Modeling of Cu_2ZnSnS_4 Solar Cells with Bismuth Sulphide as a Potential Buffer Layer

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***Abstract*—The Cu_2ZnSnS_4 is a quaternary semiconductor compound has recently been drawn the attention of extensive research as a potential absorber layer since its offers favourable optical and electronic properties along with low cost material. In this research work, the deep level defects on the performance of CZTS solar cells with Bismuth Sulphide (Bi_2S_3) buffer layer was carried out by numerical analysis using SCAPS 2802 simulator. In the proposed cell, the CZTS absorber layer was reduced that minimized the cost, saving process time and energy required for fabrication. In this study, it was found that the feasibility of this proposed ultra thin CZTS solar cells and showed higher efficiency of 17.89% (J_{sc} = 31.05 mA/cm^2, V_{oc} = 1.03V and FF = 0.562). Moreover, the thermal stability of the CZTS solar cell was examined and found that the normalized efficiency of the proposed cell was linearly decreased with the increased of operating temperature at the gradient of -0.41%/^{0}C.**

Keywords*— CZTS solar cell, Low cost material, Deep level defect, SCAPS 2802, Thermal stability.

I. INTRODUCTION

For the sustainable development in the arena of energy harvesting focus mainly on solar energy which is the most reliable and abundant form of renewable energy that serve as an alternative resource of energy for rapid raising demand of power consumption. Conventional energy sources are diminishing day by day in response of bulk demand of energy and consequently the price of these energy sources are increasing gradually. At present, it is burning question to explore the alternative source of energy having clean, environment friendly, cost effective and sustainability.

Si-based solar cells treated as first generation solar cells have been dominating in the field of solar energy harvesting for the last few decades for the property of high efficiency. Prospects of Si solar cells faced challenges due the high cost and risk to fall some of their efficiency at higher temperatures at hot sunny days than thin-film solar cells. Polycrystalline second generation thin film solar cells (CIGS and CZTS) have been considered as potential alternate to Si based solar cells. As a second generation solar cell, extensive research work is going on CIGS solar cells and 20.5±0.6% conversion efficiency is achieved by the researchers [1].

Researchers are very much promising to implement the CZTS solar cell since the abundance of Zinc (Zn) and Tin (Sn) in earth's crust. The availability of Sn and Zn are 45 times and 1500 times greater than that of Indium (In) respectively and consequently the price of Zn and Sn is too less than that of In due to its scarcity effect [2]. Subsequently, investigation has been done on CZTS thin film solar cell to explore the hidden potentiality by adding different buffer layer materials as the availability of Zn and Sn led to design cost effective solar cells. The abundance of Zn and Sn motivate to research work on CZTS solar cells since the scarcity of In and Ga are replaced by Zn and Sn respectively. CZTS has high absorption co-efficient (10^4 cm^{-1}) and optimal direct band gap energy of 1.4-1.5 eV which are highly required in solar cell materials as a high performance solar cell [3].

The structures of CZTS are stannite and kesterite considering the different locations of Cu and Zn. The kesterite structure having the property of more stability [4] and the stannite structure exhibits monocrystal found by Olekseyuk et al. [5]. Typically Cu-rich growth method provides a better grain size and performance also. Tanaka et al. mentioned that the higher ratio of Cu/(Zn+Sn) gives an improved the grain size but Cu-rich condition having low resistivity which caused unfitness for the fabrication of solar cell [6].

In this research work, numerical analysis was done to explore the possibility of ultra-thin CZTS solar cell with Bi_2S_3 as potential buffer layer utilizing SCAPS 2802 simulator to improve the different parameters of cell performance. During the research, effect of TCO, variation of the band gap of buffer layer, deep level defect in absorber layer, variation of doping concentration, effect of capture cross section and thermal stability are investigated for efficient CZTS solar cell.

II. MODELING AND SIMULATION

In this research work, the purpose of numerical modeling and simulation were done using SCAPS 2802 to investigate the possibility of ultra-thin CZTS absorber layer for low cost solar cells. By incorporating a 20 nm TCO layer (i-ZnO), a 30 nm buffer layer (Bi_2S_3) to be added in 1 µm CZTS solar cell. Mo is used as a back contact metal in this proposed CZTS solar cell structure. Fig. 1 shows the schematic diagram of the proposed CZTS solar cell structure used in this work.

