

Parameter Optimization and Efficiency Improvement of Cu(In, Ga)Se₂ (CIGS) Solar Cells

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Key words: Solar cell of CIGS, Quantum Efficiency (QE), absorbent layer of photon, simulation

Abstract: The aim of doing this research is to study and optimize the parameters I-V and increase the efficiency of solar cell of CIGS which is a proper substitute for fossil fuels. This solar cell is a combination of solution of Cu-Indium-Selenide (CIG) and Cu-Gallium-Selenide (CGS) which is a kind of semi-conductor of I-III-VI₂ that due to the high stability and the direct band gap Energy (E_g) is one of the most proper substitutes for silicon solar cell, also among other solar cells of thin layer, it has higher efficiency and lower price. In order to realize the aim of the research, optically modeling and simulating the solar cells based on thin band of Cu(In,Ga)Se₂ (CIGS) was done by using of Silvaco and AMPS software. Therefore, the methods of increasing the efficiency of solar cells of CIGS through improving the thickness of absorbent layer and changing in impurity of absorbent layer and adding another absorbent layer (Molybdenum) and changing in band gap Energy (E_g) of absorbent layers up to reach to the optimum point were studied. According to the gained results, the efficiency of 32% of solar cells of CIGS with minimum effectiveness on other parameters was gained and a solar cell of CIGS with optimum structure was created. By gaining the result of similar simulation by using of AMPS and SILVACO software, this result was gained that this solar cell practically is constructible and reliable. Achieving this efficiency can be a turning-point for more attention of generators of solar cells to this kind of solar cell.

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INTRODUCTION

With regard to the limited resources of fossil energy and increase of the energy consumption level in the world and increase of environmental pollutions, we can not rely on the existing resources of energy anymore. Due to this in the modern era, human always has sought a way for

providing the renewable energy. Due to the issues and challenges such as increase of efficiency, reduction of price, permanence and storage of energy which exist ahead of renewable energy resources, this energy has inclined many studies to itself^[1, 2].

The solar radiation energy which reaches to the Earth every day is sufficient for providing the needed energy of

the earth for a year. The solar energy directly or indirectly can be converted to other forms of energy like heat and electricity. To convert the solar energy to the electricity, the photovoltaic effect can be utilized by using of solar cells. The technology of solar cell and its applications have been expanded severely during 4 recent decades^[3,4].

Conversion of energy includes absorption of photon by a semi-conductor and in continuation, generation of electron-hole pairs and then segregation of charge carriers. In most of cases, a junction of P-N is used for segregation of charge carriers. This system currently is the only system of solar electricity generation which can have both powerhouse and non-powerhouse applications. The base unit of this system is named solar cell. In most of cases, semi-conductors are applied as the materials used in the solar cells. The main element in construction of solar cells includes semi-conductors like silicon and Gallium arsenide. At the time of photon radiation on the cell surface, much percent of radiated photons is reflected from the cell surface and it is dismantled. In the meantime, only those photons which have special energy, are absorbed and from this number of photons, a percent will be also re-combined, all of these cases are those factors which cause to reduce the efficiency of cell. Therefore with regard to these factors, for increase of the solar cells performance, solar arrays in large range are needed, thus, the cost of construction is increased^[5,6].

On the other hand, improvement of the efficiency of solar cells beside this issue that the price of construction of them should be kept low is from the important aims of solar cell industry. One important way for reduction of the cell price is to apply the thin film technology which is cognized as the second generation of solar cells and provides the possibility of generating the panels in large scale with lower cost than the cells of first generation. The most important step in simulation of a solar cell is to have the necessary knowledge of electron features and properties of its constituent layers^[5] which are cognized as the second generation of solar cells. In the solar cells of thin film, those materials are used which naturally have low price and also the techniques of construction of this kind of potential cells embrace a low cost. But their efficiency is lower than the silicon cells and it needs to be improved.

With these details, the aim of doing this research is to study, optimize and increase the efficiency of solar cell of CIGS which is a proper substitute for fossil fuels. Therefore, optically modeling and simulating the solar cells based on thin band of Cu(In, Ga)Se₂ (CIGS) is studied by using of Silvaco and AMPS software.

