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Few possible models for 19.9%efficient pCIGS solar cells

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Abstract

Device modeling and simulation studies of a CIGS thin film solar cell have been carried out using SCAPS 2902. A variety of graded band gap structures of efficiency around 19.9% are examined. The study shows that material saving models with efficiency η around 19.9% is possible.

Keywords

Thin Film Solar Cell; Open Circuit Voltage (V_{oc}); Short Circuit Current (J_{sc}); Conversion Efficiency (η).

Academic Classification

Science Physics

Subject

Physics, Solar Energy

Type

Theoretical Modeling

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1. Introduction

Much information is available in literature [1-3] regarding Cu ($In_{1-x}Ga_x$) Se_2 (CIGS) solar cells. Many attempts are being made to improve the open circuit voltage V_{oc} as solar cells with high V_{oc} suffer less interconnection losses when modules are manufactured. $CuInSe_2$ is alloyed with Ga to form CIGS thin films to utilize the higher band gap energy of CIGS to match better with solar spectrum for the optimum absorption of the incident photons. By introducing a spatial variation of Gallium content within the CIGS layer, a band gap profile can be optimized to increase the photon absorption and carrier diffusion. This optimization would improve V_{oc} and J_{sc}.

Recently, I. Repins et.al [4] has reported the experimental study on 8 solar cells with efficiency ranging from 19.2% to 19.9%. Of these 8 samples studied, three cells namely C2219213#7, C220022#1 and C221322#2 have open circuit voltage V_{oc} 714mv, 725mv and716 mV with J_{sc} being 35.1, 33.6 and 33.4mA/cm^2.

An attempt is made here to ascribe few possible structure for solar cells of this kind viz, η being around 19.9%. Such modeling will provide insight in to the possible structure of existing cells and new cells that can be synthesized. In all, 16 band gap profiles are simulated including a baseline case of uniform band gap profile.

Many softwares like SCAPS [5], AFORS-HET [6], AMPS-1D [7] are available as freewares for PV community to simulate the behavior of solar cells. In this paper, the implementation of graded band gaps in **SCAPS2902** is done and the results of various structures are analyzed to determine the impact on the performance parameters of the cell.

2. Cell Structure and Material Parameters

The CIGS cell structure considered in this study consists of the following material layers: n-ZnO, i-ZnO, n-CdS, high recombination interface, inverted surface, p-CIGS absorber and a Mo on glass substrate. In the paper of I. Repins et.al referred above, there is no reference to the existence of OVC or inverted surface but in this study this surface is assumed to be present.

The schematic energy-band diagram under equilibrium condition for a typical n-ZnO/ i-ZnO /CdS/p-CIGS solar cell with a uniform band-gap profile is shown in Figure1.

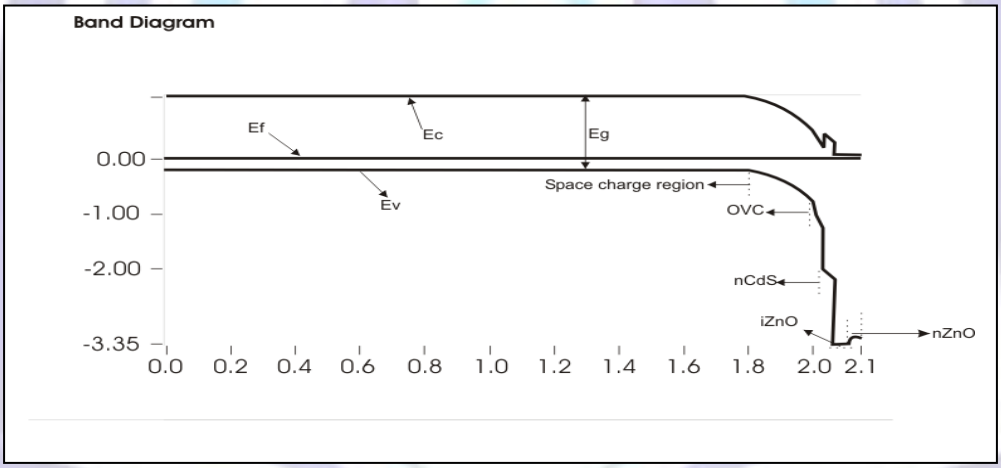

Figure 1. The schematic energy-band diagram of a typical n-ZnO, i-ZnO /CdS/CIGS solar cell under equilibrium condition.

