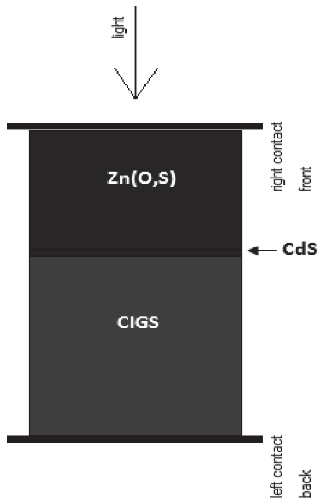

Fig. 1: Schematic structure of typical CIGS based thin film solar cells

This paper indicates a simulation study to optimize the CIGS based thin film solar cells. In this study we use SCAPS numerical simulation software to predict the changes to CIGS based solar cell performance that are introduced by the presence of the thicknesses of absorber, window and TCO (transparent conductive oxide) layer. An optimum value of the thickness of this structure has been calculated and it is shown that by optimizing the thickness of the cell, the efficiency has been increased and the cost of production can be reduced.

2. Numerical simulation

We have modeled the J–V characteristics, fill factor (FF) of graded $Cu(In_{1-x},Ga_x)Se_2$ solar cells with the numerical simulation package SCAPS [9, 10]. Electron and hole mobility's of 100 cm²/V s and 25 cm²/V s selected [10]. Poisson's equation commonly used for semiconductor device simulation is:

$$\frac{d^2}{dx^2}\psi(x) = \frac{e}{\varepsilon_0\varepsilon_r}(p(x) - n(x) + N_D - N_A + \rho_p - \rho_n). \tag{1}$$

Where ψ is electrostatic potential, e is electrical charge, ε_r is relative and ε_0 is the vacuum permittivity, p and n are hole and electron concentrations, N_D is charged impurities of donor and N_A is acceptor type, ρ_p and ρ_n are holes and electrons distribution, respectively. The continuity equations for electrons and holes are:

$$\frac{d}{dx} \quad J_n(x) - e\frac{\partial n(x)}{\partial t} - e\frac{\partial p_n}{\partial t} = G(x) - R(x) \tag{2}$$

$$\frac{d}{dx} \quad J_p(x) - e\frac{\partial p(x)}{\partial t} - e\frac{\partial p_p}{\partial t} = G(x) - R(x) \tag{3}$$

Where

$$J_n = -\frac{\mu n}{e} n \frac{\partial E_{Fn}}{\partial x} \tag{4}$$

$$J_p = \frac{\mu p}{e} n \frac{\partial E_{Fp}}{\partial x} \tag{5}$$

Where J_n and J_P are electron and hole current densities, E_{Fn} and E_{Fp} are Quasi- Fermi level for electrons and holes, G(x) and R(x) are charge generation and recombination rates. SCAPS calculates solution of the basic semiconductor equations in one-dimensional and in steady state conditions. These are the Poisson equation for electrostatic potential, and the continuity equations for electrons and holes together with the appropriate boundary conditions [8]. Recombination in deep bulk levels and their occupation is described by the Shockley–Read–Hall (SRH) formalism. The current transport mechanism of our model can be explained in general terms by considering the effect of light on the band diagram [10]. Since the calculations require the input of device parameters, the surface recombination velocities of both electrons and holes were set at 10^7 cm/s. The solar AM 1.5 radiations was adopted as the illuminating source with power density of 100mW/cm². The light refection of the front and back contacts was set at 0.1 and 1 respectively. The light absorption coefficient for CIGS layer was taken from absorption file. The other simulating parameters are given in table 1.

Table 1: Parameter values adopted for the solar cell in the simulation

Parameter	**Graded p-CIGS**		**CdS**	**Graded n-Zn(O,S)**	
Relative permittivity $\varepsilon/\varepsilon_0$	13.6		10	9	
X (ev)	4,5		4,2	4,45	
band gap Energy Eg [eV]	1	1,65	2.4	3.3	3,6
Electron mobility μ_e [cm²/Vs]	100		100	100	
Hole mobility μ_h [cm^2/Vs]	25		25	25	
Acceptor or Donor concentration[cm^{-3}]	P : $2*10^{18}$	P : $2*10^{16}$	n : 5. 10^{20}	n : 10^{17}	
Effective density of states N_C [cm^{-3}]	$2.2*10^{18}$		$2.2*10^{18}$	$2.2*10^{18}$	
Effective density of states N_V [cm^{-3}]	$1.8*10^{19}$		$1.8*10^{19}$	$1.8*10^{19}$	

3. Results and discussion

Several research groups have an attempt to improve the efficiency, of CIGS based solar cells [11]. Also, replacing toxic CdS buffer layer with other materials has been reported [12]. One of the main challenges in CIGS based solar cell is the cost of materials which it is limited the mass production of these devices that of module price in comparison with conventional single or polycrystalline silicon solar cells is too high. Typical thickness of CIGS absorber is about 1–2 µm but it is not cost efficient and thickness of the cell should be reduced. This paper indicates a study to optimize the CIGS based solar cell by considering the effects of layer thickness on the performance of the cell and the graded structure of Zn(O,S). In this respect, the structure of CIGS based thin film solar cell is shown in figure 1.