MATERIALS AND METHODS

The stages of doing the work

Numerically modeling the solar cell: All specifications of transferring a semi-conductor piece are resulted from

solving the Poisson's equation and electrons and holes continuity equation. But, some of the base equations which are used for the co-junction structures, should be reformed in the meta-junction structures for modeling different features of materials. Poisson's equation in a meta-junction structure is expressed as follows^[7]:

$$\frac{d^2\phi}{dx^2} = -\frac{q}{\epsilon}(p-n+N_D-N_A) - \frac{1}{\epsilon} \frac{d\phi}{dx} \frac{d\epsilon}{dx} \quad (1)$$

Where:

- q = The electron charge
- n = The density of free electrons
- p = The density of holes
- N_D = A density which gives impurity
- N_A = A density which receives impurity
- ε = De-electric fixed amount of semi-conductor

In this group of structures, the general form of continuity equations like co-junction structures is defined as follows:

$$\frac{\partial n}{\partial t} - \frac{1}{q} \nabla \quad (2)$$

But the component of electrical current of meta-junction structures is gained from the following relations:

$$J_n = -n\mu_n q \nabla (V + \theta_n) + KT_{\mu_n} \nabla n \quad (3)$$

$$J_p = -p\mu_p q \nabla (V + \theta_p) + KT_{\mu_p} \nabla p \quad (4)$$

In a manner that θ_n , θ_p are the band parameters in meta-junction structures and they are equal to:

$$\theta_n = \frac{x_c}{q} - \phi_0 + \frac{KT}{q} \ln \left(\frac{N_c}{n_i} \right) \quad (5)$$

$$\theta_p = -\frac{1}{q}(x_c + E_g) + \phi_0 + \frac{KT}{q} \ln \left(\frac{N_v}{n_i} \right) \quad (6)$$

Where:

- N_v and N_c = The effective densities of the states of capacity band energy and conduction band
- K = The fixed amount of Boltzmann
- T = The absolute temperature
- n_i = The density of inherent carriers
- E_g = The band gap energy
- x_c = The electron tendency
- φ₀ = The reference potential which is a fixed amount and φ is the electrostatic potential^[8,9]

Simulation of solar cell of CIGS by Silvaco software

The codes needed for simulation: Programing is done in DeckBuild environment and by Atlas module which is defined as follows:

- go atlas
- mesh auto width = 1e14
- x.mloc = 0 s = 0.5
- x.mloc = 1 s = 0.5
- region num = 1 material = ZnO bottom thick = 0.2 ny = 40 conductor
- region num = 2 material = CdS bottom thick = 0.05 ny = 15 donor = 2.2e19
- region num = 3 material = CIGS bottom thick = 1 ny = 40 accep = 1e16
- region num = 4 material = Molybdenum bottom thick = 1.5 ny = 30 conductor
- elecnum = 1 name = cathode top
- elecnum = 2 name = anode bottom
- material material = ZnO resistivity = 100
- material material = Molybdenum resistivity = 100
- material material = CdS indx.real = solarex05_0.n indx.imag = solarex05_0.k
- material material = CIGS indx.real = solarex05_1.n indx.imag = solarex05_1.k
- output opt.intens
- beam num = 1 x.origin = 0.0 y.origin = -1.0 angle = 90.0 wavelength = 0.6 tr.mat diffuse min.power = 1e+10 reflects = 1 sub
- solar iw = solarex05.log min.wave = 0.1 max.wave = 1.2 step.wave = 0.01
- tonyplot-overlay solarex05.log solarex05.dat -set solarex05_0.set
- quit

Explanation of the program lines

- The first line conducts the software to the Atlas module
- In the second line, meshing is done in the specified width automatically
- The third and fourth lines regulate the piece length with meshing distance of 0.5 μm

- The fifth, sixth, seventh and eighth lines divide the entire piece into four zones and the thickness, genus and density of each zone are specified in these four lines. The amounts which have been put in these four zones have been gained from the results of simulation by AMPS software
- The ninth line puts the first electrode on top of the piece and makes it cathode (ZnO) and the tenth line puts the second electrode below the piece and makes it anode (Molybdenum)
- The eleventh, twelfth, thirteenth and fourteenth lines specify the material of different zones that the pre-assumed amounts of software have been used
- The fifteenth line specifies the kind of output from pointwise kind
- The sixteenth line determines the specifications of the photon reached to the cell that the standard of AM1.5G has been used
- The seventeenth and eighteenth lines are for drawing the chart of QE according to the wave length from 100-1200 nm with steps of 1 nm
- And finally, the last line should be written for the end of the program

RESULTS AND DISCUSSION

The simulation results

The results of simulation by AMPS software: The photon of AM1.5G is radiated on the cell. The parameters of those materials which have been used in simulation of the base cell, have been mentioned in Table 1 and 2.