An inverted surface layer, which is refered to as an ordered vacancy compound (OVC) is taken to be present in-between CdS and CIGS layers. Schmid et al[8]have demonstrated the existance of such type of layer which is rich in Indium and thin, on the surface of as deposited CIGS layers. They assigned the origin of this layer to the stoichiometry of $CuIn_2Se_{1.5}$ or $CuIn_3Se_5$. But Herberhoz et.al [9], Guillemoles[10] feel that this thin, Indium rich layer might not be OVC and they use a more general term “surface defect layer” and accommodate the observed effect. The effect of this layer is to shift the electric junction away from the high recombination interface between CdS and CIGS layers and thus thought to be beneficial for the performance of the cell as the recombination rate is reduced. On the other hand, this surface defect layer has high defect density and resistivity. These properties may lead to the deteriotion of the cell.

For the purpose of this simulation, the solar cell has the following structure: n-ZnO,i-ZnO, n-CdS, high recombination interface between OVC and CdS, OVC,and p-CIGS for simulation purpose. The band gap of CIGS absorber is supposed to be engineered through the changing of the Ga profile by controlling the deposition process[4] . Changes in the amount of Ga present, shifts the position of conduction band minimum [11], bulk defect densities([12], hole concentration[13], absorption coefficient and electron affinities but not the room temperature mobility values [13].

Base-line values utilized in this work are given in table-1. These values(except for i-ZnO, OVC) here are made as near as possible to the values reported by Prof.James R. Sites[14]. Reported mobility values for electron and hole within OVC vary

over a large value[15,16].For OVC, the mobility values used are taken from the work of J.Song et.al[16] Parameters for i-ZnO are picked from the example provided along with **SCAPS**.

Table- 1 Values of various parameters used in the simulation

Parameter	nZnO	nCdS	OVC	pCIGS
Thickness (µm)	0.04	0.03	0.03	2
Band gap(eV)	3.3	2.42	1.35	1.16/1.30
Electron Affinity(eV)	4.65	4.35	4.6	4.5
Diele.Permittivity(rel)	9.0	10.0	10.0	13.6
Eff. Den of States CB ($1/cm^3$)	2.2E+18	2.2E+18	2.2E+18	2.2E+18
Eff. Den of States VB ($1/cm^3$)	1.8E+19	1.8E+19	2.2E+18	1.9E+19
Thermal. Vel. (elec) (cm/s)	1.0E+07	1.0E+07	1.0E+07	1.0E+07
Thermal.Vel. (hole) (cm/s)	1.0E+07	1.0E+07	1.0E+07	1.0E+07
Mobility(elec)(cm^2/Vs)	1.0E+02	1.0E+02	1.0E+01	1.0E+02
Mobility(hole) cm^2/Vs)	2.5E+01	2.5E+01	1.0E+01	2.4E+01
N_D	1.0E+17	1.0E+17	1.2E+12	0.0E00
N_A	0.0E00	0.0E00	0.0E00	2.3E+16
Abs.Coeff. A	1.0E+05	1.0E+05	1.0E+05	1.0E+05
Abs.Coeff. B	0.0E00	0.0E00	0.0E00	0.0E00

Values, nature and concentration of the defects incorporated in this study for n-ZnO, i-ZnO, n-CdS,interface and OVC are picked up from the numos baseline example provided with **SCAPS**.

A lot of information is available in literature about the defect states in p-CIGS absorber material. According to Abushama[17] the nature and concentration of defects undergo a change if the ratio (Ga/Ga+In) exceeds 0.6.

With this in mind the equation $E_g = 1.011+0.64x-0.249x(1-x)$ where E_g is the band gap of the absorber layer $Cu(In_{1-x}Ga_x)Se_2$ as suggested by Albin[18] was used to find the ratio (Ga/Ga+In) so that the E_g used did not cause changes in the defect states envisaged. Of the defects suggested by Abushama, only three defects with higher concentration are used in this simulation.The total thickness of the absorber is maintained at 2µm and simulations are carried at 25ºc using AM1.5G solar spectrum. In all these simulations, a layer of p-CIGS of thickness0.1µm is always used as terminating layer in contact with back electrode as done by I.Repins et.al[4]. In all these cases, as the interest is to examine the effect of bandgap profile, all other parameters used in this simulation are kept constant.

