Computer Simulation of The Effect of Band Cap Grading of The Cigs Absorber Layer on The Performance of Cds/Cigs Thin Film Solar Cell

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Abstract

In this paper, the effect of the band gap grading of the absorber layer Copper Indium Gallium Selenide (CIGS), which is a compound semiconductor, on the performance of the solar cell has been studied. CIGS has a tuneable band gap and it varied with the composition of the semiconductor. This study has been accomplished using the computer simulation program SCAPS-1D. The program was developed to study the photonic devices especially CIGS and CdTe thin film solar cells. The effect of the grading shape (Front, Back and Double Grading) on the performance of the cell has been studied so as to improve the efficiency of the cell.

Keywords: Band Gap Grading, CIGS, SCAPS-1D.

المحاكاة الحاسوبية لتاثير تدرج فجوة الطاقة المحظورة لطبقة الامتصاص CIGS على اداء الخلية الشمسية الرقيقة

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الخلاصة

في هذا البحث تمت دراسة تاثير تدرج فجوة الطاقة لطبقة الامتصاص نحاس انديوم كاليوم سلينيوم,و الذي يعتبر من اشباه الموصلات المركبة, على اداء الخلية الشمسية.ان مادة الـ CIGS لها فجوة طاقة يمكن ضبطها و تتغير مع تركيبة شبه الموصل هذا. هذه الدراسة انجزت باستخدام برنامج المحاكاة الحاسوبي SCAPS. البرنامج تم تصميمه لدراسة النبائط الضوئية خاصة الخلايا الشمسية CIGS و CdTe. تاثير شكل الترج (الامامي, الخلفي و التدرج المزدوج) على اداء الخلية تمت دراسته لغرض تحسين كفاءة الخلية الشمسية

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1.Introduction

Copper Indium Gallium Selenide $Cu(In,Ga)Se_2$ (CIGS) is an interesting material for solar cell applications. CIGS is an alloy between Copper Indium Selenide $CuInSe_2$ (CIS) and Copper Gallium Selenide $CuGaSe_2$ (CGS) and is described by the chemical formula $CuIn_{1-y}Ga_ySe_2$ where y is the ratio Ga/(Ga+In) . The typical structure of the CIGS solar cell is shown in Fig. (1) [1].

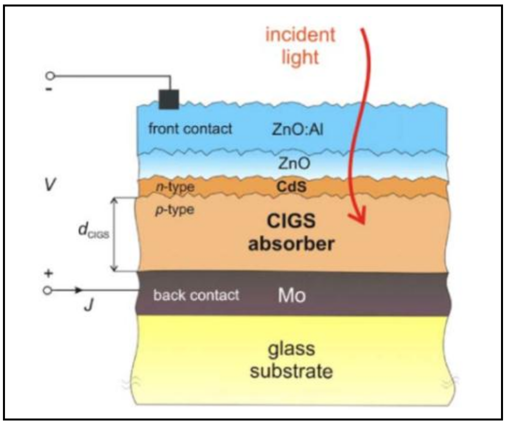

Fig. (1) Structure of the CIGS solar cell

CIGS has a direct band gap which is a very desirable in photovoltaic materials. More optimistically, the absorption coefficient (α) of CIGS is high around 10^5 cm^{-1} for a band gap of 1.4 eV.

CIGS based solar cells have shown record efficiency (~20%) for thin film devices in testing. This places CIGS solar cells at the forefront of the thin film solar cell industry. As the solar cell industry continues to expand there is great opportunity for CIGS based devices to become a significant technology in direct solar to electric conversion [2] .

A Polycrystalline CIGS semiconductor has a tunable band gap that varies with the gallium (Ga) content substituted in the CIGS material. The band gap of CIS is around 1.04 eV, whereas by adding Ga into the ternary system of CIS, the band gap energy of the CIGS quaternary system can be varied over a range of 1.04 to 1.68 eV. This property can be used to engineer the band gap of the CIGS when it used as absorber layer in the solar cell and to make a cell with a graded band gap [3]. It was experimentally observed that E_g of $Cu(In_{1-y},Ga_y)Se_2$ versus the atomic ratio *(y)* exhibits a bowing behavior, which can be described mathematically as

$$E_g(y) = E_1 + (E_2 - E_1 - b)y + by^2 \qquad (1)$$

Where E_1 and E_2 are the band gap values of CIS (y=0) and CGS (y=1), respectively, while b is the bowing factor [4]. The locally increased band gap has two effects on the photo-generated electrons. First all the recombination probability will be reduced in the regions with increased band gap since this probability is inversely proportional to the band gap. Secondly an additional electric field, E, obtained and can be described by [5].

$$E = \frac{d\Delta E_g}{dx} \qquad (2)$$

Where ΔEg is the change in band gap over the distance x due to the Ga-grading.

