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Analytical Study of High Efficient Cu(In,Ga)Se_2 Solar Cell with In_2S_3 Buffer Layer

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***Abstract*—This paper represents a lucid numerical analysis of thin film Cu(In,Ga)Se_2 (CIGS) solar cell with In_2S_3 (Indium Sulphide) buffer layer by using SCAPS-1D. The effect of band gap, concentration and thickness of both Cu(In,Ga)Se_2 absorber layer and In_2S_3 buffer layer are investigated in this simulation. This study is focused to analyze electrical performances of In_2S_3 buffer layer based Cu(In,Ga)Se_2 solar cell for a better substitute of toxic CdS buffer layer. The optimum thickness has found 40 nm for In_2S_3 buffer layer and 3000 nm for Cu(In,Ga)Se_2 absorber layer. In addition, the optimum band gap of CIGS and In_2S_3 layer has attained 1.10 eV and 2.6 eV subsequently and 25.03% efficiency has achieved along with 0.75 V open circuit voltage (V_{oc}), 39.435 mA/cm^2 short circuit current density (J_{sc}) and 84.62% Fill Factor (FF).**

Keywords—CIGS, In_2S_3, band gap, efficiency.

I. Introduction

CIGS (Copper Indium Gallium diselenide) solar cells are now leading the thin film solar cells market due to its low manufacturing cost and high efficiency compared to other thin film solar cells.. The highest lab efficiency of CdS/CIGS solar cell is 21.7% by “Solar Energy and Hydrogen Research (ZSW)” [1] and 22.3% by “Solar Frontier” [2]. It is an adulterant of copper indium diselenide (CIS) and copper gallium diselenide (CGS) which can be denoted as [Cu(In_xGa_{1-x})Se_2] CIGS. By tuning the In:Ga ratio x, the band gap of CIGS can be tuned from 1.0 eV to 1.7 eV [3].

CdS (Cadmium Sulphide) buffer layer contains toxic element Cadmium (Cd), so the excessive use of CdS in CIGS solar cells indirectly lead to serious environmental problems [4]. Moreover, the fabrication technique of the CdS as buffer layer is not compatible with other layers, resulting in a complex fabrication process for CIGS solar cells [4].

Various buffer layers have been researched in CIGS cell i.e. ZnS, ZnSe, $In(OH)_3$, In_2S_3, In_xS_y, $ZnInSe_x$, ZnMgO, ZnO, SnO_2, SnS_2. Among them In_2S_3 is a very auspicious one and β-In_2S_3 buffer layer has been applied as an ideal substitute for CdS to avoid the use of toxic Cd and to obtain an environment friendly photovoltaic system [5]. The In_2S_3 band gap ranges from 2.1 to 2.9 eV or higher values when oxygen or sodium elements is doped with it partially [5]. It has found in some report that the optical band gap of pure β-In_2S_3 in thin film form was only from 2.0 eV to 2.2 eV [6] [7]. However, In_2S_3 based CIGS cell has reached efficiency of 15.7% efficiency by CBD (Chemical Bath Deposition) process [8] and the highest efficiency 16.4% [9] is achieved by ALCVD (Atomic Layer Chemical vapor Deposition) process.

The purpose of this study is to observe performance of CIGS solar cell with In_2S_3 buffer layer and to find out the optimum performance of alternative buffer layer which can replace the toxic CdS. We study the effect of band gap, concentration and thickness of both CIGS absorber layer and In_2S_3 buffer layer.

II. Methodology

A. CIGS solar cell structure and cell parameters

The CIGS solar cell structure used is ZnO:Al/i-ZnO/In_2S_3/CIGS/Mo/substrate. Transparent conductive oxide (TCO) has been used as window layer. It is a bi-layer which comprises of intrinsic Zinc-Oxide (i-ZnO) and Aluminum doped ZnO (ZnO:Al). ZnO:Al has 95% transmission [10]. Molybdenum (Mo) is the back contact of this CIGS solar cell. It has a metal work function of 4.95 eV [11]. Its thickness depends on the required resistance of the solar cell. Solar cells are mostly fabricated on soda-lime glass (SLG) substrate. The highest efficiency of CIGS cell is obtained on glass [2].