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Table –2 Effects of Graded Band-gaps on Cell Performance

Property/ Layer	nCdS	OVC	Interface	pCIGS		
				Defect 1	Defect2	Defect3
Type	Donor	Donor	Donor	Donor	Acceptor	Acceptor
σ_e	1.0E-15	1.0E-15	1.0E-15	1.0E-15	1.0E-15	1.0E-15
σ_h	1.0E-15	1.0E-15	1.0E-15	1.0E-15	1.0E-15	1.0E-15
Energetic Details	Single	Single	Uniform	Single	Single	Single
Ref.for Defect level	>Ev	>Ev	>Ev	>Ev	<Ec	<Ec
Energy w.r.to Ref	0.6	0.6	0.6	0.28	0.12	0.63
N_t	1E18	1E18		7.5E15	8.0E16	1.4E16
Char. Energy	----	----	0.1	-----	-----	----
Total Density	----	-------	1.0E12	-------	----------	----------
Density at peak	---------	----------	1.0E13	----------	----------	----------

Initially, a simulation study was carried out on uniform band gap of 1.30eV. This establishes a baseline for comparison. Simulations were carried out for different profiles. These different profiles and the values obtained for Open Circuit Voltage (Voc), Short Circuit Current (I sc), Conversion Efficiency (η) and Fill Factors are presented in Table3.

3.1 J-V behavior

Baseline profile wherein band gap of pCIGS is maintained uniform at 1.3eV is represented as simulation 1. In simulation 2 the band gap is changed linearly from1.16eV to 1.3eV over 2µm- the thickness of the absorber material. From simulation 3 onwards a pCIGS layer of uniform band gap of 1.16eV is placed in next to back contact and the thickness of second layer of pCIGS is changed. Simulation 3 corresponds to the study reported by I. Repins et. al. 16 different simulations are carried out and results are presented in table 3.

As can be seen from the table, the values obtained for Open Circuit Voltage (Voc), Short Circuit Current (Jsc), Conversion Efficiency (η) and Fill Factors do not differ for simulation 1and 2. This means that a linear grading of band gap from 1.16eV to 1.3eV over a thickness of 2µm yields the same results as a layer of uniform band profile. This suggests that material savings can be made without sacrificing the performance with linearly graded profile.

It is further seen that when a layer of thickness 0.1 µm (referred to as layer 2 in further discussions) and band gap1.16eV is placed in contact with back electrode and remaining part of absorber is linearly graded from 1.16 to 1.3eV, there is a little change in the values of Voc, Jsc, η and fill factor. These changes are apparently within the experimental error range and hence it can be said that this profile also yields the same result as of uniform band gap profile.

When the thickness of this layer 2 is further increased, Voc continuously decreases and finally attains the value of 0.634mV – the value corresponding to the simulated value for a profile of uniform band gap1.16eV.

In the same region, J_{sc} initially decreases, reaching a minimum of 29.20mA/cm^2 for the thickness1.6 µm and then increases to37.85 mA/cm^2 – the value corresponding to the simulated value for a profile of uniform band gap1.16eV. Fill Factor also exhibits the same pattern but the minimum is reached at 1.8 µm of thickness.

Efficiency η, exhibits the same trend of reaching a minimum value 14.17% for a thickness 1.8µm and then increasing to18.43%.This value corresponds to the efficiency η of a solar cell(simulated) with absorber layer of thickness 2 µm. Both Fill Factor and Efficiency η exhibit local maxima when the layer thickness increases from1.8µm to 2.0µm. This is shown in the graph1.

ISSN 2347-3487

3.2 J-V behavior of the solar cell with substructure.

In order to see the response of the cell for the substructure, a cell with following structure was simulated. In this case pCIGS absorber layer of constant thickness was subdivided in to three layers – layer three of thickness 0.1µm and band gap 1.16eV was placed in contact with back electrode, the remaining thickness was divided in to two layers. The band gap of these two layers changed linearly from 1.16eV to 1.3 eV. The thickness of these two layers was varied from 0.1 to 1.8µm. The results are shown in table 4. As seen in the table, the value of Voc is hovering around o.75mV but the value of Jsc has drastically reduced. The value of Jsc is around26.6 mA/cm2 and efficiency is around15.3%. Only when the thickness of layer 1 which forms junction with CdS is reduced to 0.1µm, Jsc improves to 32.83mA/cm2 and η to19.82%.

