SIMULATION AND OPTIMIZATION OF CIGS SOLAR CELLS IN CONCENTRATED SUNLIGHT

Ali Alimardani, MaziyarNoei, EbrahimAsl-Soleimani and Ali Afzali-Kusha

School of Electrical and Computer Engineering, University of Tehran, Tehran, Iran

1. Abstract

Chalcopyrite Solar cells based on copper-indium-gallium-diselenide (CIGS) absorbers demonstrate the highest efficiencies of all thin film photovoltaic technologies. In the recent years, laboratory scale cells have reached efficiencies of about 20% and this technology has received significant funding to support its growth. Simulations of CIGS solar cells can help designers to examine and evaluate their limiting factors and employ proper techniques to overcome them. In this work, we simulate single-crystal CIGS solar cells with different absorber thicknesses and compositions, different grading ratios and different doping concentrations when considering some defect densities. Moreover, we have added grain boundaries in the structure of our cell's absorber layer in order to have a qualitative look at the effects of poly-crystalline boundaries in charge carriers' recombination rate and their influence on efficiency. Furthermore, we compared our results for the cells with and without boundaries. This comparison helps one to understand the impact of morphology in a CIGS solar cell on its efficiency. In addition, we performed all of our simulations in higher concentrations of sunlight in order to optimize the grading ratio and doping concentration in these conditions for obtaining the highest efficiency.

2. Introduction

Recently, commercial interests have begun to shift towards thin film solar cells where lower amounts of absorber materials are used in the fabrication processes. So far, Copper Indium Gallium (di)Selenide solar cells have received favorable attention among emerging materials for solar cell fabrication (Ugarte, et al. 1999). $CuIn_{1-x}Ga_xSe_2$, being a chalcopyrite material and belonging to P65 symmetry group, experiences direct electronic transitions and is among the materials with high production volumes. The CIGS solar cells offer the specific power of up to 919 W/Kg, which is the highest attainable value among the thin film solar cells (Otte et al. 2006). Also, their high efficiency (as a result of CIGS's direct bandgap and high optical absorption coefficient) and low cost potential, as well as their ability to be fabricated in a flexible and inexpensive way offer new possibilities for their applications. Moreover, CIGS cells also display strong radiation hardness compared to GaAs solar cells (Rudmann and Kessler, 2004). This shows promise for their further use in space applications. These features have made CIGS solar cells very attractive in the recent years.

By changing the Ga to Ga+In ratio from 0 to 1, a wide range of bandgap values (1.06eV to 1.7eV) are obtained while graded-bandgap structures, which offer even higher efficiencies can also be built. The highest reported efficiency value so far has been obtained by setting the Ga/Ga+In ratio to values of about 0.3. CIGS solar cells have reached efficiencies in the range of 20% (Bouabid et al., 2005; Ramanathan et al., 2005) and an efficiency of 21.32% has been achieved with CdS based buffer material in (Chelvanathan et al., 2010). It is found that the high efficiency CIGS cells have the absorber layer thickness of about 3µm (Pudov et al., 2005) and the optimum thickness of buffer layer is reported to be 40–50nm.

In addition to improving the open circuit voltage, incorporation of Gallium helps in improving the adhesion of absorber layer to the Molybdenum back contact. It also alters some of the material properties like lattice constant, film morphology and defect mechanisms. The composition of absorber layer can be adjusted by using different processing techniques. This is referred to as Gallium grading. Increasing the Gallium content increases the bandgap by predominantly shifting the conduction band. Therefore, Gallium grading helps to build quasi-electrostatic fields, which enhance current collection.

T. Dullweber et al. (Dullweber et al.,2000) have studied various graded absorber layers like a linearly graded absorber, multi-graded absorber and a double graded absorber. The output parameters show a strong dependency to the slope of grading in a linearly graded absorber. While in a multi-graded absorber, the current is dominated by the minimum bandgap and the open circuit voltage is dominated by the bandgap in the space charge region.

Non-radiative Shockley–Read–Hall (SRH) recombination occurs via defect states in the band gap. This recombination is higher for states near the gap center than for states near the band edges. SRH type recombination in the space-charge region not only increases the saturation current, but also increases the diode factor (Siebentritt, 2011). A special location for SRH recombination are the grain boundaries (Rau et al., 2009), which can be expected to display a large density of structural defects, like strained or dangling bonds. The density of charged defects at grain boundaries in $CuGaSe_2$ was found to be 10^{12} cm^{-2} (Schuler et al., 2002). Assuming grain sizes of about 1µm means an average defect density of 10^{16} cm^{-3}. On the other hand, it has been argued that a barrier in the valence band (Persson and Zunger, 2003) at the grain boundaries keeps the holes away from the grain boundaries and prevents recombination (Persson and Zunger, 2005).