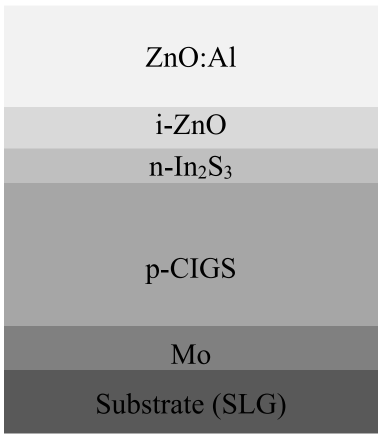

Fig.1. Schematic structure of CIGS solar cell used in the simulation.

Numerical method helps to test the results and optimize the process parameters on the device without fabrication. In this study, CIGS solar cells are modeled using the latest version

(3.0.0.2) of SCAPS (Solar Cell Capacitance Simulator) which is a one dimensional simulator developed at the university of Gent [12]. The semiconductor parameters used in this simulation is given in Table I. The CIGS solar cell is simulated with solar spectrum AM 1.5G, 100mW/cm^2 power density and 300 K of temperature. The function of current density versus voltage (J-V) characteristic curve has used for extraction of electrical parameters such as V_{oc}, J_{sc}, FF and efficiency. In this study band gap, concentration and thickness of both CIGS and In_2S_3 have been observed and all the other parameters remain constant.

TABLE I
Material properties for basic CIGS cell materials

Layer properties				
Layer	ZnO:Al	i-ZnO	In_2S_3	CIGS
Thickness (nm)	200	50	40-200	500-3000
E_g (eV)	3.3	3.3	2.1-2.8	1.01 - 1.69
χ_e (eV)	4.45	4.45	4.65-3.95	4.35 - 3.69
$\acute{\varepsilon}_r$	9	9	13.5	13.6
N_c (cm^{-3})	2.20×10^{18}	2.20×10^{18}	1.80×10^{19}	2.20×10^{18}
N_v (cm^{-3})	1.80×10^{19}	1.80×10^{19}	4.00×10^{13}	1.80×10^{19}
μ_e (cm^2/Vs)	100	100	400	100
μ_h (cm^2/Vs)	31	31	210	25
N_D (cm^{-3})	1.00×10^{20}	1.00×10^{18}	1.00×10^{16}-1.00×10^{18}	0
N_A (cm^{-3})	0	0	10	1.00×10^{16}-2.00×10^{18}
Parameter	ZnO:Al	i-ZnO	In_2S_3	CIGS
Type	Donor	Donor	Acceptor	Donor
σ_n	1.00×10^{-15}	1.00×10^{-15}	1.00×10^{-15}	5.00×10^{-17}
σ_p	5.00×10^{-13}	5.00×10^{-13}	5.00×10^{-13}	1.00×10^{-13}
Contact properties				
Contact	Mo		ZnO:Al	
SN_0 (cm/s)	1.00×10^{7}		1.00×10^{7}	
SP_0 (cm/s)	1.00×10^{7}		1.00×10^{7}	
ϕ_m (eV)	4.95		4.4	
Transmitivity	0.20		0.95	

TABLE II
Overall sign of CIGS cell material properties

Overall properties	
Bandgap	E_g
Electron affinity	χ_e
Dielectric relative permittivity	$\acute{\varepsilon}_r$
Conduction band effective density	N_c
Valence band effective density	N_v
Electron mobility	μ_e
Hole mobility	μ_h
Donor density	N_D
Acceptor density	N_A
Capture cross section of electrons	σ_n
Capture cross section of holes	σ_p
Surface recombination velocity of electron	SN_0
Surface recombination velocity of hole	SP_0
Metal work function,	ϕ_m

III. RESULTS AND DISCUSSIONS

A. Effect of CIGS absorber layer band gap

In this study CIGS band gap has varied from 1.01eV to 1.69 eV while other parameters are remain constant. Fig. 2 shows that V_{oc} has increased with the band gap and it has saturated at 0.853 V over the band gap value of 1.42 eV, whereas J_{sc} and FF decrease rapidly and efficiency increases for a while then it started to decrease. Photons which are carrying energy larger than band gap, will contribute to electron hole pair formation and remaining photons which are carrying energy lesser than the band gap will be wasted. That's why efficiency has increased for a while with the band gap and then it has decreased after a certain value. The highest efficiency that is obtained from this simulation is 21.297% at 1.10 eV.