2. Device Simulation

Simulation of ZnO/CdS/CIGS thin film solar cell was carried out using the simulation program SCAPS. This program was developed at the University of Gent for simulation of the photonic devices. The dependence of the energy band gap of the CIGS absorber layer on the composition of Ga (y) used in the program is Eq. (1). Many researchers show that the band gap of the CIGS is equal to 1.15 when the composition of Ga (y) is equal to 0.3 [6] so that the bowing factor was chosen to be equal 0.3904. An exponential law for composition grading (*Y(x)*) is well suited to describe a back ground composition in the bulk of a layer. It has the following parameters: the composition of Gallium (Ga) near the back contact region (Y_{left}, at y=0), the characteristics length of the back graded region ($L_{char/left}$), the composition of Gallium (Ga) near the junction region (Y_{right}, at y=W), the characteristics length of the front graded region ($L_{char/right}$) and the background or bulk composition (Y_o). W is the width of the CIGS absorber layer (nm).

The variation of the composition with the absorber layer thickness (x) takes the form [7]

$$Y(x) - Y_o = \frac{(Y_{left} - Y_o)\sinh\left(\frac{W-x}{L_{char}}\right) + (Y_{right} - Y_o)\sinh\left(\frac{x}{L_{char}}\right)}{\sinh\left(\frac{W}{L_{char}}\right)} \quad (3)$$

2.1 Front Grading Simulation:

Front grading is an increasing the band gap in the space charge region (SCR). The composition of Gallium (Ga) at front (Y_{right}) is varied from 0.35, i.e. Eg = 1.1752 eV, to 1, i.e. Eg = 1.68 eV, in 0.05 intervals. Due to the variation in the Composition of Ga the band gap of the CIGS absorber layer will be graded at the front side and this is shown in Fig. (2) for $L_{char/right}$ = 100 µm. The Fig. shows the variation in the conduction band.

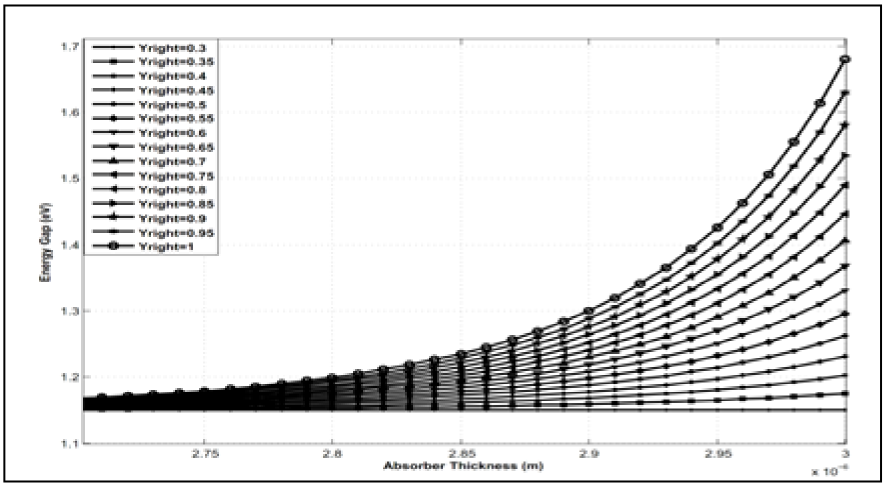

Fig. (2) Variation of the bandgap near the junction with the Ga composition

The effect of the $L_{char/right}$ on the shape of the bandgap is shown in Fig. (3) for $Y_{right} = 0.5$.

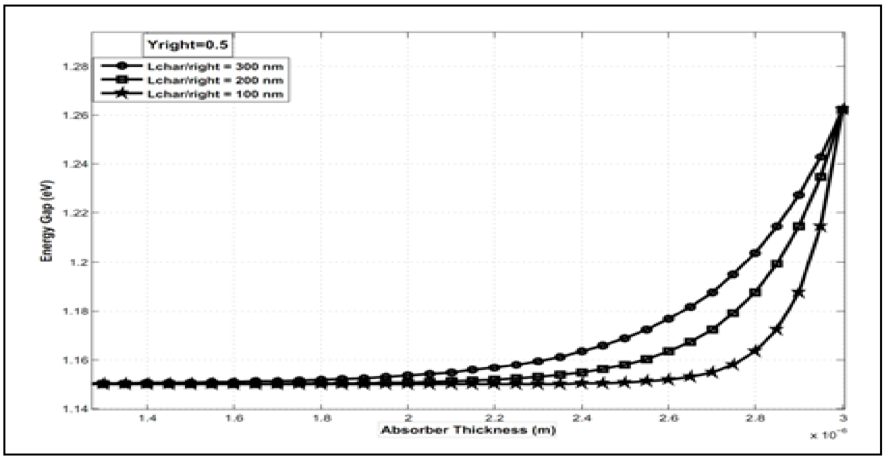

Fig. (3) Effect of the $L_{char/right}$ on the front grading band gap.

2.2 Back Grading Simulation:

The energy band gap of the CIGS absorber varies with the composition of Ga near the back contact region (Y_{left}) as shown in Fig. (4). Fig. (5) illustrates the effect of the characteristic length ($L_{char/right}$) on the back graded energy band gap of the absorber.