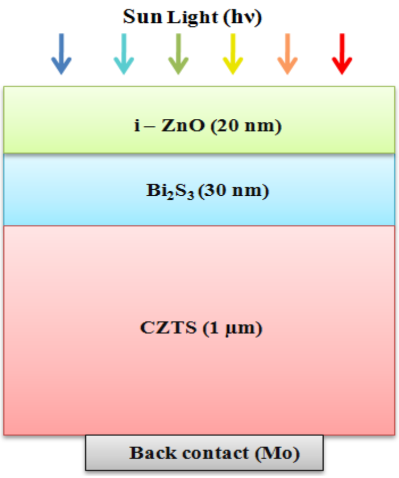

Fig.1 The proposed structure of CZTS solar cell

The material parameters used in this research work are shown in Table I which are selected based on experimental data, literature values, theory, or in some cases reasonable estimation [7].

TABLE I MATERIAL PARAMETERS USED FOR NUMERICAL ANALYSIS OF THE PROPOSED CZTS SOLAR CELLS

Parameters	i-ZnO	n-Bi_2S_3	p-CZTS
Thickness, W (µm)	0.02	0.03	0.5-3
Permittivity, $\varepsilon/\varepsilon_0$	9	13	10
Electron mobility, μ_c (cm^2/Vs)	100	200	100
Hole mobility, μ_p (cm^2/Vs)	25	1100	25
Carrier concentration, n, p (cm^{-3})	1×10^{19}	3×10^{18}	1×10^{14}
Band gap, Eg (eV)	3.3	1.1-1.5	1.5
Density of state in conduction band, Nc (cm^{-3})	2.2×10^{18}	1.5×10^{18}	2.2×10^{18}
Density of state in valence band, Nv (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Electron affinity, χ (eV)	4.6	4.5	4.5

Numerical analysis was done by SCAPS simulator through Poisson equation and Continuity equation. In this research work, recombination in three different layers is explained by the Shockley-Read-Hall (SRH) formalism. Bethe theory described the transport of majority carriers at the metal-semiconductor interfaces [8] and transport of minority carriers is characterized by their surface recombination velocity [9]. The presence of TCO layer and the band gap variation of Bi_2S_3 are investigated along with the deep level defect in the absorber layer with the variation of doping concentration. The effect of capture cross section and thermal stability are also investigated to design higher performance CZTS solar cell.

III. RESULT AND DISCUSSION

A. *Effect of the presence of TCO layer*

In solar cells, the function of TCO is to provide a highly transparent and conductive contact to buffer layer and intrinsic ZnO (i – ZnO) is used as TCO in this work. A comparative study of cell models with Bi_2S_3 buffer layer along with and without TCO layer has been illustrated in Table II. It can be observed form Table II that i-ZnO/Bi_2S_3/CZTS provides the best cell performance structure having TCO layer placed above buffer layer.

TABLE II COMPARISONS BETWEEN CZTS CELLS WITH AND WITHOUT TCO

Parameters	Voc (V)	Jsc (mA/cm^2)	FF	Eff. (%)
With TCO	1.03	31.05	0.562	17.89
Without TCO	0.88	17.03	0.638	9.59

B. *Effect of Buffer layer band gap*

For thin-film solar cell the magnitude of the band gap of buffer layer acts a significant role to improve the performance. In this research work, the band gap value for Bi_2S_3 buffer layer is varied between 1.1 eV to 1.5 eV. The reason for choosing slightly lower band gap value than the typical for Bi_2S_3 is due to the effect of band bending in the TCO/Bi_2S_3 interface. Fig. 2 depicts the magnitude of *Voc, Jsc,* FF and efficiency with the variation of band gap value for the Bi_2S_3.

