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Analysis of Absorber and Buffer Layer Band Gap Grading on CIGS Thin Film Solar Cell Performance Using SCAPS

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ABSTRACT

A numerical simulation and analysis was performed to investigate the effect of absorber and buffer layer band gap grading and on a Copper-Indium-Gallium-Diselenide (CIGS) solar cell. The software used is the Solar Cell Capacitance Simulator (SCAPS). The absorber and buffer layer energy band structures' effect on the cell's output parameters such as open circuit voltage, short circuit current density, fill factor and efficiency were extensively simulated. Two structures of the energy band gap were simulated and studied for each of the absorber and buffer layer. The simulation was done on the uniform structure in which the energy band gap is constant throughout the layer. It was then continued on the cell with graded band structure, where the energy band gap of the material is varied throughout the layer. It was found that the cell with graded band structure in absorber and buffer layer had demonstrated higher efficiency and better performance in comparison with the cell with uniform band gap structure.

Keywords: Band gap, CIGS absorber, Grading, SCAPS

INTRODUCTION

Copper-Indium-Gallium-diSelenide (CIGS) thin-film solar cell is known as a promising alternative to expensive conventional silicon-based solar cells. Its characteristics for high performance and low cost have led to the direct increase in the interests in this type of thin film solar cells. The cell, consisting of the CIGS layer, is a p-type semiconductor material. The role of this layer that is to absorb incoming photons which reach the layer. According to the theoretical considerations proposed by Loferski and also based on Shockley–Queisser limit, the maximum theoretical efficiency of a solar cell can be obtained by the absorber

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layer band gap in the range of 1.2 eV to 1.5 eV (Loferski, 1956; Shockley & Queisser, 1961). This has led to the interest in using CIGS material due to its energy band gap, which is in the range of 1.06 eV to 1.7 eV. This feature firmly makes CIGS as a promising semiconductor material to be used as an absorber layer in a thin film solar cell.

The other important layer of the CIGS solar cell structure is the buffer layer. The role of a buffer layer in a heterojunction is to form a junction with the absorber layer, while leading maximum amount of incoming light to the absorber layer. The buffer layer should have minimal absorption losses, low surface recombination and minimal electrical resistance when transporting the photo generated carriers to the outer circuit (McCandless & Hegedus, 1991). The most important features of the buffer layer are protecting the junction against the chemical reactions and mechanical damage, as well as optimizing the band alignment of the cell, electrical properties and making a wide depletion region with the p-type absorber layer. This eventually can minimize the carriers tunneling and maintain higher open circuit voltage value to establish higher contact potential (Contreras *et al*., 2002). In order to satisfy such desired features, the buffer layer should have a wider band gap in comparison with the CIGS layer. The most common used material as a buffer layer in CIGS solar cells is Cadmium Sulfide (CdS). Recently, the efficiency of a CdS/CIGS solar cell was recorded at 20.4% and this was achieved when it was fabricated on flexible polymer substrates (Tiwari, 2013). This achievement was compared to the previous 20.3% efficiency which was gained with a CdS/CIGS solar cell on glass substrate (Jackson *et al*., 2011). Despite the highest efficiency of CIGS cells recorded, the cell was with CdS buffer layer. This has been a contrast to some developments of solar cells with Cd-free buffer layer which is important because of CdS toxicity was found to be harmful to human health (Siebentritt, 2004). Thus, the Indium Sulfide is one of most promising alternative materials to be used as the buffer layer in CIGS cells due to its band gap that can vary in the range of 2 eV to 2.9 eV (Ernits *et al*., 2007; Revathi, Prathap, Subbaiah, & Reddy, 2008; Saadallah, Jebbari, Kammoun, & Yacoubi, 2011). The highest efficiency level that has been achieved up to now from a CIGS thin film solar cell with In_2S_3 buffer layer is 16.4% (Naghavi, Spiering, Powalla, Cavana, & Lincot, 2003). Accordingly, there is still a gap between the highest reported efficiency of cells with In_2S_3 and CdS buffer layers.

One technique that can be used to improve the efficiency of In_2S_3/CIGS cell performance is band gap grading. The band gap grading usually is done on absorber layer band gap. Since the band gap of In_2S_3 can vary in a certain range, this technique can be done on buffer layer band structure in an In_2S_3/CIGS cell as well. In this study, the effects of absorber and buffer layer band gap grading were investigated separately.