Figure 2 shows the variation of efficiency and fill factor versus CIGS thickness. It is shown that by increasing the thickness from 0.05µm to 0.3 µm, efficiency increase from 14.91 to 24.22% efficiency increase about 10% and after 0.3 µm falls down. From the simulation, results were found that the optimized value of the graded p-CIGS is 0.3 µm which leads to a thinner and cheaper solar cell.

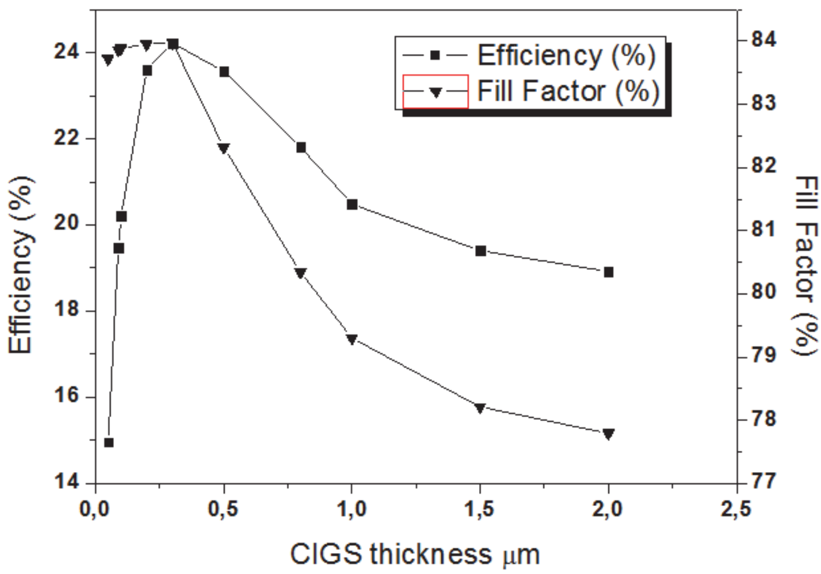

Fig. 1: Variation of efficiency and fill factor as a function of graded CIGS thickness

Figure 3 shows variation of transparent conductive oxide (TCO) thickness, n-Zn(O,S), versus fill factor (FF) and efficiency. It is shown that by decreasing the thickness of graded n-Zn(O,S), cell efficiency increases. It is due to this fact that n-Zn(O,S) is not fully transparent for light and this layer always absorbs and reflects the sunlight. As shown in Figure 3, by increasing the Zn(O,S) thickness, light absorption increases and leads to lower efficiency. By decreasing the Zn(O,S) layer from 1µm to 0,001µm, it is predicted that cell efficiency increases from about 20.10 % to 20.80 %. Also, FF curve has the same increasing rate as shown in Figure 3 .Calculation shows that variation of the Zn(O,S) thickness has no effect on the current density. Simulation results shows optimized value of CIGS and graded n-Zn(O,S) thickness is 0.3 µm and 0.002 µm respectively. The figure 4 shows the J-V characteristics for optimized values such as J_{SC} (short circuit current), V_{OC} (Open circuit voltage), Fill Factor FF and efficiency η are 40.28 mA/cm², 0.7198 V, 83.56% and 24.23% respectively.

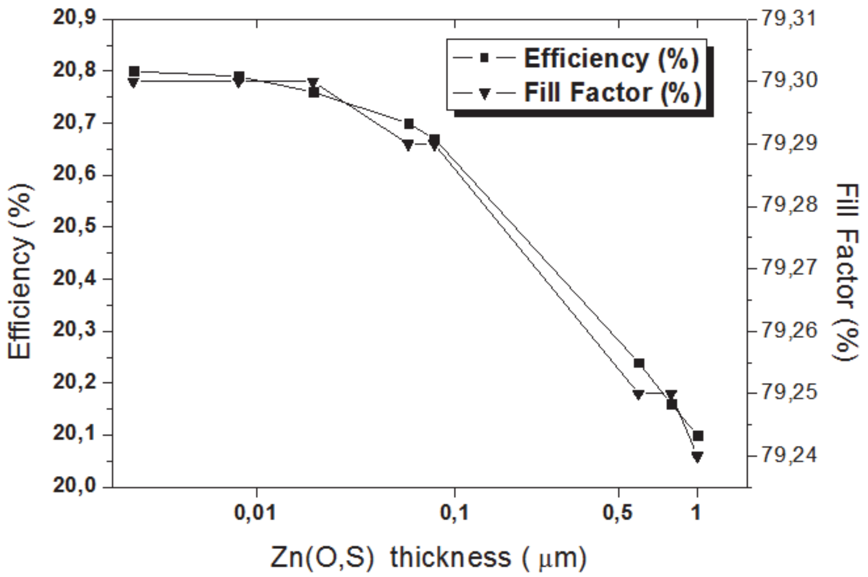

Fig. 2: Variation of efficiency and fill factor as a function of graded Zn (O, S) thickness