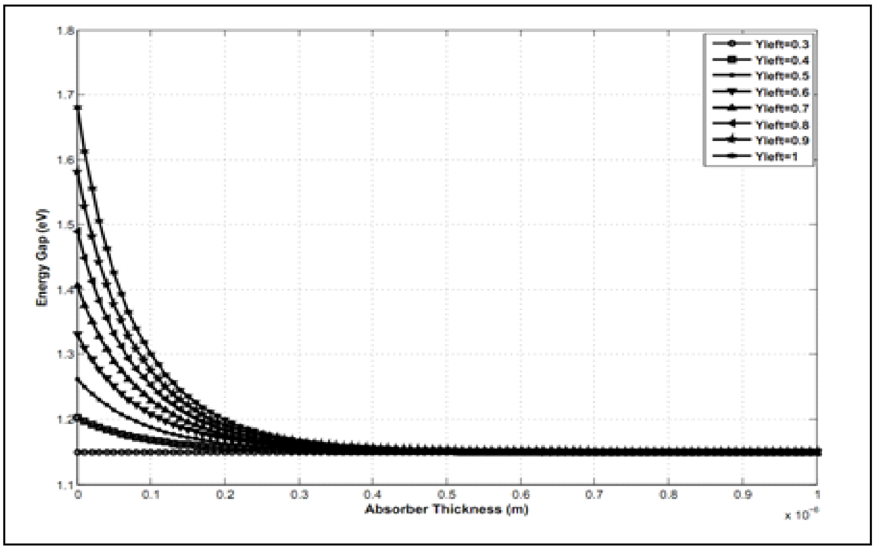

Fig. (4) Variations of the energy band gap near the back contact with the composition of Ga**.**

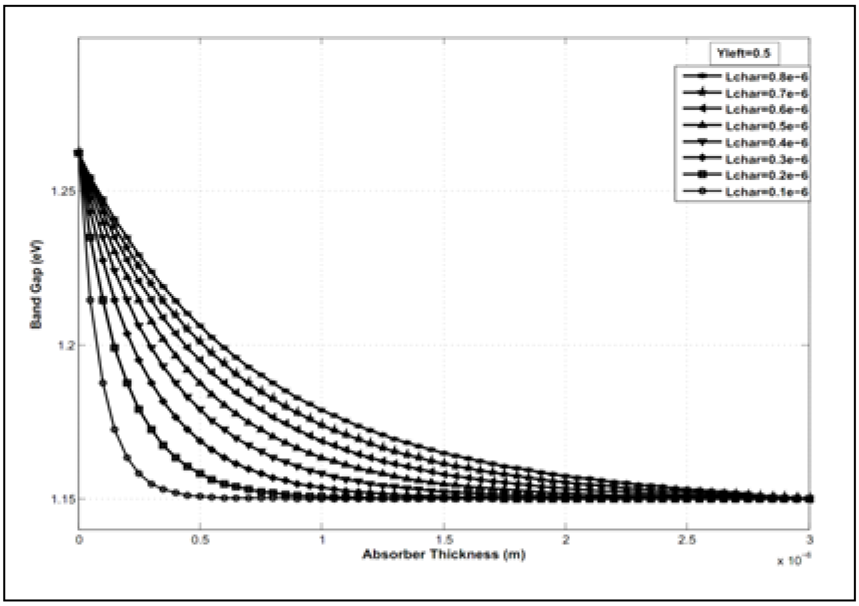

Fig. (5) Effect of the $L_{char/right}$ on the shape of the back grading band gap for Y_{left} = 500 nm.

3. Results and Discussion:

The output parameters of the base line cell with a uniform band gap equal to 1.15 eV are V_{oc}=638.8 mV, J_{sc}=34.307 mA/cm^2, FF%=79.59 % and η=17.44%.

3.1 Front Grading

At open circuit conditions the dominant part of the recombination is expected to occur in the space charge region (SCR). When the band gap increased within the SCR the recombination processes can be reduced due to the increasing in the barrier height resulting in improved V_{oc} as shown in Fig.(6). For $L_{char/right}$ = 100 nm. V_{oc} increased from (0.64 V) for Y_{right} = 0.35 (i.e. E_g = 1.1752 near the junction when Y_{right}=0.35), to (0.6732 V) for Y_{right} = 1 (i.e. E_g = 1.68 eV near the junction when Y_{right}=1), and V_{oc} also increased when $L_{char/right}$ values increased due to the higher band gap value beside the space charge region (SCR), for large $L_{char/right}$ values as shown in Fig. (5). For Y_{right} = 1 (E_g = 1.68 eV) V_{oc} increased from 0.6731 V for $L_{char/right}$ = 100 nm to 0.7596 V for $L_{char/right}$ = 200 nm.

