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Numerical studies on $Cu_2BaSn(S,Se)_4$ absorber based thin film solar cells

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ABSTRACT

$Cu_2BaSn(S, Se)_4$ (CBTSSe) is emerged as most promising absorber layer for the thin films solar cells due to its exotic properties such optimum band gap (~1.5 eV), high absorption coefficient (> 10^4 cm^{-1}), less number of stable secondary phases, p-type conductivity etc. In the present article, device modelling of CBTSSe solar cell is carried out using one dimension solar cell capacitance simulator (1D-SCAPS) program. The JV characteristics of Mo/p-CBTSSe/n-CdS/ZnO/ITO (in substrate configuration) is analyzed by varying thickness and optical band gap of CBTSSe.The maximum efficiency of the optimized device is 10.5% with V_{OC} of 658 mV.

INTRODUCTION

Photovoltaic (PV) technology: generating direct current (DC) electricity from theoptical energy of the Sun, is well proven to be reliable, dependable, reasonably efficient and clean energy source. The main point of focus in PV research is on the environmentally clean raw materials, processes and on the reduction of cost. The PV technology is mature and is being adopted widely (in Giga watts) among several developed and developing countries, still, significant efforts need to be expended on the enhancement of efficiencies and reducing process costs. While addressing economics, the viable option is to develop thin film PV technology. The main factors in thin film PV devices are the cost, stability and efficiency. Among the severalPV materials, the promising materials are$Cu(In,Ga)(S, Se)_2$ (CIGSSe)andCdTe that have demonstrated a remarkable record PV efficiency 22.6% and 22.1% respectively on lab scale[1]. Due to scarce availability of In (0.160 ppm), Te (0.001 ppm) and Cd (0.15 ppm), these solar cells face some challengeson a large-scale production.Alternatively, Cu-based quaternarychalcogenide semiconductor$Cu_2ZnSn(S,Se)_4$(CZTSSe) is considered as the chalcopyriteCIGSSe. Till date, CZTSSe absorber based photovoltaic deviceshave attained maximum efficiency of 12.4%[2] which is lower than thetheoretical Shockley-Queisser efficiency limit for a single p-n junctionCZTSSe solar cells. The main reason for the lowefficiency is due to presence of stable secondary phases in CZTSSe.

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Recently, Cu_2BaSnS_4 emerged as alternate to the current absorber layers. The electronic studies on trigonal CBTS compoundssuggest thatcopper vacancy (V_{Cu}), a shallow acceptor, is the dominant point defect withthe leastformation energy (formation energy 0.6 eV) in Cu-poor/S-rich conditions[3].Band structure studies show that CBTS exhibits both direct band gap (1.79 eV) and indirect band gap (1.77 eV), but the energy difference is very small(~20meV)which cannot significantly influence the absorption characteristics at room temperature[3]. The band gap is larger than the optimal value (1 to 1.5 eV) for a high-efficiency single p-n junction solar cell[4]. Experimentally, Shin *et al* demonstrate thatthe $Cu_2BaSnS_{4-x}Se_x$ (CBSTSSe) exhibits trigonal structure ($P3_1$) for $x \leq 3$ and band gap can been varied from 1.95 eV (x = 0) to 1.55 eV (x = 3)[5]. For pure selenide compound (x = 4), it transforms to the orthorhombic structure (*Ama2*) and the band gap is 1.72 eV which is larger than the 1.28 eV value calculated by Hong *et al* assuming trigonal structure[3].This tunable band gap 1.28–1.95 eV are appropriate for singlep-n junction and multi junction photovoltaic application.

The crystal structure, electronic properties and band structure studies highlight the suitability of CBTSSe as a potential PV absorber material for thin film photovoltaics. Also, the constituting elements of the compound are earth-abundant (Cu 68 ppm, Ba 340 ppm and Sn 2.2 ppm) and non-toxic. The first CBTSSe absorber base solar cell was reported by Shin *et al* with device structure(device area 0.425 cm^2): Glass/Mo/CBTS/CdS/i-ZnO/ITO/Al-Ni[5]. The CBTS thin film was prepared by co-sputtering of Cu, Sn and BaS targets followed by sulfurization at 570 C for 10 hours.The maximum PV efficiency achieved was 1.62% having V_{OC}, J_{SC}, FF equals to 713 mV,4.11 mA/cm^2 and 55.32%.Ge *et al*showed an improvement of PV efficiency from 1.57% to 2.03% (0.08 cm^2 device area) by incorporating a CdS:O/CdS bilayer and also yielded larger V_{OC} of 0.93 V but low J_{SC} (5.08 mA/cm^2) and FF (43%)[6], [7].Recently, Sin *et al* incorporated Se in CBTS and successfully enhancedthe PV efficiency to 5.2% (on device area 0.425 cm^2) with V_{OC}, $J_{SC}$and FF of 611 mV, 17.4 mA/cm^2 and 48.9% respectively demonstrating the highest efficiency among the CBTSSe absorber based thin film photovoltaics [8]. The rapid rise of the PV performance of the CBTSSe solar cells drawsa singnificant potential towards a cost-effective, non-toxic and high-efficiency solar cells.