Studying the effect of thickness change of absorbent layer of CIGS on the output parameters such as efficiency. The results of simulation with different thicknesses of absorbent layer can be observed in Table 3 and as it is also clear from the results, reduction of the thickness of absorbent layer causes the back contact surface to approach to the discharge zone more, therefore, the electrons are absorbed to the back contact surface easily and due to their partnership in re-combination phenomenon, the amount of electrons influencing on efficiency is lessened and consequently, Jsc, Voc, FF and

Table 1: The parameters used in simulation of the base cell of CIGS in the temperature of 300°K

Layer properties	n-ZnO	n-CdS	P-CIGS
Layer thickness w (nm)	200	50	3000
Affinity (ev)	4	4.4	4.5
Relative permittivity (ϵ_r)	9	10	13.6
Electron mobility ($\mu\text{cm}^2/\text{V.s}$)	100	100	100
Hole mobility ($\mu\text{p cm}^2/\text{V.s}$)	25	25	25
Acceptor or donor concentration (cm^{-3})	Nd = 10e18	Nd = 2.2e19	Na = 1e17
Band gap Energy (E_g ev)	3.3	2.42	1.15
Effective density of state ($N_c \text{ cm}^{-3}$)	2.20E+18	2.20E+18	2.20E+18
Effective density of state ($N_v \text{ cm}^{-3}$)	1.80E+19	1.80E+19	1.80E+19

Table 2: The parameters used in simulation of the base cell of CIGS in the temperature of 300°K

Layer properties	i-ZnO	n-MgZnO
Layer thickness w (nm)	50	300
Affinity (ev)	4.6	4.05
Relative permittivity (ϵ_r)	9	10.5
Electron mobility ($\mu_n \text{ cm}^2/\text{V.s}$)	100	300
Hole mobility ($\mu_p \text{ cm}^2/\text{V.s}$)	25	20
Acceptor or donor concentration (cm^{-3})	Nd = 1×10^{14}	Na = 1×10^{18}
Band gap Energy (E_g ev)	3.3	4.1
Effective density of state ($N_c \text{ cm}^{-3}$)	2.20×10^{18}	2.20×10^{18}
Effective density of state ($N_v \text{ cm}^{-3}$)	1.80×10^{19}	1.80×10^{19}

Table 3: The results of simulation with different thicknesses of the absorber layer

Thickness	Voc	Jsc	FF	Efficiency
1.0	0.675840	34.258889	80.522757	18.643863
1.5	0.680141	34.720171	80.741397	19.066765
2.0	0.680733	34.827951	80.860687	19.170884
2.5	0.680877	34.834041	80.887888	19.184747
3.0	0.680905	34.817140	80.895370	19.178012
3.5	0.680906	34.799045	80.897373	19.168545
4.0	0.680902	34.784006	80.897774	19.160228

Efficiency are reduced. In Fig. 1 a-c, due to this issue that the photon absorption and real generation of charge carriers occur only in this layer, this layer has high importance, due to this, this layer can not be taken less than a specified amount. Therefore with regard to the discussion of optimization, economic issues and results gained from simulation, the optimum thickness of this layer is 2.5 μm . As it is observed in the Fig. 1d with more increase of the thickness of this layer, the efficiency will not have tangible increase.

Studying the effect of increase of CIGS thickness on QE (Quantum Efficiency): Theoretically with increase of the thickness of absorber layer, the number of absorbed photons is increased, larger length waves of radiated photon are accumulated (QE), consequently, more number of electron-hole pairs of absorbed photons is generated, therefore, the quantum efficiency is increased but since, our thickness change is very inconsiderable as it is seen in Fig. 2a, b increase of the quantum efficiency with thickness change of absorber layer is very intangible.

Improvement of efficiency with increase of impurity density of absorber layer: By selection of the optimum thickness of absorber layer (2.5 μm), we achieved the efficiency of 19.184%. In Fig. 3 and 4, the effect of impurity density change of absorber layer on efficiency and performance of CIGS cell have been shown. Since, bipolar around the junction of P-N should have equal number of changes in both sides increase of the hole density causes to reduce the width of discharge zone in P-side. As we know, those carriers which are generated in the discharge zone and distance of one length of its

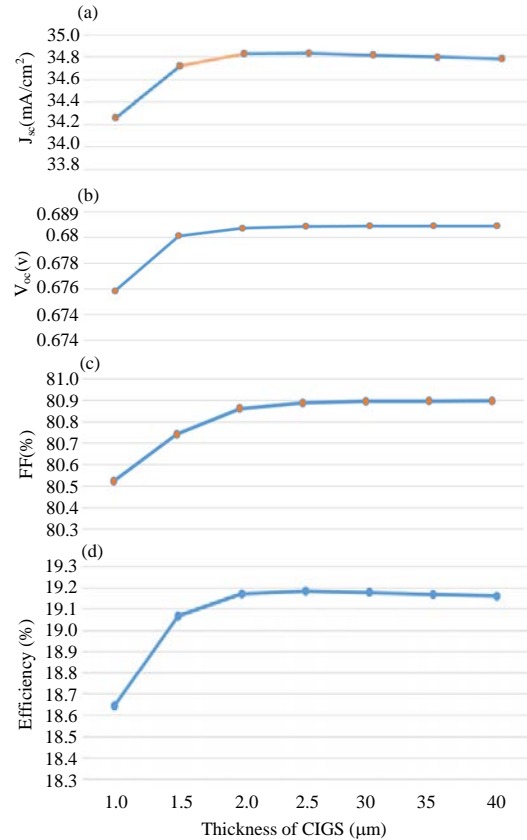


Fig. 1(a-d): (a) The results of J_{sc} with different thicknesses of absorber layer, (b) The results of V_{oc} with different thicknesses of absorber layer, (c) The results of FF with different thicknesses of absorber layer and (d) The results of Efficiency with different thicknesses of absorber layer