The large band gap in the front region will also reduce the absorption in this region this can be componsated for by an incresed absorption further into CIGS absorber layer, where the band gap not is incsreased. Photoelectons generated deeper into the CIGS absorber layer will on the other hand have lower collection probabilty and this will reduse J_{sc} from 34.3233 mA/cm^2 for Y_{right} = 0.35 to 32.6867 mA/cm^2 for Y_{right} = 1. This reduction becomes more pronounced whene the energy band gap increases within the SCR by increasing $L_{char/right}$, since the low energy photons will not bsorbed, as shown in Fig. (7)

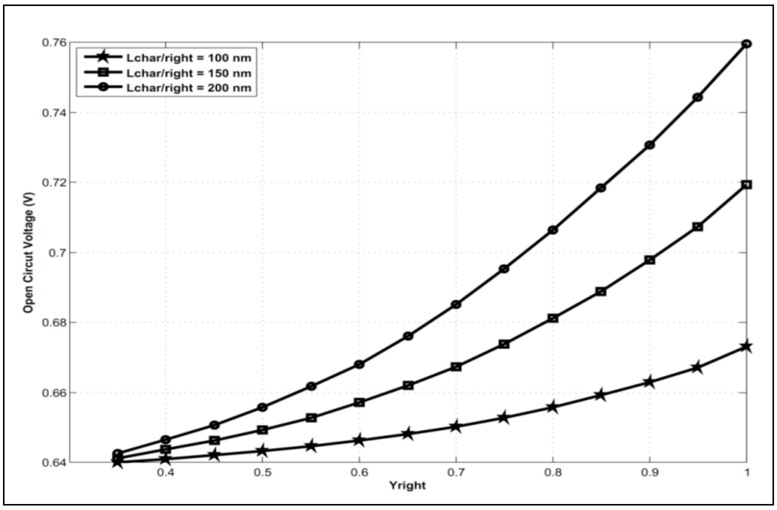

Fig. (6) Improvement in V_{oc} with increased Ga composition at the front side for different $L_{char/right}$.

Fill factor shows significant reduction due to V_{oc} and short J_{sc} losses as shown in Fig. (8). The efficincy of the cell will also reduced, Fig. (9), and the losses in the efficincy is high for large $L_{char/right}$ due to the high losses in the short circuit current density as compared with the improvement in V_{oc} for large $L_{char/right}$.

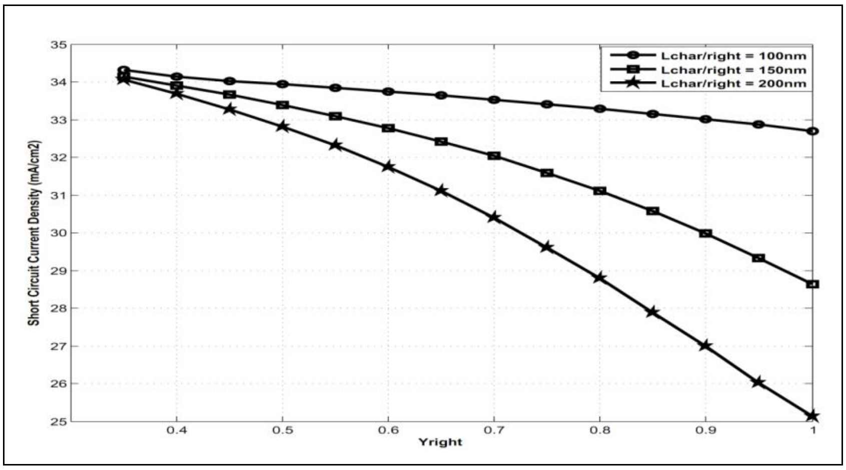

Fig. (7) Reduction in J_{sc} due to the icreased band gap at the front side

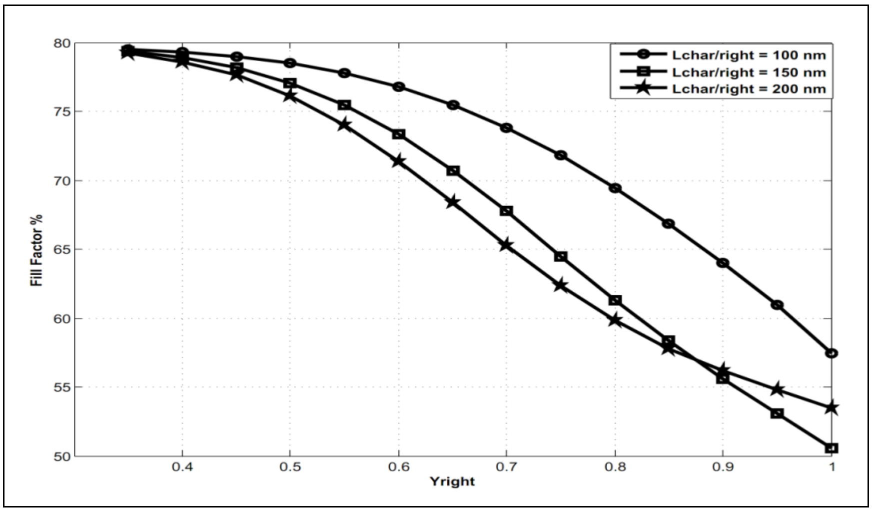

Fig. (8) Variation of the FF% due to the front grading for different $L_{char/right}$