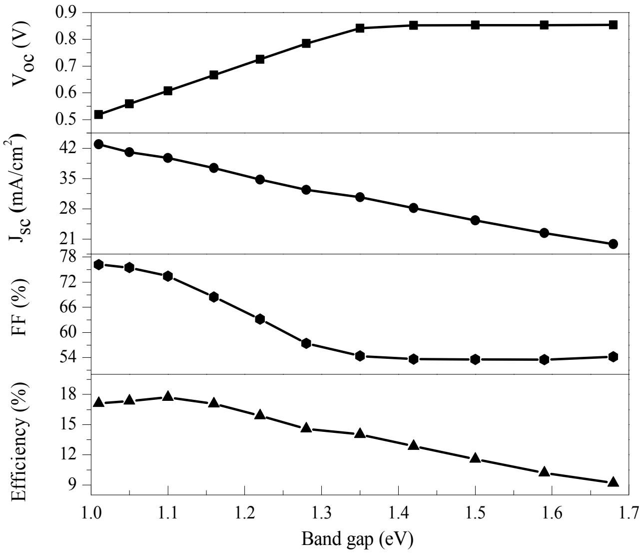

Fig.2. Solar cell electrical parameters with variable CIGS band gap.

Fig. 3 depicts the quantum efficiency of CIGS solar cell with variable band gap. Conduction band is varies with band gap. For a high band gap materials it is much higher compared to a low band gap material. Hence for higher band gap, more photons energy will require to free the electrons. That's why absorption rate is reduced due to higher band gap as well as long wavelengths.

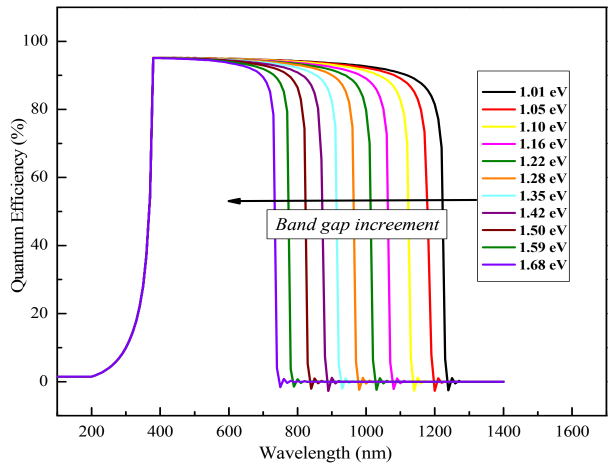

Fig.3. Quantum efficiency with variable CIGS band gap.

B. Effect of CIGS absorber layer concentration

In this section, CIGS concentration is varied from 1×10^{16} cm^{-3} to 2×10^{18} cm^{-3} and the optimum CIGS band gap 1.01 eV is set. As we increase the concentration FF, V_{oc} increases rapidly and J_{sc} reduces slightly which in turns lead to the rise in efficiency from 17.72% to 23.89% as shown in Fig. 4.

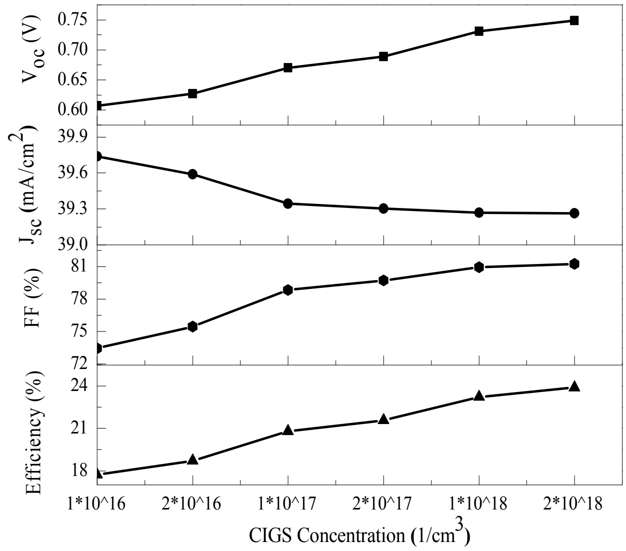

Fig.4. Solar cell electrical parameters with variable CIGS Concentration.

C. *Effect of CIGS absorber layer thickness*

CIGS solar cell output parameters have shown an upward trend with the rise in thickness as exhibits in Fig.5. Its thickness has varied from 500nm to 3000nm while the CIGS concentration is set 2×1018 cm-3 and other parameters remain same. When the thickness of CIGS absorber layer has increased, more photons will be absorbed here which results growth in Voc, Jsc, FF and efficiency. The optimum thickness of absorber layer has found 3000 nm in this simulation.