distribution are segregated from each other by electrical field and lead to the current pass in the external circuit, but since with increase of the hole density, the width of the strong field zone is shortened more, less carriers can be accumulated in the contacts, consequently, the short circuit current is reduced.

On the other hand, according to Fig. 4, whatever the amount of impurity density of the hole is more, the density of the absorber minority carriers is lessened, consequently, the re-combination partners are reduced, so, the rate of re-combination in the semi-conductor is reduced, therefore with increase of the hole impurity, the voltage of the open circuit of the cell is exposed to be increased. In Fig. 4, at first, the effect of increase of absorber impurity is more than the wastes of its current and therefore increase of the hole density can improve the efficiency of cell and FF.

According to Fig. 3 but when the amount of absorber density approaches to the impurity density of

Table 4: The effect of the increase of impurity density in the absorbent layer

Nd Cds (constant) (cm ⁻³)	NaCIGS(cm ⁻³)	J _{sc} (Ma/cm ²)	V _{oc} (V)	FF(%)	η(%)
2.20E+19	1.00E+17	34.834041	0.680877	80.887888	19.184747
2.20E+19	1.00E+18	32.886346	0.73998	82.933501	20.182075
2.20E+19	1.00E+19	31.950030	0.799275	84.556591	21.593089
2.20E+19	1.00E+20	31.652424	0.860484	86.279111	23.499333
2.20E+19	1.00E+21	26.607891	0.920264	102.519378	25.103175
2.20E+19	1.00E+22	24.850008	0.979888	110.367071	26.874620
2.20E+19	1.00E+23	24.677383	0	130.368452	28.689077

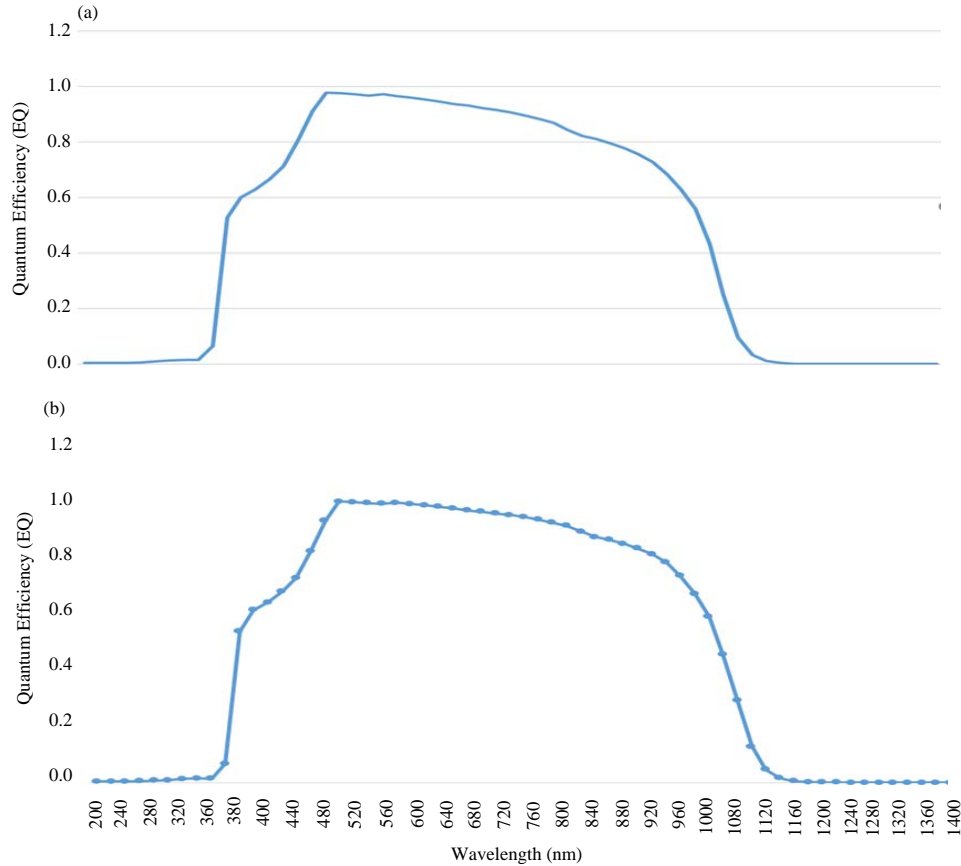


Fig. 2(a, b): (a) The results of QE change in the thickness of absorbent layer of 1 μm and (b) the results of QE change in the thickness of absorbent layer of 2.5 μm

the valve layer or becomes more than it, due to the high impurity density of absorbent, absorption occurs in the valve layer, so in this state, reduction of the current has prevailed over increase of voltage and efficiency is reduced severely. In the Table 4, the most optimum state has been specified with darker color.