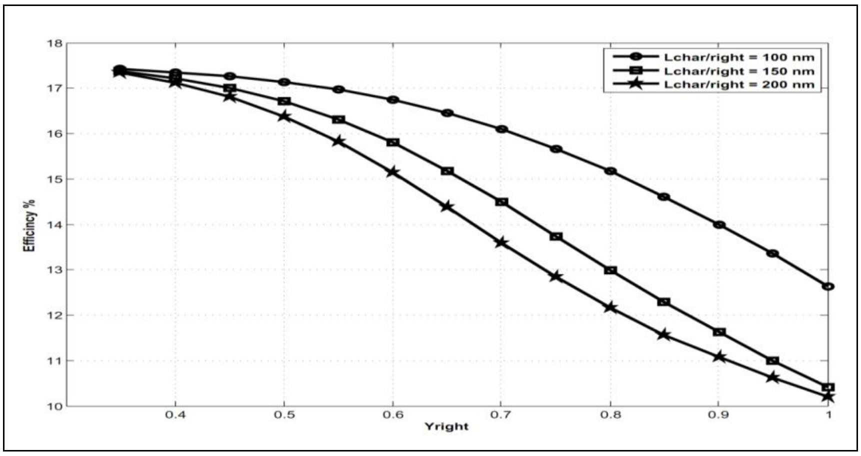

Fig. (9) Reduction in η% due to the front grading for different $L_{char/right}$

3.2 Back Grading

At short circuit conditions, the dominant part of the recombinations is expected to occur near the back contact. With the incorporation of the high Ga content in the CIGS absorber layer near the back contact region, additional drift fields for minority electrons can be establish in the back region of the absorber, and thus the back surface field is created in the cell. The photo generated minority carriers away from the space charge region count on the diffusion mechanism to be collected for the contribution to the current. Therefore, the performance of the baseline cell with the back surface field is expected to improve by reducing the recombination processes near the back contact and increasing the effective minority carriers diffusion length, resulting in an efficient carriers collection. Both the short circuit current density (J_{sc}) and the open circuit voltage (V_{oc}) of the baseline cell with the back surface field are enhanced as shown in Fig. (10) and Fig. (11) respectively. In Fig. (10) the short circuit current density (J_{sc}) increased from 34.3088 mA/cm^2 for Y_{left} = 0.35, i.e. E_g = 1.1752, to 34.3191 mA/cm^2 for Y_{left} = 1, i.e. E_g= 1.68, for $L_{char/left}$ = 100nm. A less improvement will also occur in the open circuit voltage (V_{oc}), as shown in Fig. (11), for $L_{char/left}$ = 100nm because the energy band gap will be small beside the back contact (the graded region is narrow) and the graded region will be far away from the space charge region (SCR). The fill factor approximately constant at $L_{char/left} \leq$ 300nm because the increment in V_{oc} and J_{sc} has been annealed by the increment in the maximum output voltage (V_m) and the maximum current density (J_m) and this is clearly shown in Fig. (12). The improvement in the efficiency is small for $L_{chsr/left} \leq$ 300 nm as shown in Fig. (13). The improvement in the cell output parameters will be more pronounced at high characteristic length due to the high energy band gap beside the back contact region. The graded region will be close from the SCR for high $L_{char/left}$ so that V_{oc} is more enhanced. As shown in Fig. (10) V_{oc} increased from 0.6391 V for $L_{char/left}$ = 100 nm to 0.6518 V for $L_{char/left}$ = 800 nm and Y_{left} = 1 in both cases. The generated photoelectrons far from the SCR will drift near the SCR and J_{sc} is also increase. As shown in Fig. (11) J_{sc} increased from 3.3191 mA/cm^2 for $L_{char/left}$ = 100 nm to 34.752 mA/cm^2 for $L_{char/left}$ = 800 nm and Y_{left} = 1 in both cases. This will causes in an increasing in the fill factor from (79.59%) to (80.07%) and the efficiency from (17.45%) to (18.14%) for the same cases.