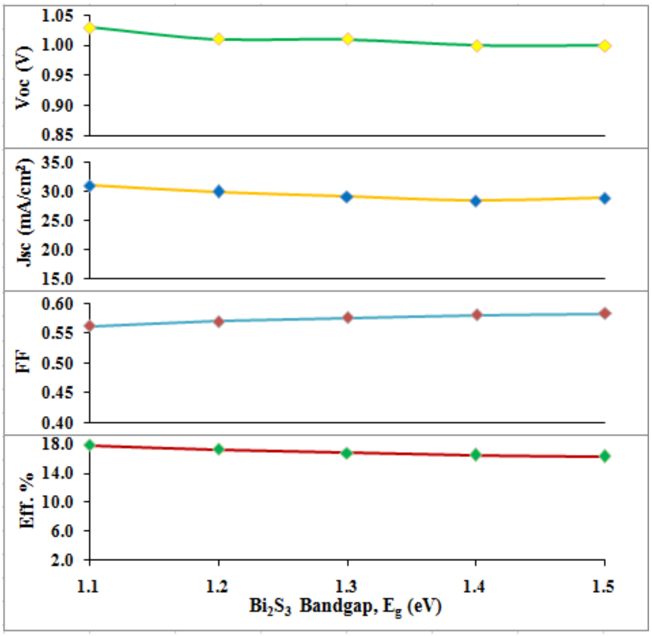

Fig.2 CZTS cell performance with different Bi_2S_3 band gap

C. *Effect of CZTS layer thickness*

It has been investigated the effect of CZTS absorber layer thickness reduction by numerical calculations for the i-ZnO/Bi_2S_3/CZTS configuration. Fig. 3 illustrates the simulation results during the variation of CZTS absorber layer thickness from 0.5 µm to 3 µm. The magnitude of *Voc* and *Jsc* show increasing trend as expected with the increase of CZTS layer thickness whereas FF are decreasing trend. In this research work during the variation of absorber layer, cell conversion efficiency mainly affected by the open circuit voltage.

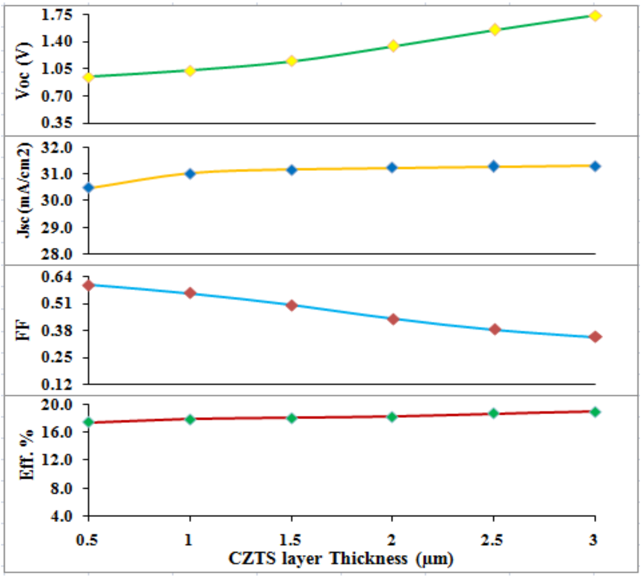

Fig.3 Effect of CZTS thickness variation for the proposed cells

D. *Effect of Doping Concentration*

The p-type doping of CZTS absorber layer is varied from 1×10^{10} to 1×10^{14} cm^{-1}. Fig. 4 shows the effect of the CZTS doping concentration on cell performance parameters.

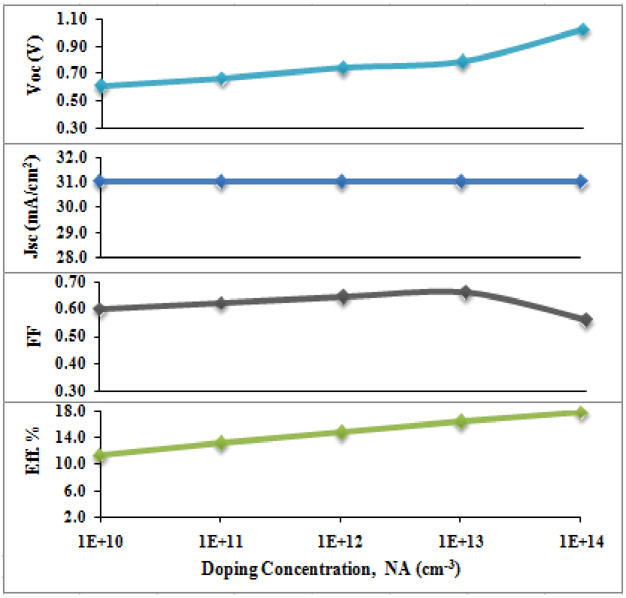

Fig.4 Effect of the CZTS doping concentration on cell performance

It is clear from the Fig. 4 that the cell conversion efficiency is increased with the increase of doping concentration of the absorber layer. With the increase of doping concentration in absorber layer, the *Voc* is increased but FF is decreased after certain doping concentration whereas *Jsc* is unchanged.