Improvement of efficiency and increase of the specifications of I-V with increase of impurity density of absorbent layer can be observed in the Fig. 5 and 6:

Improvement of efficiency with change of the band gap energy of absorbent layer: Eg is about 1ev for CIS layer which can be changed up to 1.7ev by

adding Ga to CIS model of the band gap energy. In this stage with change of the amount of Ga in CIGA cell from CIS (x = 0)-CIGS (x = 1), we change the band gap energy of absorbent layer from about 1ev to about 2ev. With regard to the results gained from simulation, it will be observed that increase of the band gap energy of absorbent layer reduces the photon absorption in this layer that this affair will cause to reduce Jsc. Although, the amounts of Voc and FF are changed and increased with increase of the linear prohibited band gap energy, by establishment of a compromise between reduction of current and increase of voltage, we select the optimum amount of Eg = 1.17 that with this

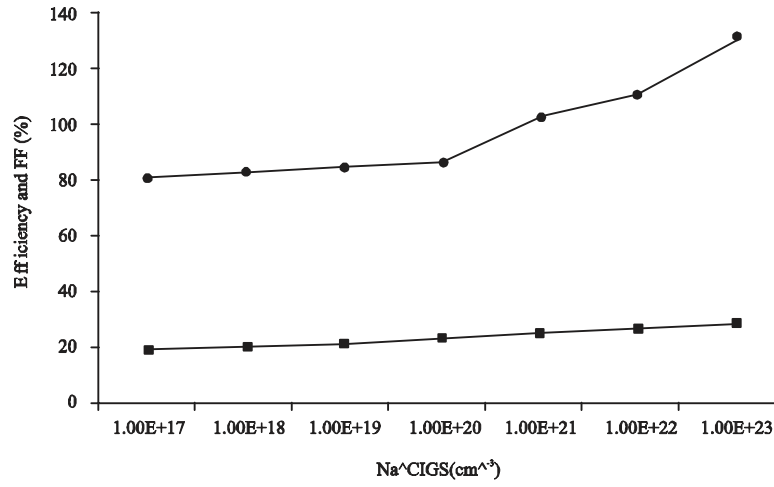


Fig. 3: The effect of increase of impurity density in the absorbent layer on parameters of FF and Efficiency

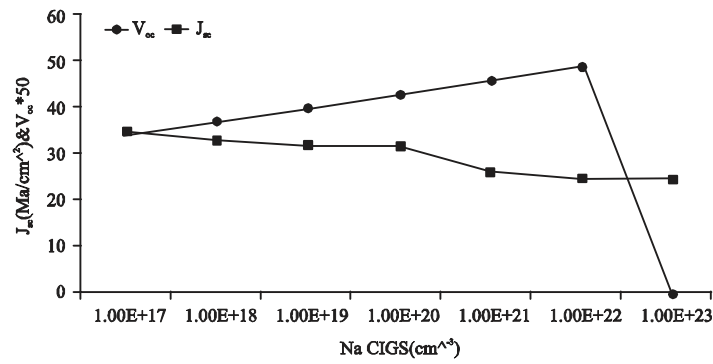


Fig. 4: The effect of increase of impurity density in the absorbent layer on the parameters of J_{sc} and V_{oc}

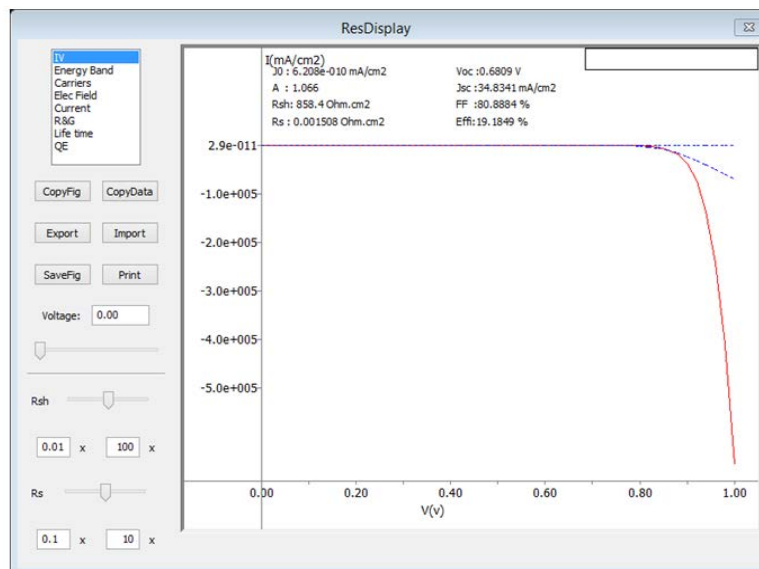


Fig. 5: The specifications of I-V and efficiency before increase of impurity density of absorbent layer