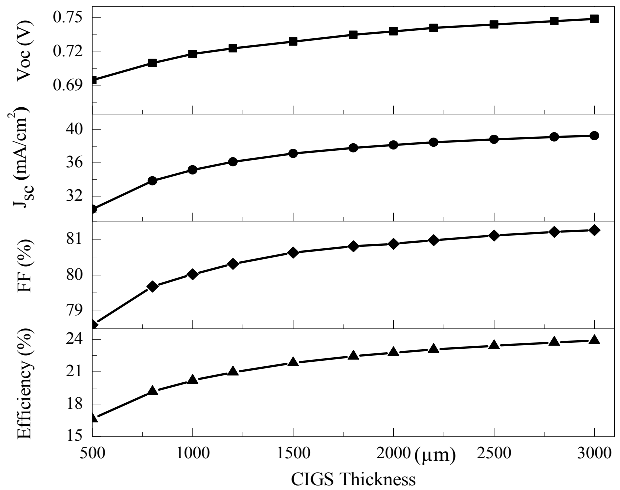

Fig.5. Solar cell electrical parameters with variable CIGS Thickness.

Fig. 6 depicts the quantum efficiency of the solar cell with variable CIGS absorber layer thickness. Thicker absorber layer quantum efficiency is much higher than the thinner one as shown in Fig.6. Because, in thicker absorber layer generation process held very far from back contact while in thin absorber layer it is much nearer to back contact.

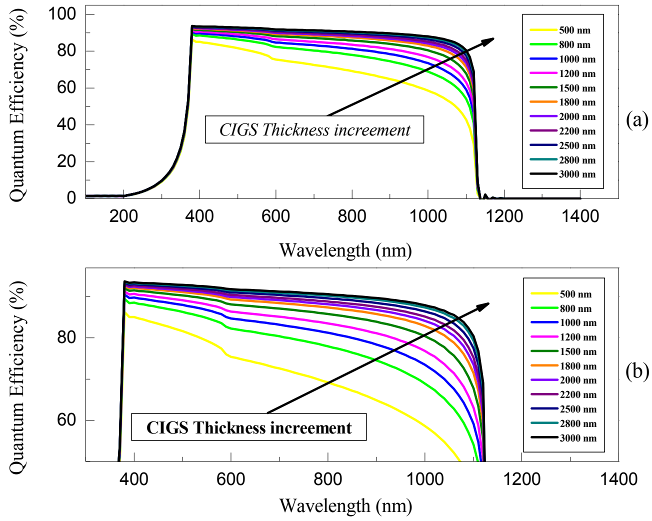

Fig.6. Quantum efficiency with variable CIGS Thickness
(a) in full scale (b) in optimized scale.

D. *Effect of In_2S_3 buffer layer band gap*

In this part, the band gap of In2S3 has been varied from 2.1 eV to 2.8 eV whereas the optimum CIGS thickness is set at 3000 nm. Voc is plateaued with the rise in band gap and a slight increment in Jsc. However efficiency increases with band gap and peaks at 2.6 eV with 25.03% highest efficiency. This is because of higher bandgap of n-type region will allow maximum number of photons to be absorbed in the absorber layer. Further increment in band gap results reduction in efficiency and with 2.8 eV efficiency reaches at 17.32% as given in Fig.7.

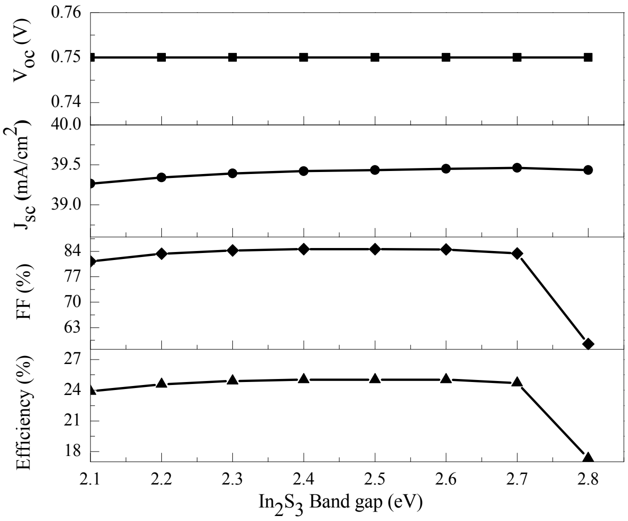

Fig.7. Solar cell electrical parameters with variable In_2S_3 band gap.