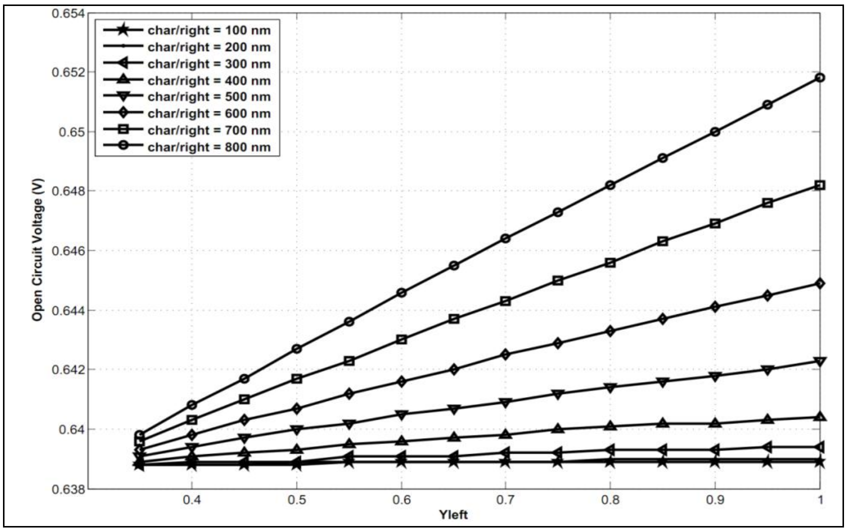

Fig. (10) The dependence of V_{oc} of the baseline on the composition of Ga at the back (back grading) side for different values of $L_{char/left}$

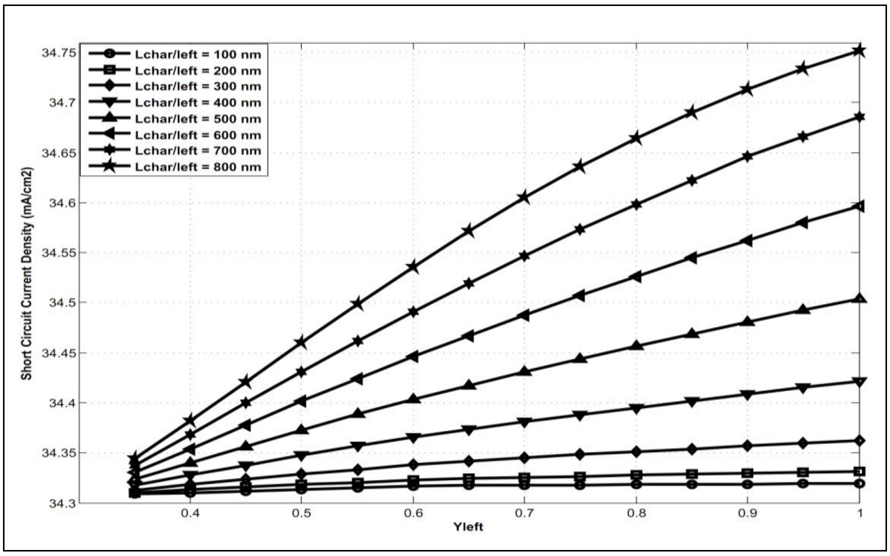

Fig. (11) The dependence of J_{sc} of the baseline on the composition of Ga at the back side (back grading) for different values of $L_{char/left}$

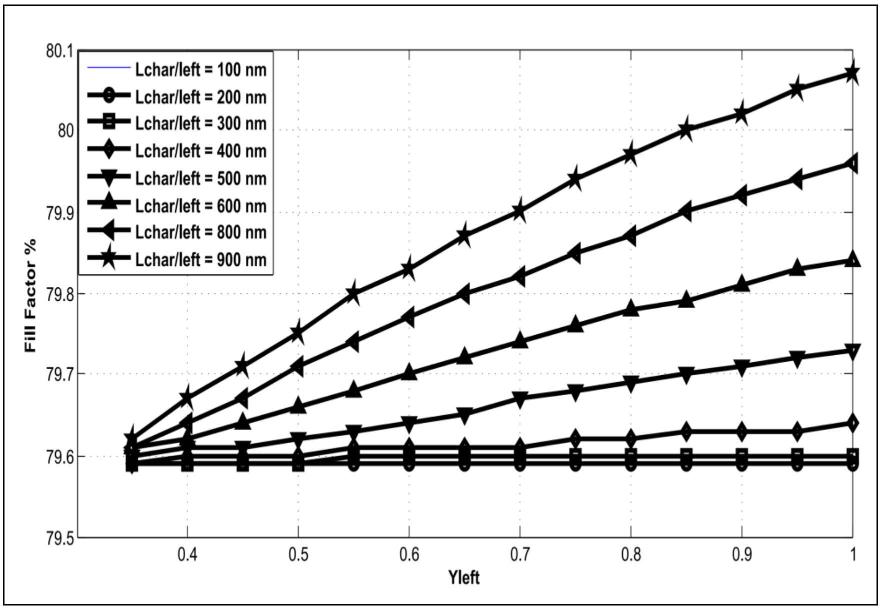

Fig. (12) The dependence of FF% of the baseline on the composition of Ga at the back side (back grading) for different values of $L_{char/left}$