Higher sunlight concentrations bring two advantages for solar cells. Firstly, the required area can be reduced which lowers the cost. This allows us to use more expensive technologies to produce more qualitative cells. On the other hand, open circuit voltage of the cell increases as well as its short circuit current, enhancing the cell’s efficiency. The efficiency however may be adversely affected or saturated due to other loss mechanisms present in these cells. As a result, it is obvious that design optimization of a CIGS solar cells requires the study of all of these effects.

Our purpose in this paper is to have a comprehensive study on CIGS solar cells, therefore, we organize this paper as follows. After the introduction, in Section 2 we present the cell structure which will be simulated in our work. In order to do so, we find the highest possible efficiency by simulating the device for different composition values and different absorber layer thicknesses. Using the constructed cell structure, in Section 3 we demonstrate the effects of graded-bandgap. Section 4 is devoted to the impact of absorber layer’s doping concentration on its performance, while Section 5 gives a qualitative look at the effects of poly-crystalline thin film grains and the recombination centers at their boundaries. Conclusions are finally drawn in Section 6.

3. Defining the Cell Structure

Schematic of a typical CIGS solar cell structure is depicted in Fig.1. The device consists of a typically 1µm thick Molybdenum layer which is deposited on a soda-lime glass substrate of 1-3 mm thickness and serves as the back contact.

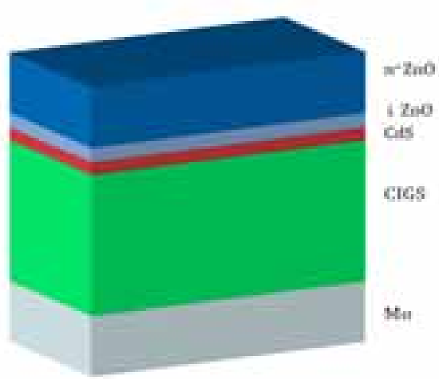

Fig.1: CIGS cell structure

The p-type absorber layer is deposited on the back contact, where a thin layer of CdS acts as buffer and forms a heterojunction with CIGS absorber film. A thinner CdS film minimizes the spectral loss caused by its light absorption, and the highest conversion efficiencies in CIGS so far have been achieved by CdS thicknesses of 30-70nm. A second buffer layer, which is a nominally undoped (intrinsic) i-ZnO (usually of thickness 50-70 nm) and then a heavily Al-doped ZnO layer are deposited on top of the structure. As ZnO has a bandgap energy of 3.3eV, it is transparent for the main part of the solar spectrum and hence is denoted as the window layer of the solar cell.

Table 1. Parameters assumed for CIGS cell simulation

	n^+ ZnO	iZnO	CdS	CIGS
Width (d)	400 nm	50 nm	40 nm	3000 nm
Dielectric constant (ε_r)	9.0	9.0	10	13.6
Electron mobility (μ_e)	100	100	100	100
Hole mobility (μ_h)	25	25	25	25
Acceptor concentration (N_A)	0	0	0	$2 \times 10^{16}\ cm^{-3}$
Donor concentration (N_D)	$4 \times 10^{18}\ cm^{-3}$	$1 \times 10^{18}\ cm^{-3}$	$1 \times 10^{17}\ cm^{-3}$	0
Electron effective DOS (N_C)	$2.22 \times 10^{18}\ cm^{-3}$	$2.22 \times 10^{18}\ cm^{-3}$	$2.22 \times 10^{18}\ cm^{-3}$	$2.22 \times 10^{18}\ cm^{-3}$
Hole effective DOS (N_V)	$1.78 \times 10^{19}\ cm^{-3}$	$1.78 \times 10^{19}\ cm^{-3}$	$1.78 \times 10^{19}\ cm^{-3}$	$1.78 \times 10^{19}\ cm^{-3}$
Affinity level (χ)	4.0	4.0	3.8	4.1
Bandgap (E_g)	3.3	3.3	2.4	$1.06 - 1.70$
	Front Surface		Back Surface	
Surface recombination for electrons	$10^7 cm/sec$		$10^7 cm/sec$	
Surface recombination for holes	$10^7 cm/sec$		$10^7 cm/sec$	
Reflectivity	0.1		0.9	

In this work, all of the simulations are done in 2-dimensions. This allows us to consider some of the lateral effects as well. Firstly, we define the structure of our cell based on the values of physical parameters that are brought in Table.1.