MATERIALS AND METHODS

SCAPS Numerical Simulation Programme

SCAPS (Solar Cell Capacitance Simulator) software was designed and introduced by the University of Gent (Burgelman, Nollet, & Degrave, 2000). It is used for numerical analysis of solar cell performance and characteristics. Multiple measurements of solar cells' output parameters can be done through SCAPS. It can simulate the open circuit voltage (Voc), short circuit current density (Jsc), output J-V characteristic, fill factor (FF), quantum efficiency (QE), cell's output efficiency (η,), generation and recombination profiles, band alignment, etc. SCAPS simulation software does all these measurements by solving the fundamental semiconductor equations such as the Poissons equation and the continuity equation for the electrons and holes. These equations are solved via numerical techniques. It needs an initial prediction for the calculations and to get the solution. Thus, SCAPS will calculate several situations at the first measurement point and under the set working point. Fig.1 is a flow chart that shows the strategy of SCAPS performed for getting to the working point and the first calculation point. Each calculation begins at the start point. The initial assumption to get to the equilibrium situation is zero quasi-Fermi levels throughout the structure and no potential drop over the structure. In the case of the calculation under dark condition, this equilibrium is used as an initial condition to calculate the solution. While under light condition (with illumination), the short circuit situation is calculated in an intermediate step to serve as the next initial guess. The convergence of the Gummel type iteration scheme with Newton-Raphson algorithm is used in SCAPS for numerical calculations. This scheme's parameters can be set in the numerical setting panel as convergence settings. In order to improve the convergence, the number of iteration steps can be increased. Obviously, this can decrease the calculation speed and consequently increase the processing time, especially in batch calculations.

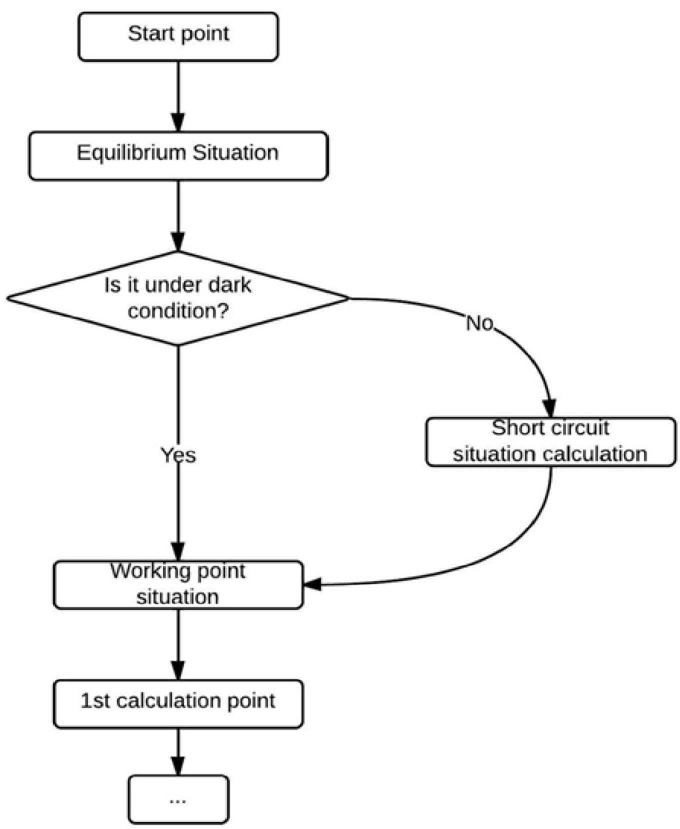

Fig.1: Strategy of getting to the working point and first calculation point

One of the most important facilities available in SCAPS is the possibility of defining layers with graded parameters. The mechanism of a graded layer definition is that the layer is considered to have composition $A_{1-y}B_y$. The properties of pure compounds A (y=0), B (y=1) and the composition grading y(x) over the thickness of the layer should be set as input values. The material properties that may vary from pure A to pure B in the layer thickness are defined as a function of y, as shown in equation (1):

$$P = f[y(x)] \tag{1}$$

Several grading functions available in SCAPS that can be used for grading over the layer are linear, logarithmic, parabolic (two laws), power law, exponential, effective medium, etc. These significant features of SCAPS are used to investigate the effects of absorber and buffer layers' band gap grading on CIGS solar cell's output performance.