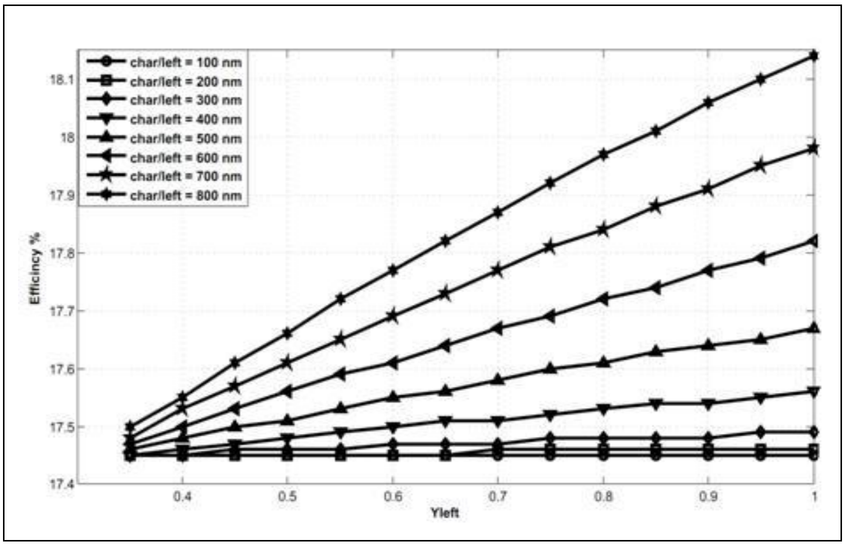

Fig. (13) The dependence of η% of the baseline on the composition of Ga at the back side (back grading) for different values of $L_{char/left}$

3.3 Double Grading

The baseline cell with the double grading band gap profile incorporate both the front side grading for increasing V_{oc} and back side grading for increasing J_{sc}. The double grading has been achieved on the eight cells which shown an optimum efficiencies in the back grading conditions with the addition of a graded region at the front side. The parameters of the front graded region is (Y_{right} = 1, i.e. E_g = 1.68 eV, and $L_{char/right}$ = 10nm). The composition's value for the back side is (Y_{left} = 1, i.e. E_g = 1.68 eV). The variation will occurs for the characteristic length for the back side ($L_{char/left}$)

The enhancement in the V_{oc}, J_{sc}, FF% and η% is shown in Fig. (14), Fig. (15), Fig. (16) and Fig. (17) respectively as compared with the back grading baseline cell.

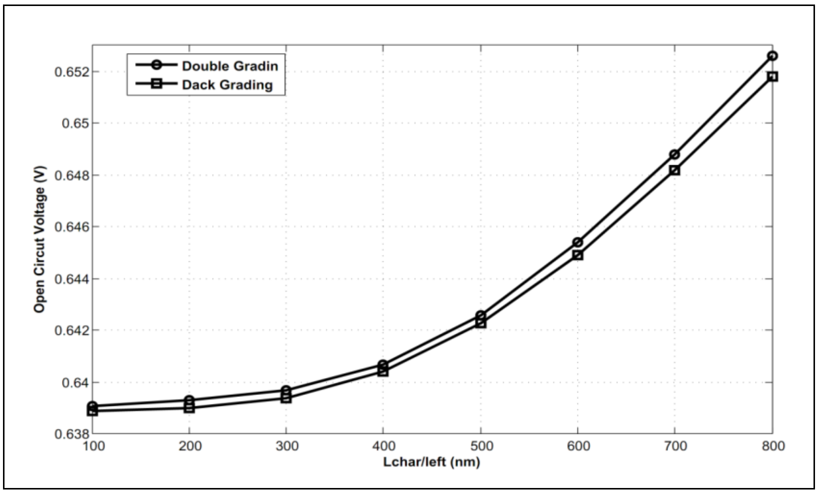

Fig. (14) The enhancement in V_{oc} of the baseline due to the double grading in the energy band gap as compared with back grading.

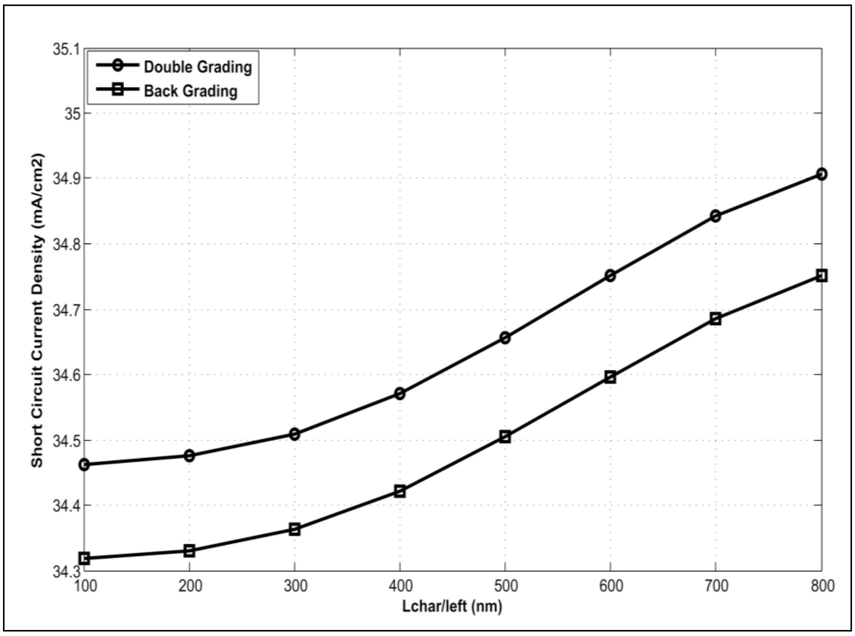

Fig. (15) The enhancement in J_{sc} of the baseline due to the double grading in the energy band gap as compared with back grading.