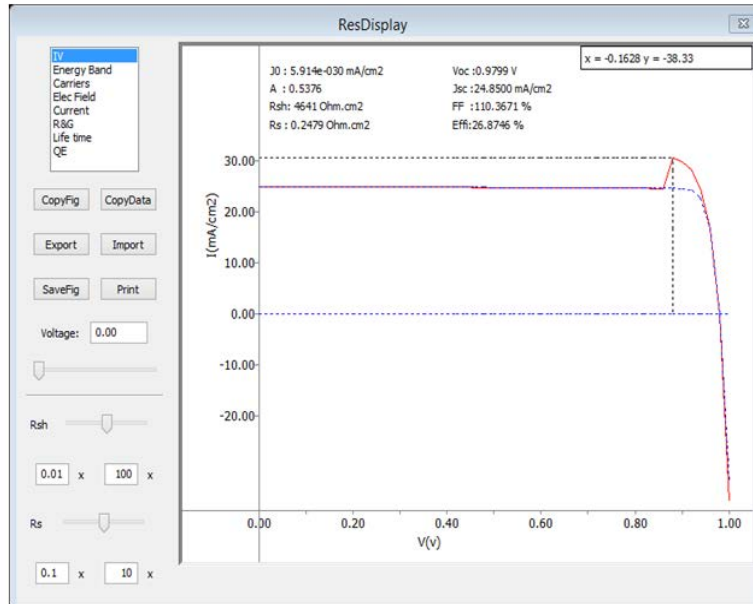


Fig. 6: The specifications of I-V and efficiency after increase of impurity density of absorber layer

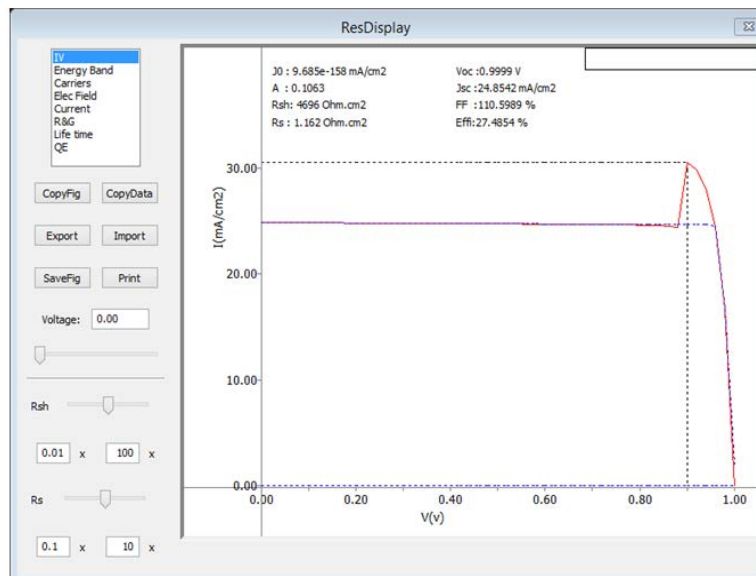


Fig. 7: Change of the specifications of I-V and efficiency after increase of the band gap energy of absorber layer

change, E_g of solar cell is changed from 1.15-1.17 and also the efficiency will reach from 26.874-27.485. The specifications of I-V and other specifications after change of the band gap energy of absorber layer are observed in Fig. (7).

From the main factors of carriers wastes in solar cells of CIGS, high speed of superficial re-combination (11^7 cm sec⁻¹) in the terminal contact of cell can be mentioned. Reduction of re-combination in the back

contact of CIGS cell can help in reduction of the thickness of absorber layer and consequently, reduction of the price of this element, therefore, different methods have been studied in numerous articles for reduction of re-combination in the back contact of CIGS cells. Quantization of the band gap of CIGS absorber and creation of a back superficial field in the intersection between absorber and back contact of cell can be mentioned as some of them. The back superficial field can