3.3 C -V behavior

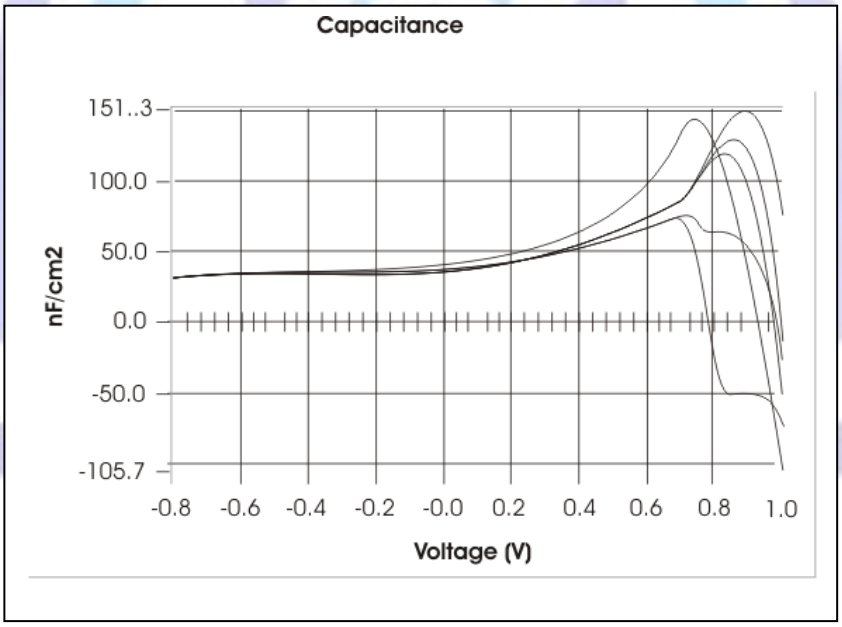
The C-V behavior of profiles f3tof12 when simulated over the range -0.8 to 1.0v exhibit a trend in which capacitance gradually increases with voltage, reaches a maximum value and falls sharply.

Generally at low voltages, current is much smaller than the saturation current of the contact diode (at the back); hence there is no voltage drop over the contact. This results in voltage dropping entirely over CdS/CIGS junction. Consequently junction capacitance would be the capacitance measured- cj: and this increases with voltage.

At high voltages, the current is limited to the saturation current of the contact diode; the CdS/CIGS junction and all the additional voltage drops over the contact diode. The capacitance now switches over to the value of contact capacitance Cc.

At intermediate values, the applied voltage is divided between CdS/CIGS junction and the contact, and the capacitance is the series connection of the junction and the contact capacitance. This series capacitance would be smaller than the either of the two capacitance. If the width of the intermediate region is not too narrow, the C v/s V plot would exhibit a minimum between two maxima.

But in the present study for models s3 to s12 such a behavior is not exhibited in the region -0.8 to 1.0V. The C values would reach a maximum value and then fall sharply without going through a minimum and then a second maximum. Profiles s13, s14 and s15 show a variation from this behavior in the sense that over a small region of V values they exhibit a constant value of capacitance and then again a decrease is observed. In graph 1 few typical curves are shown.



GRAPH1: Graph shows the simulated C-V behavior of few representative profiles.

3.4 Acknowledgement

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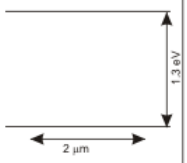
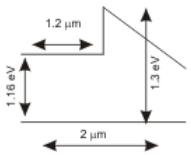
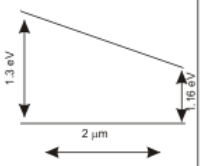
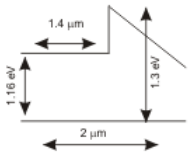
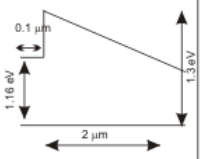
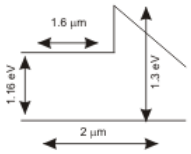
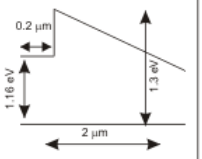
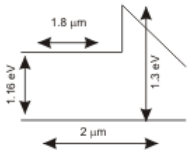
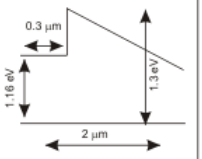
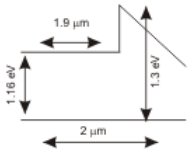
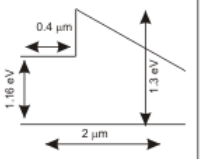
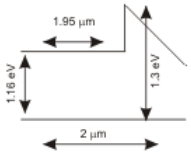
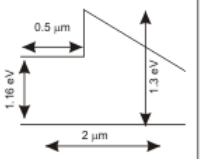
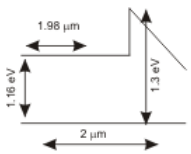
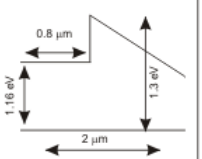
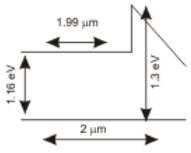
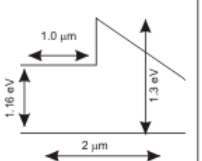
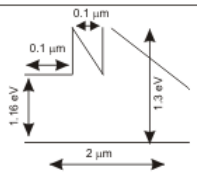
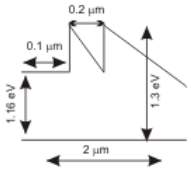
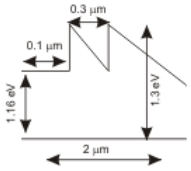
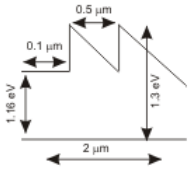
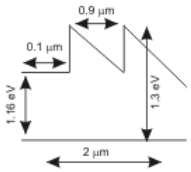
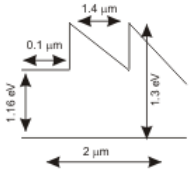
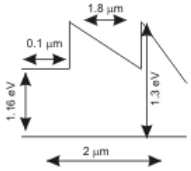
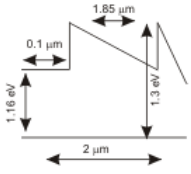
TABLE3. Simulated performance parameters of the CIGS solar cells with various absorber band-gap profiles.