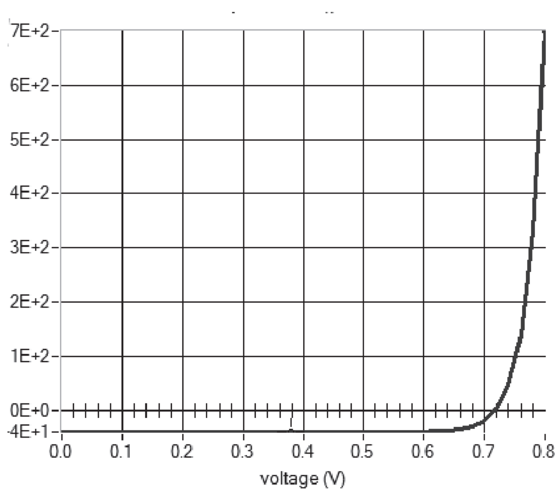

Fig. 3: J-V characteristics of optimized graded CIGS

We note when the doping concentration of the absorber layer increase the efficiency of the solar cell increase. The characteristics of the semiconductor materials are strongly influenced by the impurities. They are added to increase the electrical conductivity or the control of the duration of life, but these often these impurities or imperfections in the network, from a certain threshold, act as factors loss, therefore a high concentration of defects discriminates the carrier transport, thereby reducing the conversion efficiency.

Figure 5 shows the variation of efficiency and fill factor versus doping of CIGS. It is shown that by increasing the doping of CIGS from 2.10^{16} to 9.10^{20} cm^{-3}, efficiency increase from 20.44 to 28.77% efficiency increase about 8% and after 10^{21} cm^{-3} falls down. This simulation results have a good agreement with the theoretical estimation. But we note that for this value of the doping, fill factor is small so it does not correspond to the optimal value. The best value that gives good performance and fill factor for doping 2.10^{20} cm^{-3}.

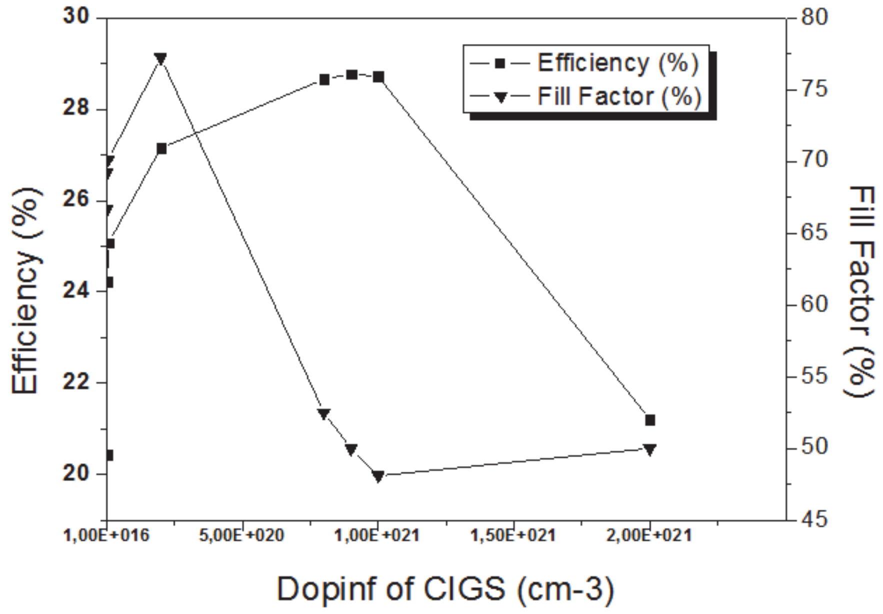

Fig. 4: Variation of efficiency and fill factor as a function of doping of graded CIGS cm^{-3}

The optimum parameters of the optimum structure obtained by our simulation for the two thin layers (Zn (O, S), CIGS) are presented in the following table 2.

Table 2: The optimum parameters obtained by our simulation

Zn(O,S)		CIGS		V_{OC}	J_{SC}	FF	η
0.002µm	10^{17} cm^{-3}	0.3µm	2.10^{20} cm^{-3}	0.92 V	38.33mA/cm²	77.23%	27.51 %

4. Conclusion

This paper indicates a numerical investigation of graded CIGS based solar cells. Numerical optimizations have been done by adjusting parameters such as the combination of band gap, as well as the specific structure of the cell. From the simulation result, it was found that by optimization of the considered structure, optimized value of graded CIGS and graded Zn(O,S) thickness is 0.3 um and 0.002 um and an improvement of conversion efficiency has been observed in comparison to the conventional CIGS which cell efficiency increase to 24.23%.When the doping of CIGS is 2. 10^{20} cm^{-3} the efficiency is 27.51%. CIGS layer thickness is very important since it influence through efficiency and through manufacturing costs. Because of these two facts, the argument has been made that highly absorbing, thinner thickness, and inexpensive absorbers may give the best optimization.

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