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Research Article

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Theoretical analysis of CZTS/CZTSSe tandem solar cells.

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Abstract: Kesterite $\text{CZTS}_x\text{Se}_{1-x}$ has a band gap range from 1 to 1.5eV depending upon S/Se ration. The tandem of kieserite solar cell is proposed and simulated in SCAPS-1D for device configuration and analysis of the performance. CZTS of bandgap 1.5eV as top cell and CZTSSe of bandgap 1.1eV as bottom cell are stacked in tandem for the structure. The thickness of the two layer are optimized for matching the short circuit current J_{SC} in the tandem. This study shines light on alternative technique of thin film multijunction for enhancing the efficiency of $\text{CZTS}_x\text{Se}_{1-x}$ solar cells.

Keywords: Multijunction, SCAPS-1D, Simulation, Chalcogenide solar cell, Bandgap tuning.

1. Introduction

Single junction solar cell with constant bandgap absorbs only a portion of solar spectrum. Its efficiency is mainly limited by non-absorption and thermalization losses and is 33% [1] also known as Shockley-Queisser limit (SQL). List of techniques are suggested to decrease these losses and thus overcome SQL. Light concentration, Spectrum conversion, Multiple temperature, Multi-absorption and Multi-energy level, Multi-junction are some techniques for beating SQL [2]. Theoretical efficiency of photovoltaic is 33-68% by various techniques under 1 sun.[1] Among all these only multijunction (MJ) technology have achieved efficiency $\leq 45\%$ way beyond any other technology. This technology is less used for terrestrial application however its impact will be immense if implemented in low-cost manner. DSSC/CIGS [3], CGS/CIGS [4], Perovskite/CZTS [5] are some experimentally reported attempts. Efforts should be made to lower the cost of these technologies, cost effective implementation of MJ in thin film solar cells can be one viable approach.

The Chalcogenide $(\text{Cu}_2\text{ZnSn}(\text{S}_x\text{Se}_{1-x})_4$ solar cell which is derivative of CIGS, by replacing rare In, Ga with earth abundant Zn, Sn and considered a replacement for CIGS. The complex defect physics of CZTS has limited its efficiency to 12.6% as of now. Passivating defect of bulk CZTS and optimizing device structure are the current engagement. The $\text{CZTS}_x\text{Se}_{1-x}$ has a well reported bandgap tuning by varying ratio of S/Se in range of 1-1.5eV [6]. Pure sulphide CZTS ($x=1$), Pure selenide CZTSe ($x=0$) and sulpho-selenide ($0 < x < 1$) empirical dependence of bandgap on the S/Se ratio is given by

$$E_g = xE_{gCZTS} + (1 - x)E_{gCZTSe} - bx(1 - x)$$

Where E_{gCZTS} is 1.5eV, and E_{gCZTSe} =1eV, b is the bowing factor =.1ev [6]. The $CZTS_xSe_{1-x}$ band gap tuning is advantageous for absorbing effectively the solar spectrum. Mechanically stacked arrangement of two thin films, to share same incoming radiation can effectively capture the solar radiation. Photons of energy 1.1eV and 1.5eV will be contributing in generating photo-voltage in two cells.

2. Simulation

The stack of junction arranged one over other in decreasing bandgap order absorbs sun light efficiently. The i^{th} cell in the Multijunction stack will generate current equal to number of photons absorbed in that energy range of E_{g_i} (bandgap of the i^{th} cell) to $E_{g_{i+1}}$ (bandgap of the $i+1$ cell). Neglecting absorption of light emitted by other solar cell. The power will be given by product of current and total Voltage in the stack and empirically by

$$P = \sum_{i=1}^n IV_i.$$

The current will be limited by the lowest current producing cell in the stack i.e. the value of current flowing through each cell in the whole stack. Each cell should be adjusted to their maximum performances and then operated at common current and individual voltage. The CZTS (1.5eV) and $CZTS_xSe_{1-x}$ (1.1eV) are attached in tandem sharing the same incoming light. The high wavelength part of spectrum transmitted light from the top (large band gap) cell will be the illumination for the bottom cell (low band gap). The current in the two cells is given by

$$J_{CZTS} = q \int_{\frac{E_{gCZTS}}{hc}}^{\infty} \phi_{AM1.5}(\lambda) d\lambda$$

$$J_{CZTSe} = q \int_{\frac{E_{gCZTSe}}{hc}}^{\frac{E_{gCZTS}}{hc}} \phi_{AM1.5}(\lambda) d\lambda$$

Where $\phi_{AM1.5}$ is the spectral photon flux. Solar cell capacitance simulator SCAPS-1D [7] version 3.3.02 is used for the simulation of the multijunction [8]. The SCAPS-1D simulation for the CZTSSe [9] and CZTS [10] is widely reported. The CZTS solar cell and CZTSSe cell are simulated separately. Multivalent defect of charge state $\{3+/2+, 2+/+, +/0\}$ in CB at $E_t=1.40$ eV and charge state $\{0/-, -/2-, 2-/3-\}$ at VB. Defect density of $5 \times 10^{14} \text{ cm}^{-3}$, capture cross section of 10^{-13} cm^2 recombination coefficient (cm^3/s) 10^{-13} and auger recombination coefficient is $10^{-28} \text{ cm}^6/\text{s}$. Interface neutral defect density of 10^{12} cm^{-3} is taken at CZTS/CdS junction. The device is illuminated with AM1.5

spectrum. In tandem same current will flow through two cells, this current matching is done by varying thickness of the two cells. The J-V of tandem is obtained by series connects of two cell using SCAPS script “tandem connection.script”. It calculates the transmitted spectrum from top cell and applies that spectrum to bottom cell as illumination. The J-V of the two cells is added to get the J-V of the Tandem cell. The material parameters used here are listed in Table1 [9-11].