E. *Effect of Deep level Defect*

Deep defect level may lie closer to the mid-gap and consequently they can hold carriers more strongly than shallow levels. Deep defect levels can reside throughout the energy band gap [10]. In this research work, both Uniform and Gaussian energetic distributions have been taken to analysis the performance of CZTS solar cell. During the research work, deep level defect has been assumed to be of neutral type, capture cross section of electron and hole has been taken initially to be of a moderate value (1×10^{-15} cm^2). The performance of Bi_2S_3/CZTS structure has been investigated for containing TCO and without TCO. It is evident from Table III that i-ZnO/Bi_2S_3/CZTS structure gives the best results for both uniform and Gaussian distribution.

TABLE III COMPARISONS BETWEEN CZTS CELLS WITH DEEP LEVEL DEFECT

Parameters	**Energ. Dis.**	**Voc (V)**	**Jsc (mA/cm²)**	**FF**	**Eff. (%)**
With TCO	Uniform	1.02	31.05	0.562	17.87
Without TCO		0.88	17.03	0.637	9.58
With TCO	Gaussian	1.02	31.05	0.562	17.86
Without TCO		0.88	17.03	0.637	9.57

F. *Effect of Capture Cross Section*

In this research work, the hole capture cross section has been varied numerically to observe the effect on the cell performance of CZTS solar cells. Fig. 5 shows the graphical representation of capture cross section of hole. A variation of hole cross section (Cp) have been investigated keeping the electron capture cross section (Cn) constant. It is evident from Fig. 5 that the efficiency of cell is degraded with the increase of capture cross section of hole (Cp). A rapid deterioration has been observed for Cp above 1×10^{-11} cm^2.

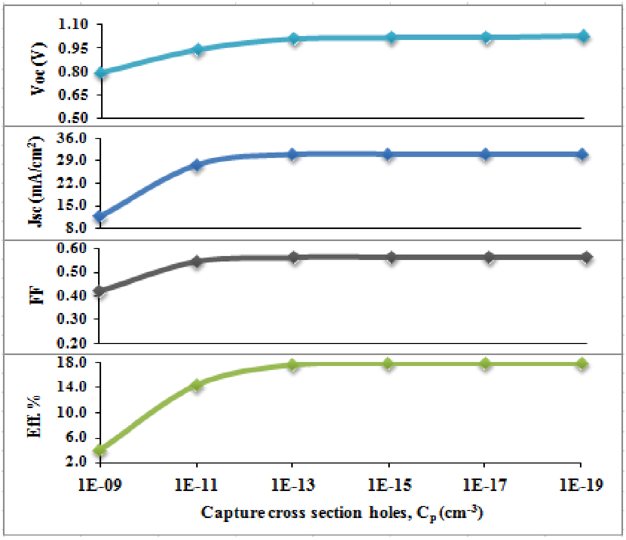

Fig.5 Effect of capture cross section of hole on cell performance

G. *Effect of Temperature*

The thermal stability of the proposed cells at higher operating temperatures is investigated as the operating temperature plays a very vital role in practical case and it affects the performances of the solar cell. It is clear from Fig. 6 that the normalized efficiency of the proposed CZTS cell is linearly decreased with the increase of operating temperature at a temperature coefficient (TC) of -0.41%/°C. This TC indicates better stability of the cells at higher operating temperature.

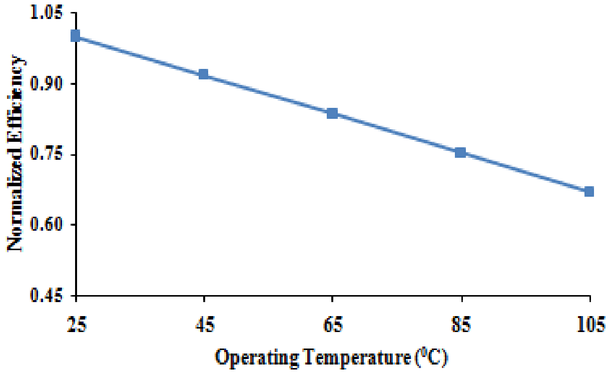

Fig.6 Effect of operating temperature on normalized efficiency

IV. CONCLUSION

The potential buffer layer material Bi_2S_3 was investigated in ultra-thin CZTS solar cell with an addition of 20 nm i-ZnO as TCO layer. The highest efficiency was found for 1 µm CZTS absorber layer along with 30 nm Bi_2S_3 buffer layer showed the best conversion efficiency of 17.89% (Jsc = 31.05 mA/cm^2, FF = 0.562, Voc = 1.03 V). A linear TC of -0.41%/°C was shown for the proposed CZTS solar cell with Bi_2S_3 buffer layer that indicated better thermal stability.

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