E. *Effect of In_2S_3 buffer layer concentration*

It can be seen from Fig. 8 on increasing the concentration efficiency rises swiftly. In this section In_2S_3 concentration varied from 1×10^{16} cm^{-3} to 1×10^{18} cm^{-3} and its band gap is set at 2.5 eV. With the rise in concentration J_{sc} and also FF increases gradually whereas V_{oc} remain constant at 0.75 V.

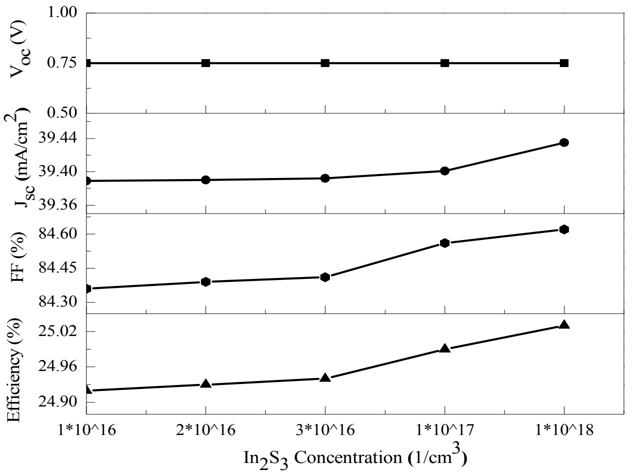

Fig.8. Solar cell electrical parameters with variable In_2S_3 Concentration.

F. *Effect of In_2S_3 buffer layer thickness*

In this section, In_2S_3 buffer layer has been varied from 40 nm to 200 nm. Efficiency and J_{sc} has decreased with rise in In_2S_3 thickness, and V_{oc} remain same at 0.75 V and a slight increment in FF has observed. Due to buffer layer increment, more energy carrying photons will be absorbed in this layer. It will reduce the number of photons which could reach the absorber layer. Hence the efficiency has been decreased from 25.03% to 23.38% as illustrates in Fig. 9. .

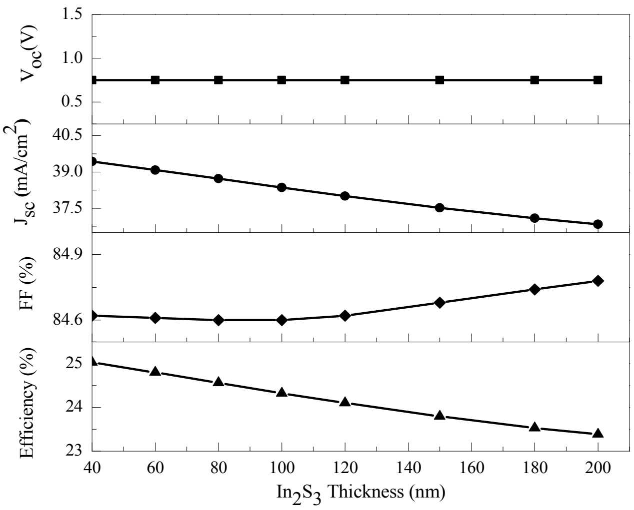

Fig.9. Solar cell electrical parameters with variable In_2S_3 Thickness.

In_2S_3 based proposed CIGS cell efficiency has reached over the previous best efficiency.

TABLE III
Proposed simulated In_2S_3/CIGS cell parameters and previous study

	Efficiency (%)	**V_{oc} (V)**	**FF (%)**	**J_{sc} (mA/cm^2)**
Proposed In_2S_3/CIGS	25.03	0.75	84.62	39.43
CBD process [8]	15.70	0.59	74.60	35.50
ALCVD process [9]	16.40	0.66	78.00	31.50
AMPS simulation [13]	16.00	0.65	75.20	32.57

IV. Conclusion

The electrical performances of CIGS solar with variation in band gap, concentration and thickness of both absorber layer and buffer layer has been carried out through numerical analysis. In_2S_3 has shown great performances as buffer layer which can be a better substitute of toxic CdS. The optimum band gap of CIGS and In_2S_3 layer has detected 1.10 eV and 2.6 eV respectively. In_2S_3 thickness increment results fall in efficiency, whereas the opposite scenario has seen in case of CIGS and optimum layer thickness is found 40 nm and 3000 nm accordingly. 25.03% efficiency with 84.62% FF has perceived in In_2S_3/CIGS solar cell. These results can be helpful to fabricate a desired In_2S_3/CIGS solar cell. But some other parameters need to be investigated in further studies.

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