These values are chosen based on experimental data, literature values, theory and reasonable estimates. Using these values, to get a reference structure, the conventional CIGS cell is simulated for different fractions of gallium content in order to find the optimum value for the composition of absorber layer. Fig.2.a shows the I-V characteristics of our cell when simulated with different composition fractions. It is observed that by increasing the incorporated content of gallium in the absorber layer, its energy gap and consequently open-circuit voltage increases, while the short circuit current decreases as a result of lower wavelength cut off. In Fig.2.b, the obtained efficiencies are plotted as a function of composition fraction. It can be seen that the efficiency reaches an optimum value in Ga to Ga+In ratio of about 0.4.

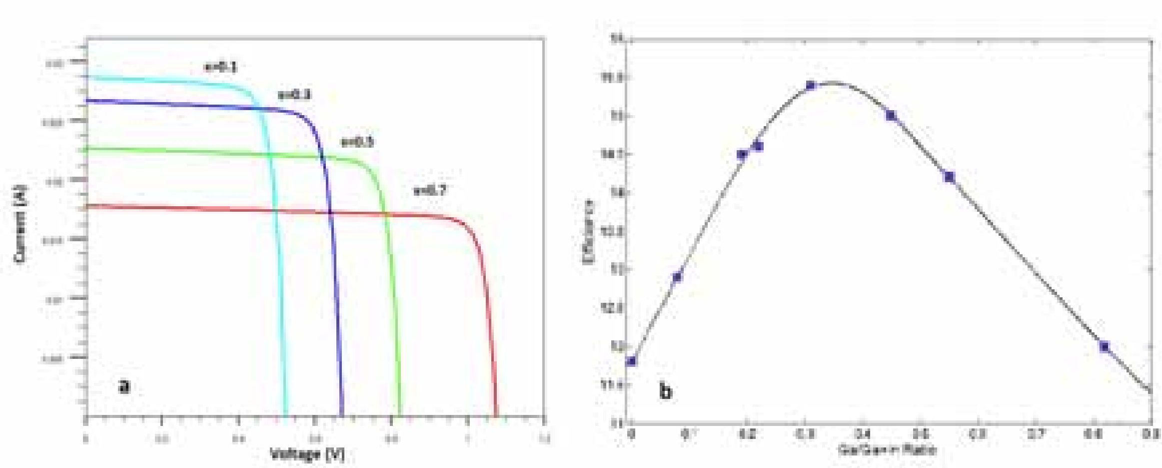

Fig. 2: Effect of changing composition fraction in CIGS a) I-V curves for some fractions b) Efficiency

Having specified the optimum composition fraction for the presented cell, the next step is to perform our simulations for different thicknesses of absorber layer. As it can be seen in Fig.3, the efficiency of cell increases with the thickness of absorber layer, but the rate of improvement is much slower for thicknesses of over 4000nm. A thicker absorber layer has more cost with very little improvement in efficiency. Therefore, the optimum value for thickness of this layer is about 3-4μm. The reference cell structure for our following simulations has thickness of 3μm for CIGS layer, 50nm for intrinsic ZnO layer, 400nm for the Aluminumdoped ZnO window and 40nm for CdS layer (Ward et al., 2001).