Device modelling provides a deeper understanding of transport of charge carriers in thin film solar cells. In the modelling, basic transport equations (continuity equation and Poisson's

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equation) are solved numerically. There have been many device modelling programs developed such as SCAPS [9], AMPS [10], PC-1D[11] etc. In the present work, device modelling on CBTSSe absorber based solar cell is carried out using SCAPS-3.3.05 simulation program. SCAPS (Solar cell CAPacitance Simulator) is a 1D solar cell simulation program developed byMarc Burgelman et. al. [9].The current-voltage (JV) characteristics of CBTSSe solar cell has been analyzed by varying thickness and bandgap of CBTSSe.

MODELLING OF THIN FILM SOLAR CELL

The proposed device structure in substrate configuration (light falls on the substrate after passing through all layers) is illustrated in Fig. 1.It consists of mainly four layers: substrate (molybdenum), absorber layer (p-type CBTSSe), buffer layer (n-type CdS), window layer (Sn-doped indium oxide). The IV-characteristics of the solar cell depends on the various properties these layers. The properties of the layers are used as parameters to for modelling the device.The parameters are given in Table 1.

Optimization of thickness and optical band gap of CBTSSe absorber layer:

Working point conditions

Temperature 300.00 K

AM1.5 G Illumination

Material parameters:

Surface work function of back contact (Molybdenum): 5.5 eV

Electron surface recombination velocity (SRV): 10^7 cm/s

Hole SRV: 10^5 cm/s

Table 1: Parameters of p-CBTSSe, n-CdS, ZnO and ITO used for the simulation.

	CBTSSe	**CdS**	**ZnO**	**ITO**
Thickness (μm)	Varied	0.05	0.05	0.2
Electron affinity (eV)	4.58	4.2	4.55	4.7
Band gap (eV)	Varied	2.45	3.3	3.4
Dielectric permittivity (relative)	9.5	8.9	8.12	8.12

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CB DOS (N_C) (cm^{-3})	1.75×10^{18}	1.00×10^{18}	1.00×10^{18}	1.00×10^{18}
VB DOS (N_V) (cm^{-3})	3.41×10^{19}	1.00E$\times10^{18}$	1.00×10^{18}	1.00×10^{18}
e mobility (μ_e)(cm^2/V/s)	12	50	100	100
h mobility (μ_h)(cm^2/V/s)	1	20	20	20
Acceptor density (N_A) (cm^{-3})	1.00×10^{15}	----------	--------------	-------------
Donor density (N_D) (cm^{-3})	----------	1×10^{17}	1×10^{10}	1×10^{20}
Absorption (A) (cm^{-1} $eV^{1/2}$)	1×10^4	5×10^4	5×10^4	1×10^5
e thermal velocity ($V_{th, n}$) (cm/s)	107	107	107	107
h thermal velocity ($V_{th, h}$) (cm/s)	10^7	10^7	10^7	10^7
	CBTSSe	**CdS**	**ZnO**	**ITO**

RESULTS AND DISCUSSION

In the optimization process, thickness and optical band gap of CBTSSe is varied. Thickness of CBTSSe is varied from 500 nm to 2.5 µm. The optical band gap of CBTSSe is varied from 1 eV to 1.5 eV.

Fig. 2shows that the short circuit current density (J_{SC}) increases with thickness of absorber layer (CBTSSe) due to the absorption of more photons and consequently generation of large number electron-hole pairs. It is observed from the figure that J_{SC} decreases with the increase of band gap of CBTSSe. With the increases of band gap the absorption coefficient decreases and thus photo-generated charges decreases.

Fig. 3shows that open circuit voltage (V_{OC}) is nearly independent of thickness at lower band gap (< 1.2 eV). At higher band gap, the V_{OC} is large. The behavior can be understood using Eq. 1[12]

$$V_{OC} = \frac{E_g}{q} + \frac{k_B T}{q} ln\left(\frac{I_L + I_0}{I_0 e^{-\frac{E_g}{k_B T}}}\right) \qquad \text{Eq. 1}$$

where, E_g, k_B, T, q,$I_L$and $I_0$is optical band gap of CBTSSe, Boltzmann constant, temperature, electron charge, current under illumination and reverse saturation current. The equation suggests

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that the maximum V_{OC} can be equal to the band gap of absorber layer. Since the second term is negative, the V_{OC} is measured to be lower than the band gap.