Cell Structure and Materials Properties

The cell structure simulated is shown in Fig.2. The TCO window layer is actually a bi-layer made by an intrinsic zinc oxide (i-ZnO) and an aluminium- doped zinc oxide (ZnO:Al) deposited on In_2S_3 buffer layer. The absorber layer is $Cu(In_{1-x}, Ga_x)Se_2$ (CIGS) which is a compound and direct band gap semiconductor material. The band gap and consequently the electron affinity of $Cu(In_{1-x}, Ga_x)Se_2$ vary in the range of 1.06 eV- 1.7 eV and 4.6eV - 3.4 eV, respectively, due to the variation of Gallium ratio in the layer composition (x) (Saji, Lee & Lee, 2011). As mentioned in the introduction section, the band gap and electron affinity of In_2S_3 can vary in the range of 2 eV to 2.9 eV. The adjustable properties of these materials give the opportunity of band gap grading in absorber and buffer layers.

In this study, the absorber and buffer layer band gap and their corresponding electron affinity are varied in the mentioned range at individual simulation steps. There are other electro-optical properties of materials need to be set for each layer in SCAPS. Table 1 shows the summary of material properties that are used in SCPAS for this simulation. All the parameters are extracted from reliable numerical models and experimental studies (Barreau, Marsillac, & Berne, 2001; Gloeckler, Fahrenbruch & Sites, 2003; Rau & Siebentritt, 2006; Robles *et al*., 2005; Shan & Yu, 2004).

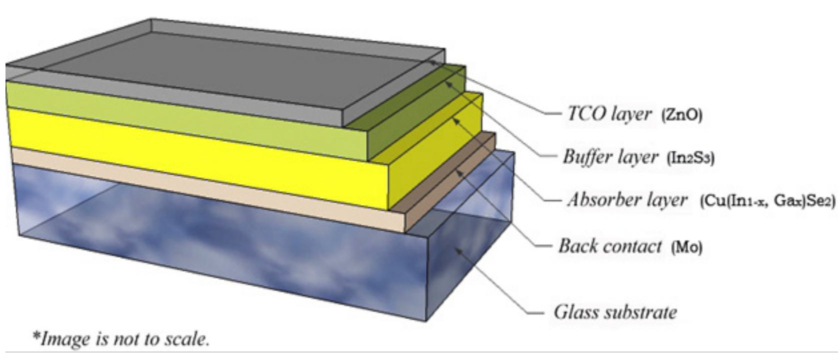

Fig.2: The CIGS thin film solar cell's structure (Khoshsirat & Md Yunus, 2013)

TABLE 1 : Summary of the parameters used in SCAPS for CIGS solar cell simulation

	Layers			
Properties	CIGS	In_2S_3	i-ZnO	ZnO:Al
Thickness (μm)	2	0.03-1	0.1	0.8
Energy Band gap (eV)	1.2	2.1-2.9	3.3	3.3
Electron Affinity (eV)	4.25	4.65-3.85	4.6	4.6
Dielectric permittivity	13.6	13.5	9	9
Conduction band effective density of states (1/cm^3)	2.2E+18	1.8E+19	2.2E+18	2.2E+18
Valance band effective density of states (1/cm^3)	1.8E+19	4.0E+13	1.8E+19	1.8E+19
Electron mobility (cm^2/Vs)	1.0E+2	4.0E+2	1.0E+2	1.E+2
Hole mobility (cm^2/Vs)	2.5E+1	2.1E+2	2.5E+1	2.5E+1
Acceptor concentration (1/cm^3)	1.0E+16	1.0E+1	0	0
Donor concentration (1/cm^3)	0	1.E+16-5E+18	1.0E+16	1.0E+18

RESULTS AND DISCUSSION

The Effect of Absorber Layer Band Gap Grading on Cell Performance

In this stage of simulation, the effect of using non-uniform band absorber layer was investigated as the band gap of CIGS absorber layer varied. In other words, the goal of this step is to study the effect of absorber layer band gap grading due to Ga content grading on the cell performance. There are several models for graded band CIGS absorber layer. One of them is the partially back grading, where the absorber layer is divided into two parts; the first part is near to the p-n junction which has uniform band gap and the second part is thinner and closer to the back contact and it has linear graded band gap and the highest band near back contact. In this simulation, the band gap of uniform part is considered 1.2 eV corresponding to the optimum energy band gap of CIGS layer. The graded part's band gap appears to increase on one occasion from 1.2 eV to 1.4 eV and next from 1.2 eV to 1.7 eV. Meanwhile, the thickness of the graded band section (d_{grd}) also varied from 0.1μm to 0.5μm and the thickness of uniform band section was kept constant at 1μm. At the last step a cell with whole back graded band absorber layer was simulated and the results of the simulation are shown in Table 2. The band diagram of cells with partially and whole back graded absorber layers are shown in Fig.3. As shown, the lower edge of conduction band varies with the variation of band gap due to Ga grading in the absorber layer. The difference between the minimum and maximum conduction band edges is shown by ΔE_g.