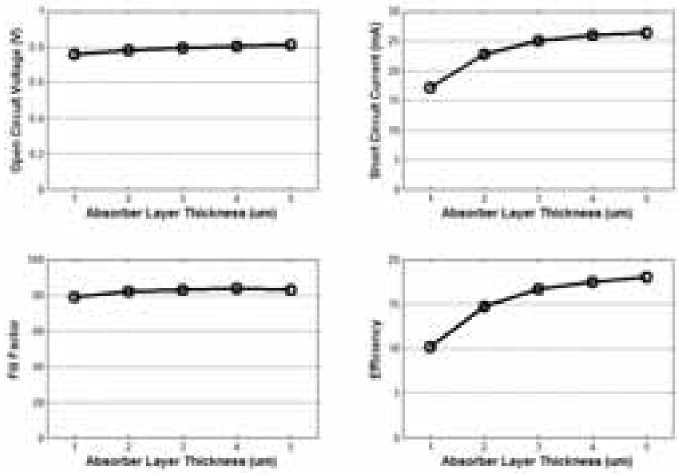

Fig. 3: Effect of the cell thickness

4. Effect of Different Grading Ratios

In this section, in order to demonstrate the effects of bandgap grading on efficiency, a certain grading profile with different grading ratios is simulated in various sunlight concentrations. In these simulations, the composition fraction of CIGS layer is varied from 0.25, 0.50, 0.75 and 1 to zero. The band diagram for these different grading ratios (in the units of Ga to Ga+In ratio per absorber layer thickness) is shown in Fig.4. This figure shows that the changes in composition fraction have a significant impact on the valence band of CIGS layer. These changes can result in quasi-electrostatic fields that affect the short circuit current to a great extent.

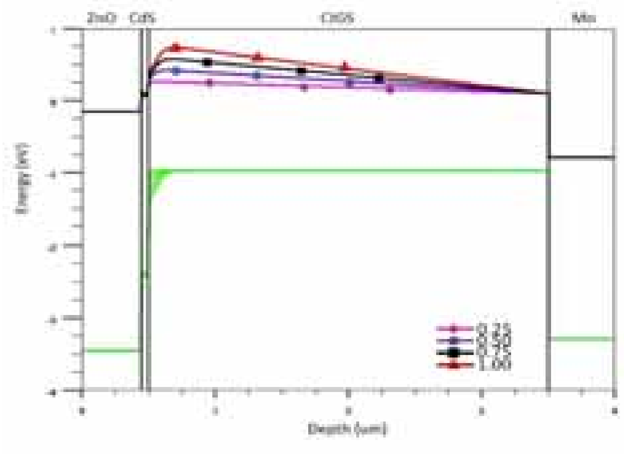

Fig. 4: Band diagram of CIGS Solar cell for different grading ratios

A higher sunlight concentration enhances the efficiency of the cell by generating more carriers. This improvement is more significant for cells with lower series resistance. Fig.5 depicts the simulated efficiency of our solar cell in different sunlight concentrations and grading ratios.

From Fig.5, it can be seen that under 1 sun concentration, efficiency increases in higher grading ratios. When the spatial variance in bandgap is not large, there's almost no significant change in the absorption coefficient and consequently the cell's current. Therefore, the electric field associated to bandgap grading will enhance the open circuit voltage, and efficiency increases. However, when the spatial variance in bandgap is large, absorption coefficient decreases and we get less short circuit current. By improving open circuit voltage, efficiency will enhance lesser than before.

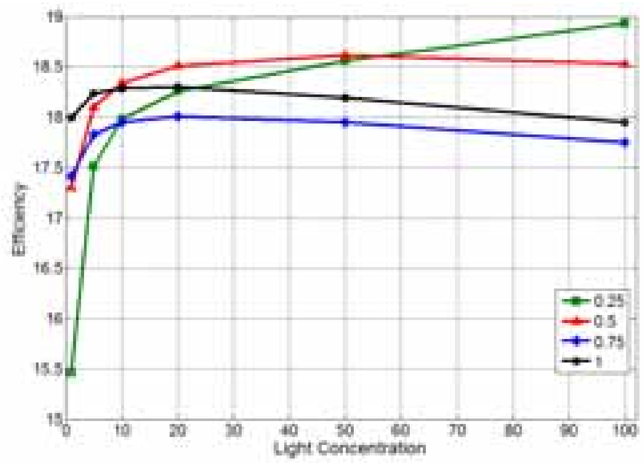

Fig. 5: Efficiency versus light concentration for different grading ratios

Higher concentrations of light generate more carriers and short circuit current almost changes proportional to the sunlight concentration. It is shown that open circuit voltage also changes in a logarithmic manner with sunlight concentration. These changes should improve the efficiency in higher concentrations if fill factor is constant throughout the enhancement of sunlight concentration. However, fill factor depends on resistivity of the cell and due to higher resistivity in the cells with higher grading ratios, by increasing the current under higher concentration of light these cells have more power loss. This causes a significant reduction in fill factor and efficiency. Maximum efficiency of the cell in each grading ratio occurs in a different sunlight concentration, because resistive losses which manifest themselves in the fill factor, take over the enhancing mechanisms in different sunlight concentrations, depending on various properties of the cell such as its grading ratio. We see that for grading ratio of 0.5, maximum efficiency occurs in 50suns, while for 0.75 it occurs in 20 suns. This can be explained by considering that the former case has a lower resistivity and compared to the latter one, it takes more increase in the cell's current for loss mechanisms to dominate. It can be seen that for grading ratio of 0.25, efficiency of the cell improves with increasing sunlight concentration even up to 100suns.