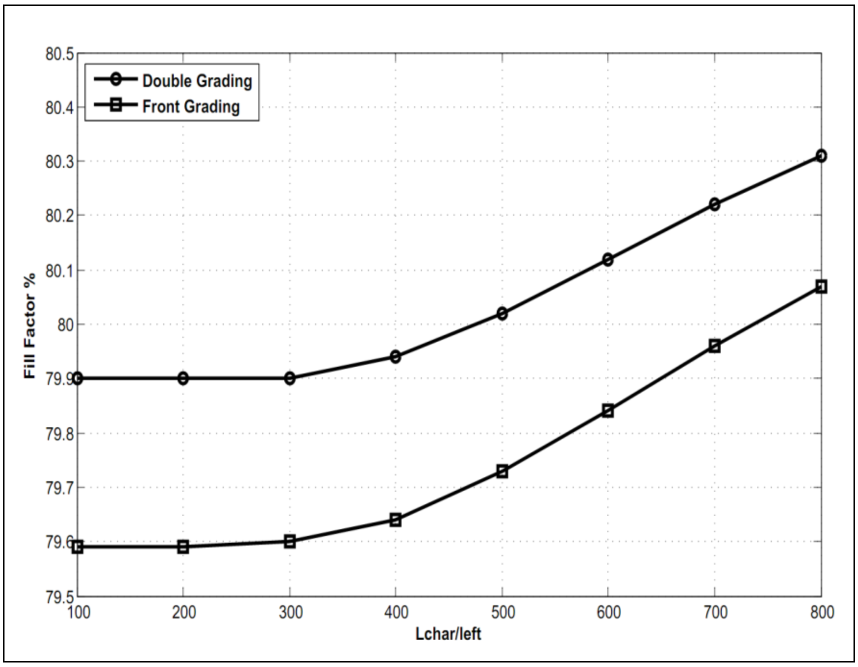

Fig. (16) The enhancement in FF% of the baseline due to the double grading in the energy band gap as compared with back grading

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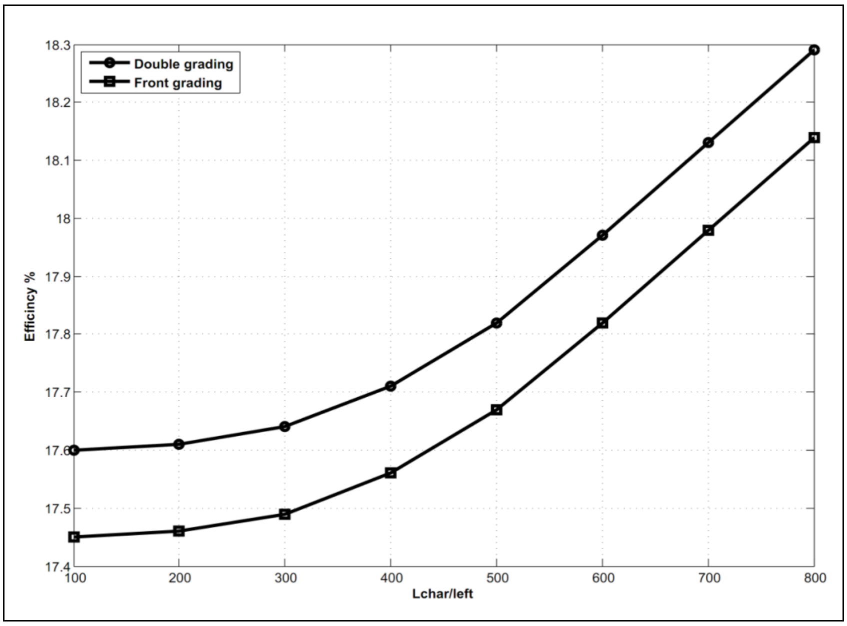

Fig. (17) The enhancement in η% of the baseline due to the double grading in the energy band gap as compared with back grading**.**

4.Conclusions

The dependence of the energy band gap of the absorber layer on the gallium content can be used to increase the energy band gap near the high recombination regions (grading). These regions are, the region between the back contact and the CIGS absorber layer (back grading) and the region between the CIGS absorber layer and the CdS buffer layer (front grading). Front grading enhanced the open circuit voltage (as shown in Fig. (6)) but reduced the short circuit current density (J_{sc}) and the efficiency (as shown in Fig. (7) and Fig. (9) respectively). Back grading enhanced both the open circuit voltage and the short circuit current density (as shown in Fig. (10) and Fig. (11) Respectively) and this leads to increasing the efficiency (as shown in Fig. (13)). By combing the benefit of front and back grading this results in enhancing the efficiency of the cell more than what found in the front and back grading.

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The work was carried out at the college of Engineering. University of Mosul