The photovoltaic efficiency (power conversion efficiency) of the solar cell is presented in Fig. 4. It is noted that the highest efficiency is observed in the region of higher thickness and medium band gap range (1.2 to 1.4 eV). The efficiency of a photovoltaic device is given by Eq. 2

$$\eta = \frac{J_{max} V_{max}}{P_{in}} = \frac{J_{SC} V_{OC} FF}{P_{in}} \qquad \text{Eq. 2}$$

where, J_{max}, $V_{max}$and P_{in} are current density (at maximum power), voltage (at maximum power) and input power (~ 100 mW/cm^2).

The IV characteristics of the CBTSSe solar cell after optimizing thickness and optical band gap is shown in Fig. 5. The optimum value of thickness and band gap obtained after the simulation are 2.5 µm and 1.2 eV. The maximum photovoltaic efficiency corresponding to the optimized parameters is 10.5% with J_{SC} = 26.7 mA/cm^2, V_{OC} = 658 mV and FF = 60%. The value is higher than the experimental value[8]. It is also noteworthy that there is a JV cross-over between dark and illuminated curves. The distortion of the JV curve is anticipated due to the large offsets at the interface of the Mo/CBTSSe and CBTSSe/CdS interface.

CONCLUSION

$Cu_2BaSn(S,Se)_4$ (CBTSSe) absorber based solar cell is investigated using SCAPS-1D numerical simulation program. The device is optimized by varying thickness and optical band gap of absorber layer (CBTSSe). The evaluated device parameters; short circuit current density, open circuit voltage, fill factor and efficiency of the optimized cell are 26.7 mA/cm^2, 658 mV, 60% and 10.5% respectively. A crossover of JV curve from illumination to the dark region is observed due to the band offsets. This crossover can be overcome by optimizing electron affinity of the layers which would help in proper band alignment.

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FIGURES AND CAPTIONS

Fig. 1 Device structure of CBTSSe based thin film solar cell

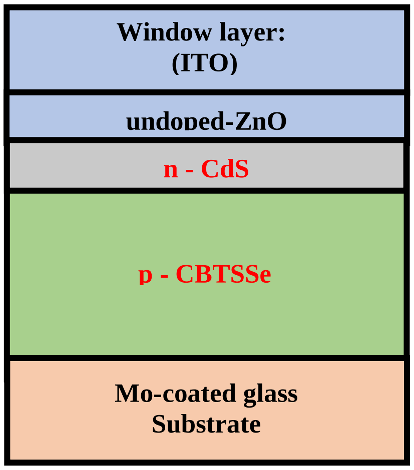

Fig. 2Variation of short circuit current (J_{SC}) with optical band gap and thickness of CBTSSe absorber layer.

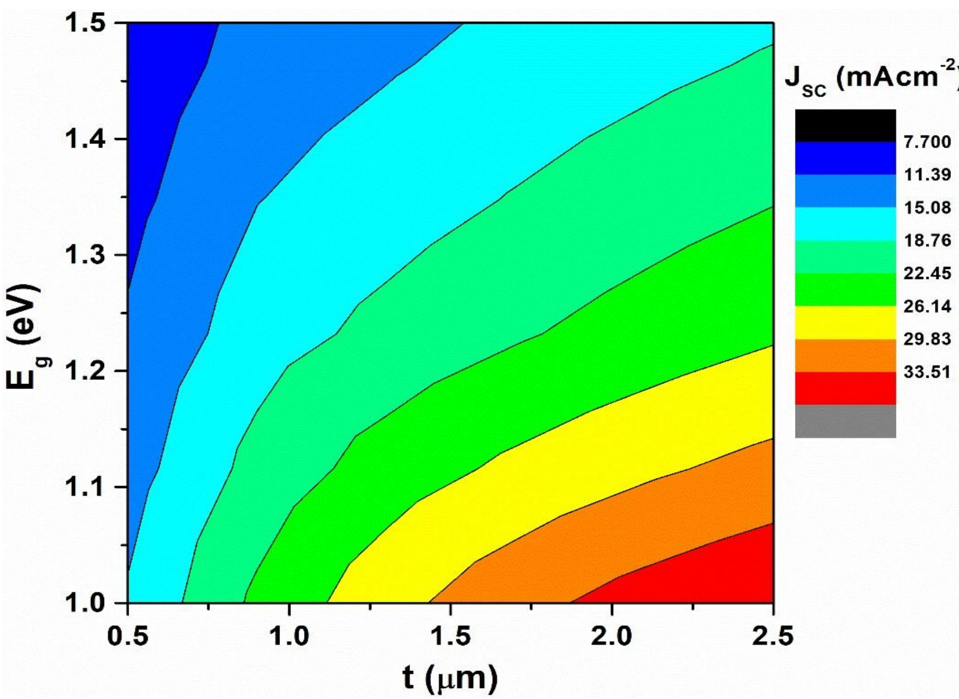

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Fig. 3Variation of open circuit voltage (V_{OC}) with optical band gap and thickness of CBTSSe absorber layer.