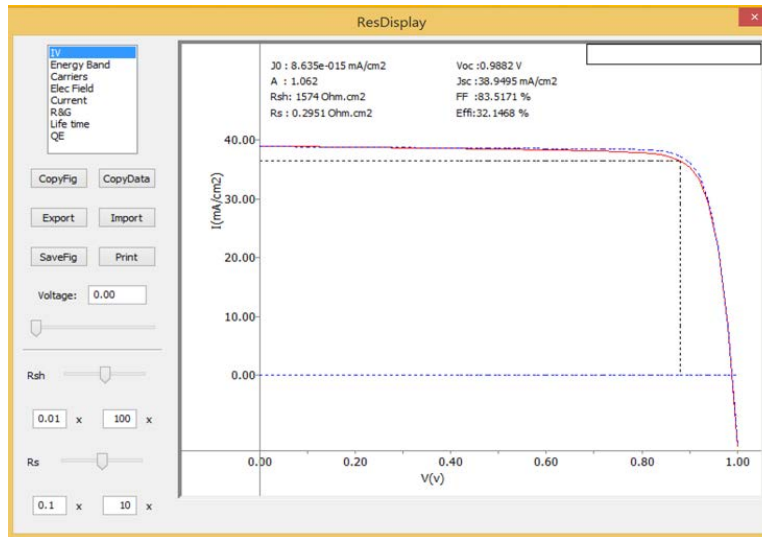


Fig. 8: Improvement of the specifications of I-V and efficiency after adding another layer

be created in the intersection of CIGS/Mo by adding a layer with Ga density more than the density of absorbent Ga or by using of the sediment of a different material with energy gap larger than absorbent. But, one of the ways influencing on increase of the back contact field is to add a layer with much impurity density (one layer of P+) at the end of absorbent layer.

Studying the effect of adding a layer of P+ with different thickness and impurity at the end of absorbent layer: Generally, adding a layer with high impurity density after absorbent layer causes to create additional field in the back contact. This field propels the electrons from the back contact toward absorbent, consequently, re-combination is reduced in the back contact which leads to increase the voltage of open circuit of cell. Also, by creating additional field in absorbent, the carriers distribution length is increased which leads to increase the photon current of cell and also reduction of the back contact re-combination causes to accumulate more number of carriers in the contacts, consequently, the amounts of current and efficiency are increased. In this part, we put a layer from the genus of absorbent layer of CIGS with different thickness and impurity at the end of absorbent. But in the meantime, improvement of the cell efficiency depends on the thickness and amount of impurity of CIGS and CIGS+layers. Selection of the correct amount of impurity and thickness of layer of P+ for improvement of performance and increase of efficiency necessitates to study 4 following states:

- Thickness and impurity of the layer of P+ are more than the thickness and impurity of the layer of P

- Thickness and impurity of the layer of P+ are less than the thickness and impurity of the layer of P
- Thickness of the layer of P+ is less than the thickness of the layer of P and impurity of the layer of P+ is more than the impurity of the layer of P
- Thickness of the layer of P+ is more than the thickness of the layer of P and impurity of the layer of P+ is less than the impurity of the layer of P

By studying and comparing the parameters gained from simulation for four above states, we will reach to four important results: Thickness of layer of P+ should be more than the thickness of layer of P that the amounts of optimum thickness for P+ and P have been gained in order = 1.5 and 1 μm .

Impurity of the layer of P+ should be more than the impurity of the layer of P that the amounts of optimum impurity have been gained for (1E21)P+ and (1E16)P layers. Eg of the layer of P+ is equal to 1.35eV and Eg of the layer of P is equal to 1.5eV. We should change the thickness of these two layers in a manner that the total thickness of absorbent is kept equal to the fixed amount of 2.5 μm . By adding a layer from the genus of absorbent layer but with more thickness and impurity in the intersection of back contact and absorbent layer, we will reach from the efficiency gained from the previous stage namely, 27.485 to the efficiency of 32.146 as you observe in Fig. 8.

The results of simulation by Silvaco software: In Fig. 10, the chart of QE has been shown according to the wave length, as it is also observed in the figure increase of the quantum efficiency can be seen well and by