Simulation No	Bandgap Profile	Performance Parameter	Simulation No	Bandgap Profile	Performance Parameter
1)		Voc = 0.7683 mv Jsc = 32.93 mA|cm^2 FF = 78.66 η = 19.90%	10)		Voc = 0.7603 mv Jsc = 31.68 mA|cm^2 FF = 77.84 η = 18.75%
2)		Voc = 0.7683 mv Jsc = 32.93 mA|cm^2 FF = 78.66 η = 19.90%	11)		Voc = 0.7527 mv Jsc = 30.77 mA|cm^2 FF = 77.12 η = 17.86%
3)		Voc = 0.7680 mv Jsc = 32.87 mA|cm^2 FF = 78.63 η = 19.85%	12)		Voc = 0.7376 mv Jsc = 29.21 mA|cm^2 FF = 75.02 η = 16.16%
4)		Voc = 0.7679 mv Jsc = 32.85 mA|cm^2 FF = 78.62 η = 19.83%	13)		Voc = 0.6816 mv Jsc = 35.64 mA|cm^2 FF = 58.35 η = 14.18%
5)		Voc = 0.7677 mv Jsc = 32.82 mA|cm^2 FF = 78.61 η = 19.80%	14)		Voc = 0.6450 mv Jsc = 37.22 mA|cm^2 FF = 75.41 η = 18.10%
6)		Voc = 0.7675 mv Jsc = 32.78 mA|cm^2 FF = 78.59 η = 19.77%	15)		Voc = 0.6409 mv Jsc = 37.54 mA|cm^2 FF = 77.84 η = 18.73%
7)		Voc = 0.7672 mv Jsc = 32.73 mA|cm^2 FF = 78.57 η = 19.73%	16)		Voc = 0.6379 mv Jsc = 37.30 mA|cm^2 FF = 78.14 η = 18.79%
8)		Voc = 0.7657 mv Jsc = 32.49 mA|cm^2 FF = 78.43 η = 19.51%	17)		Voc = 0.6357 mv Jsc = 37.76 mA|cm^2 FF = 77.69 η = 18.65%
9)		Voc = 0.7638 mv Jsc = 32.19 mA|cm^2 FF = 78.23 η = 19.23%			

ISSN 2347-3487

TABLE 4. Simulated performance parameters of the CIGS solar cells with various substructure absorber band-gap profiles.

Simulation No	Bandgap Profile	Performance Parameter
1)		Voc = 0.7680 mv Jsc = 32.87 mA|cm^2 FF = 78.63 η = 19.85%
2)		Voc = 0.7680 mv Jsc = 32.86 mA|cm^2 FF = 78.63 η = 19.85%
3)		Voc = 0.7680 mv Jsc = 32.86 mA|cm^2 FF = 78.63 η = 19.84%
4)		Voc = 0.7680 mv Jsc = 32.85 mA|cm^2 FF = 78.63 η = 19.84%
5)		Voc = 0.7680 mv Jsc = 32.84 mA|cm^2 FF = 78.64 η = 19.83%
6)		Voc = 0.7680 mv Jsc = 32.81 mA|cm^2 FF = 78.64 η = 19.82%
7)		Voc = 0.7680 mv Jsc = 32.83 mA|cm^2 FF = 78.59 η = 19.81%
8)		Voc = 0.7680 mv Jsc = 32.84 mA|cm^2 FF = 78.63 η = 19.83%