5. Effect of Different Doping Concentrations

The constructed CIGS cell is simulated for different doping concentrations of absorber layer in several sunlight concentrations. The results are depicted in Fig.6.

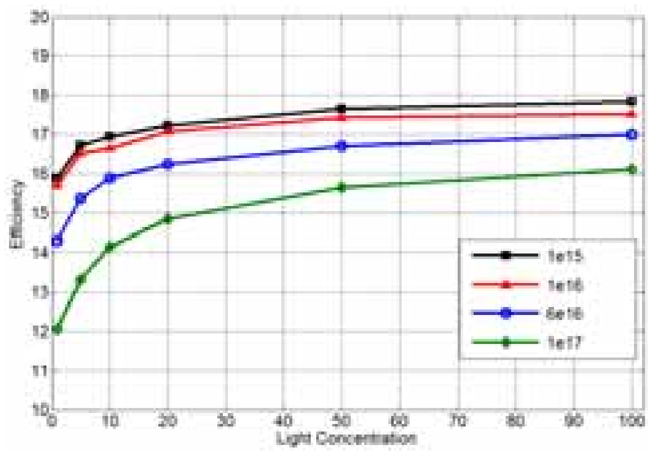

Fig. 6: The cell efficiency versus sun light concentration in four doping concentration

In higher levels of doping concentration, the cell's efficiency is degraded as a consequence of increased recombination that decreases the separation of electrons and holes. It can be seen that by changing the doping concentration of absorber layer, efficiency changes as well. Precise modeling of the dependency of efficiency on the absorber layer's doping concentration can be done in future works.

6. Effect of Grain Boundaries

To understand the behavior of poly-crystalline solar cells, in this section we consider some of the non-idealities that may exist in the structure of a CIGS solar cell. Experimental results have shown that defects and grain boundaries play an important role in the output characteristics of a poly-crystalline CIGS solar cell. Moreover, the surfaces in a CIGS solar cell may have a considerable amount of dangling bonds and Se vacancies, which act as compensating donors and recombination centers. In order to simulate the higher recombination rates in interface regions, we have defined a higher surface recombination velocity in our cell's structure. In addition, the influence of grain boundaries is taken into account by departing crystalline regions with very thin regions of high-concentration traps. In these grain boundaries, recombination has a comparatively high velocity.

We have defined three cells with different grain sizes and calculated their efficiencies both in the presence of internal defects and without them. A comparison is also made between these cases and the ideal crystalline cell. Fig.7. shows the obtained results.

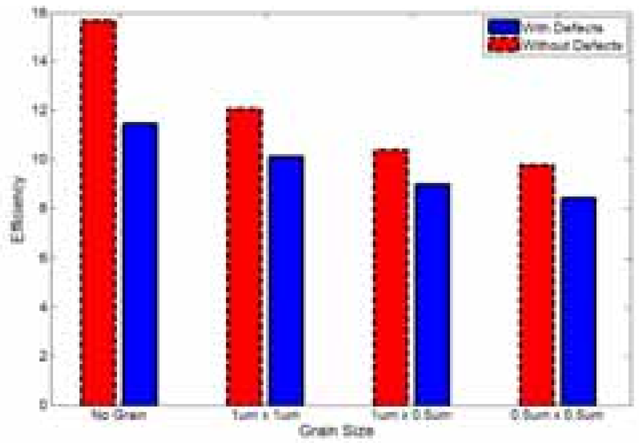

Fig.7: The cell efficiency with different grain sizes with and without defects.

Fig.7 shows that both defects and grain boundaries considerably reduce the efficiency in a CIGS solar cell, yet the impact of defects is more significant.

7. Conclusions

In this paper a conventional structure of CIGS solar cell was simulated in different grading ratios and doping concentrations. Bandgap grading and optimization of doping concentration are two important methods that are used to improve the efficiency of these cells. Increasing sunlight concentration also enhances the efficiency. Studying the impacts of higher sunlight concentration can help designers to understand the trends and mechanisms of a CIGS solar cell's performance. By considering the relation between said parameters in the design of a CIGS solar cell, we can attain the highest possible efficiency in a specific structure.

Finally, two effective non-idealities - defects and grain boundaries - were studied in the constructed cell's structure to examine the influence of material morphology on a CIGS cell's performance.

8. References

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