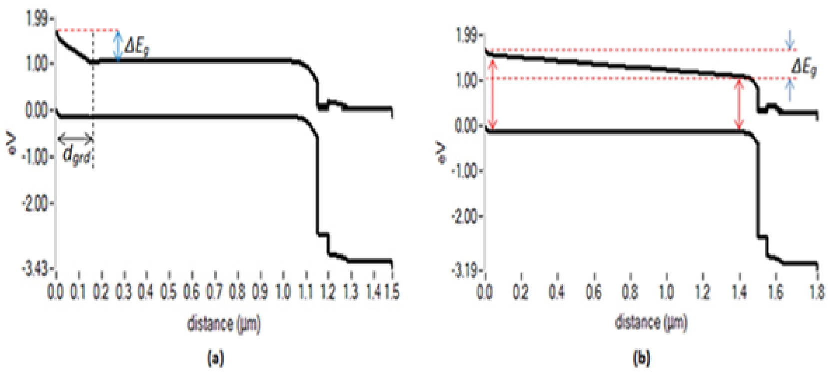

Fig.3: Band diagram of the cell with graded band absorber layer; (a) Partially back graded, (b) Whole back graded

According to the simulation results shown in Table 2 the short circuit current density is more sensitive to the variations of the graded band section's thickness and ΔEg. However, generally the cell performance will be improved by using back graded band absorber layer.

TABLE 2 : Comparison of the cells with uniform and graded band absorber layer

Band structure	ΔE_g	d_{grd}	V_{oc}	J_{sc}	FF%	η%
Cell with uniform Band absorber layer	-	-	0.7188	27.62	68.51	13.6
Cell with partially back graded band absorber layer	0.2	0.1	0.7213	29.11	68.72	14.43
Cell with partially back graded band absorber layer		0.5	0.7516	29.08	68.67	15
Cell with whole back graded band absorber layer		1.5	0.7528	32.1	74.73	18.06
Cell with partially back graded band absorber layer	0.5	0.1	0.7218	29.09	68.72	14.43
Cell with partially back graded band absorber layer		0.5	0.7219	29.214	68.69	14.49
Cell with whole back graded band absorber layer		1.5	0.7806	35.46	77.71	21.51

The results revealed that the enhancement of the cell output parameters at higher ΔE_g is more obvious. This is due to an increase of conductivity that leads to the increase of short circuit current density. Fig.4 shows the increase of cell conductance due to increase of graded section thickness. The most important benefit of using a whole graded band configuration for the CIGS absorber layer is its lower back contact recombination probability. Based on the simulation results in a cell with 1.5µm uniform band gap of 1.2 eV, the back contact recombination current density at the maximum power point voltage (V_{mpp}) is 3.66 (mA/cm^2), whereas it is $7.77E^{-4}$

(mA/cm^2) in a cell with 1.5µm absorber layer that its band gap is graded linearly from 1.4 eV to 1.2 eV. This significant reduction in the difference of back contact recombination current density gives the possibility to reduce the thickness of absorber layer. Thus, higher levels of efficiency can be obtained from the cells with thinner absorber layer (<1.5 µm). This will lead to the reduction in material usage and consequently the cell fabrication cost.