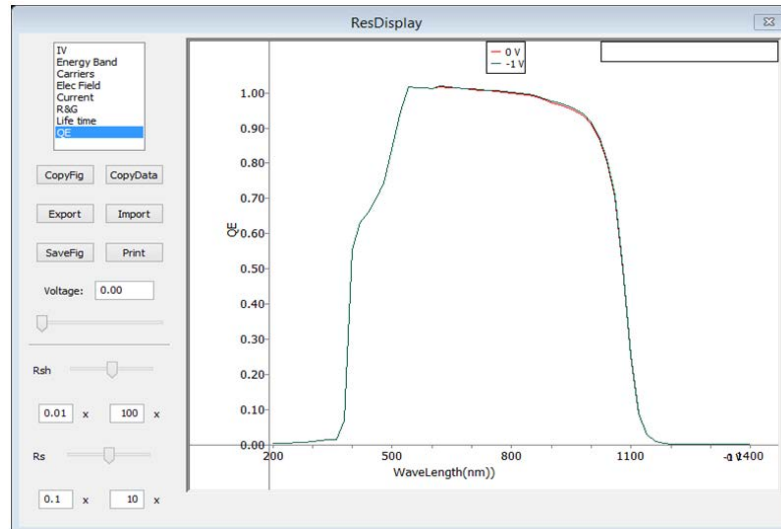


Fig. 9: Improvement of the specification of QE after adding another layer

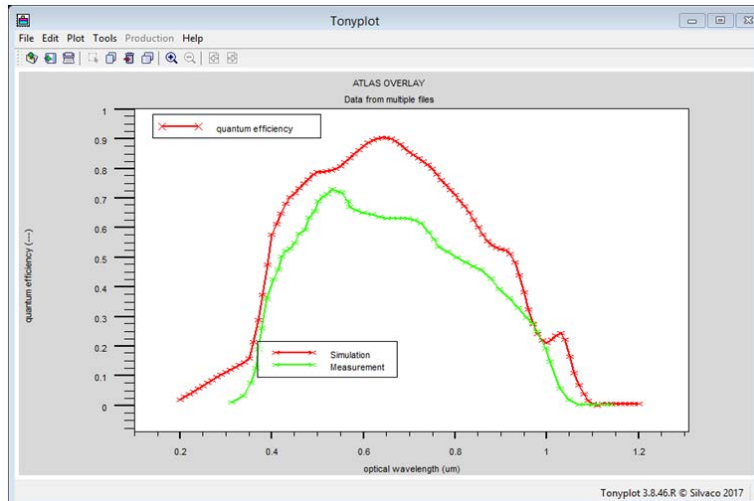


Fig. 10: The chart of QE according to the wave length

comparing with Fig. 9 which is the chart of QE according to the wave length simulated by software AMPS, we will find out this issue that the results of simulation by both software have been very close to each other which indicates that a cell with mentioned specifications and elements not only theoretically is reliable but also practically is constructible and utilizable completely.

From the results gained by Krc etc, measurement has been shown in the above chart and simulation accomplished in this research and changes in the quantum efficiency can be seen well.

CONCLUSION

By studying the performance of the solar cell with nano-structure of CIGS, a cell of CIGS was simulated by using of AMPS Software. The thicknesses of the buffer and absorber layers are in order equal to 200, 50 nm and 3 μm , the efficiency of the base cell of CIGS was 19.184%. Increase of the thickness of absorber layer increased QE and increase of the impurity density of absorber layer caused the increase of V_{oc} and reduction of J_{sc} and improved the efficiency up to 26.874%. Increase more than this amount causes that the effect of reduction of current to prevail over the increase of voltage

and the efficiency is reduced severely. Another factor influencing on efficiency was E_g of absorbent layer. In this stage with increase of E_g up to 1.7 eV, the amount of QE is increased and the efficiency reached to the amount of 27.485%, excessive increase of E_g will cause to destruct the cell performance.

In the solar cells with thin layer of CIGS, due to the very low thickness of absorbent and buffer layers, many photons reach to the back contact, high speed of carriers (10^7 cm sec⁻¹) and the superficial re-combination are accounted from the main factors of wastes and reduction of efficiency of these cells and on the other hand, the layer of transparent oxide of ZnO which is semi-conductor from the kind of n in its connection point to the metallic contact (cathode) by creating the Schottky barrier is as another factor in creating the wastes of cell.

To improve the efficiency of these cells by the method of increasing the doping of a part of absorbent layer for creating the superficial field, the electrons were propelled toward absorbent layer in order to reduce the carriers re-combination in the back contact that by adding this layer with thickness of 1.5 μ m and impurity of $1e^{21}$, reduction of thickness and impurity of absorbent layer up to 0.5 μ m and impurity of $1e^{16}$, the efficiency of 32% was resulted and a solar cell of CIGS with optimum structure was created. By gaining the similar simulation result by two AMPS and SILVACO Software, this result has been gained that this solar cell practically is constructible and reliable.

SUGGESTIONS

With regard to the results of simulation by AMPS and SILVACO Software in the charts of quantum efficiency, it can be seen well that the waves lengths influencing on the quantum efficiency are between 400-900 nm, therefore by putting an optical spectrum filter, the remained additional wave lengths can be eliminated that by doing this act, the probability of re-combination will become less.

Other dispersed generation resources like wind energy should be used, a hybrid generator should be created and the efficiency should be increased. Un-interrupted battery and sources should be used for storage and recovery of energy and the amount of increase of efficiency should be studied. High speed of charge carriers and superficial re-combination is accounted as the main factors of wastes and reduction of efficiency of these cells, a solution should be found for reducing or dismantling the wastes and consequently increasing the efficiency.

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