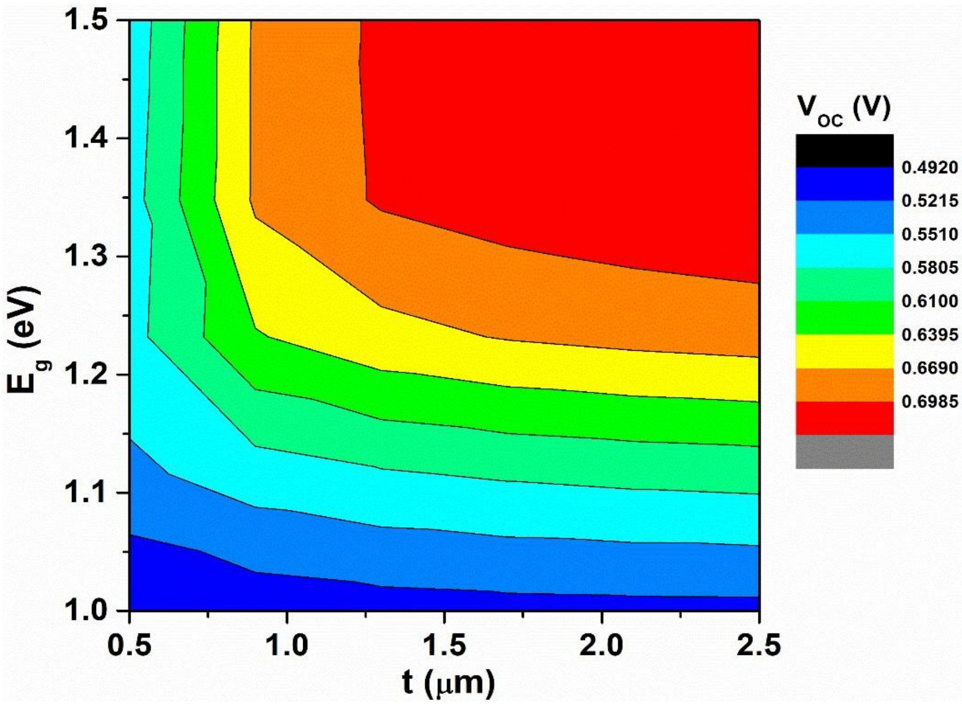

Fig. 4Variation of open circuit voltage (VOC) with optical band gap and thickness of CBTSSe absorber layer.

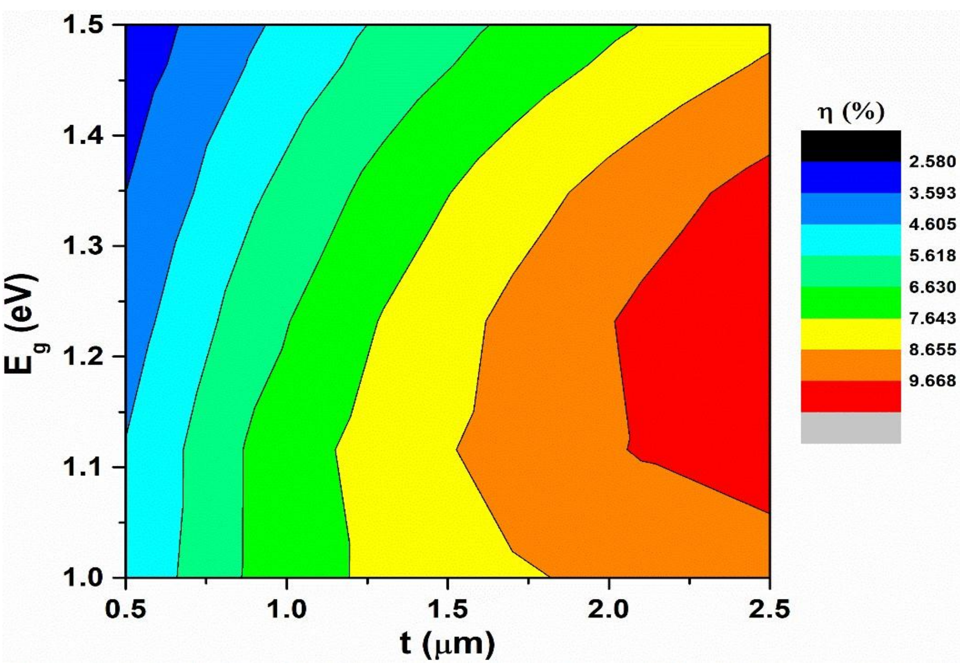

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Fig. 5Current density-voltage (JV) characteristics of optimized CBTSSe solar cell.