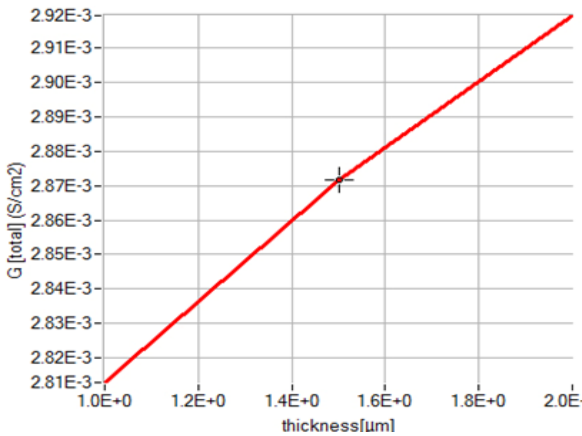

Fig.4: Increase of cell conductance due to increase of graded section thickness

Effect of Buffer Layer Band Gap Grading on Cell Performance

In this step, the effect of buffer layer band gap grading was simulated. Table 3 shows the output parameters of a cell with 0.04 µm graded band buffer layer. The electron affinity of the layer starts from 4.05 eV at areas that are closed to the absorber and increases linearly to 4.65 eV at the end of the buffer layer. As shown in Table 3, the variation of the J_{sc} resulting from the changes in the buffer layer's band gap structure is small. Therefore, J_{sc} can be considered almost constant. Both V_{oc} and FF% increased due to the buffer layer band gap grading. As tabulated, the effect of using graded band buffer layer on the cell's fill factor is significant, and this could be attributed to the lower series resistance in the cell with graded band buffer layer. The cell's output efficiency increased in consequence of increase of open circuit voltage and Fill-Factor. Accordingly, the buffer layer band gap grading could improve the performance of the cell. Fig.5 shows the difference in the J-V curve of two cells; one with a uniform band buffer layer and the other with a graded band buffer layer which refers to the series resistance difference of two structures.

TABLE 3 : Comparison of the cells with uniform and graded band buffer layer

Band structure	V_{oc}(v)	J_{sc}(mA/cm2)	FF%	η%
Cell with graded band buffer layer	0.7566	26.43	82.44	16.49
Cell with uniform band buffer layer	0.7515	26.53	78.78	15.6

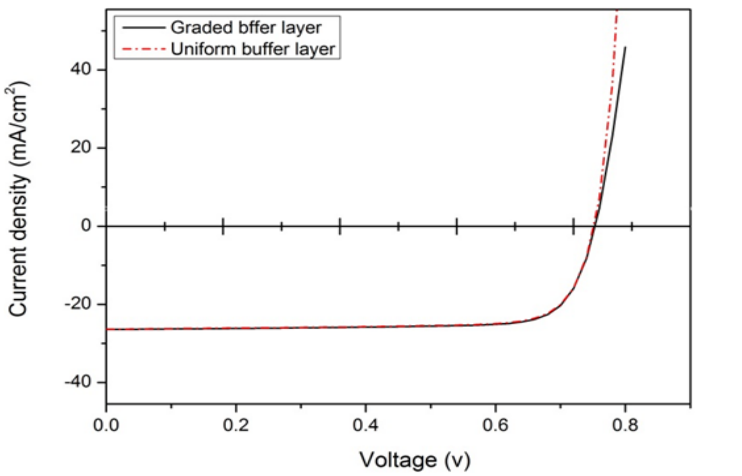

Fig.5: The J-V characteristic of cells with uniform and graded band buffer layer

As mentioned in the introduction section, the maximum efficiency reported for a CIGS thin film solar cell with In_2S_3 buffer layer is 16.4%, which was obtained from the cell with a uniform band structure for both absorber and buffer layer. Nevertheless, based on the Loferski's theoretical concerns, the maximum possible theoretical efficiency of the cell with CIGS absorber layer is about 25%, which is considered high for this kind of cell. This is still 5% lower than Shockley–Queisser limit for the single-junction solar cell efficiency.

The simulation results of this study show that an increase of the cell efficiency is possible without the growth of absorber layer thickness using the graded band structure for the absorber and buffer layer band gap. This can reduce the gap between the current efficiency record of a CIGS/In_2S_3 solar cell and the maximum theoretical efficiency of the CIGS cell.

In this study, the simulation results (see Tables 2 and 3) show that by using graded band absorber and buffer layer, losses due to back contact recombination and parasitic resistive can be reduced. Therefore, higher levels of efficiency closer to the theoretical limits are achievable. These results are exclusive and in a good agreement with experimental studies, which have been done on CIGS/CdS solar cell with graded band absorber layer (Dullweber, Anna, Rau, & Schock, 2001; Lundberg, Edoff & Stolt, 2005).

CONCLUSION

The cell performance was analyzed and simulated by the functions of absorber and buffer layer band gap grading. The numerical simulation results obtained with SCAPS showed that the cell with graded band structure in absorber and buffer layer gave higher performance as compared to the cell with uniform band gap structure. Besides, the effect of the absorber layer band gap grading on cell performance was found to be more significant. It is shown that the cell with back graded band absorber layer represents higher conductivity, lower back contact recombination and thus higher efficiency. Hence, as a result found in this structure, this study has proposed the back graded band configuration to be used for thin and ultra-thin CIGS solar cells.

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