3. Result and discussion

The schematic of the tandem cell is shown in the figure 1a. Tandem cell comprised of CZTS (1.5eV) as top cell and the CZTS_{0.25}Se_{0.75} (1.1eV) is the bottom cell. The cells are mechanically stacked one over other sharing the spectrum. The inter-connect between two cell is thought to be an ohmic, optically transparent and conductive layer [12-13]. J-V of individual cells is simulated in Fig.1b. Individual performance of CZTS is 8.37% and CZTS_xSe_{1-x} 12.67%. Bottom cell with low bandgap has higher J_{sc} and lower V_{OC} as compared to top cell. QE and cutoff wavelength are shown in figure1c, 1d respectively. Below cutoff wavelength are absorbed by the cell. The tandem cell will have more than one current source region. Current generating from the two cells must be equal for SCAPS to calculate the tandem cell parameters. The Short circuit current flowing in the circuit can be made similar by varying thickness of the two layers. Top layer will act as the filter for solar spectrum for bottom cell. Current is limited by the junction/cell producing the lowest current. Voltage generated in individual cell can be directly added. Optimum thickness is obtained by using simulation to match the J_{CZTS} and J_{CZTSSe} at short circuit condition. Fig. 2a shows the tandem IV of the cell run using ‘tandem connection.script’. Current of the bottom cell is higher than the top cell. The tandem IV does not extrapolating the current in current mismatch region as shown in Fig. 2a. The bottom cell at lower bandgap, current value will be higher due to availability of large spectrum thus bottom absorber thickness needs to reduce. Figure 2b shows the J_{sc} with thickness of bottom cell. Thickness corresponding to short circuit value in top cell is the optimizing thickness of the two absorber, current in tandem cell is matched. At current matching condition optimum value of thickness for bottom layer (1.1eV) is 0.148 micron and top layer (1.5eV) thickness is 0.6 micron.

The final IV at the current matched condition for the CZTS_xSe_{1-x} is shown in the Fig. 3. The voltage of the tandem is the linear sum of the two cells. Current remain the same in device. The cell parameters for top cell, Bottom cell are shown in Fig. 3. Tandem cell parameter are V_{OC} 1.21V, J_{sc} 18.6mA/cm², FF 66% and Efficiency 15.12%. To obtain same short circuit current cell thickness optimization is the crucial step involved in designing the multijunction solar cell.

4. Conclusion

Kesterite is one among possible thin film solar cell suitable for MJ. Analysis of MJ for kesterite ($\text{CZTS}_x\text{Se}_{1-x}$) bandgap pair (1.1 and 1.5 eV) is presented here. Simulated results shows large value of voltage 1.21 and high efficiency of 15.12%. Thickness of the absorber layer in two solar cell layers in tandem is optimized to obtain current matching condition. This work is analyzing a suitable structure strategy which could implement thin film multijunction by solution processed way. Experimental realization of such work could possibly be a cost-effective way to enhance efficiency.

Declaration of Interest

Author declare no conflict of interest.

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Figure 1. (a) Schematic of the mechanically stacked Tandem solar cell, CZTS is top cell and CZTSSe is the bottom cell, (b) Individual IV of the CZTS cell and CZTSSe cell, (c) Individually simulated Quantum efficiency of the CZTS solar cell and the CZTSSe solar cell. (d) The derivative of the quantum efficiency with respect to wavelength ($dQE/d\lambda$) for the two cells. $dQE/d\lambda$ bring out the cutoff wavelength of the two device below which the solar cell absorb light.

Figure 2. (a) The J-V for the CZTS, CZTSSe and tandem solar cell. The current is highly mismatched; SCAPS does not plot Tandem JV for the mismatched region. (b) shows the short circuit current with the thickness of bottom cell.

Figure 3. The optimized J-V of the tandem cell. The individual J-V of the CZTS and CZTSSe is also shown, at optimum thickness for current matching condition.

Table 1. Material parameter of the layer used in the simulation [9-11]

Fig. 1

Fig. 2

Fig. 3

Table 1.

Parameter	CZTS _x Se _{1-x}		CdS	ZnO
	x=.25 (CZTS _{.25} Se _{.75})	x=1 (CZTS)		
Thickness(nm)	variable	variable	80	400
Bandgap(eV)	1.1	1.5	2.4	3.3
Electron affinity(eV)	4.1	4.2	4.25	4.5
Dielectric permittivity	10	7	9	9
CB effective density of state $N_C(\text{cm}^{-3})$ ($\times 10^{18}$)	2.2	2.2	1.8	2.2
VB effective density of state $N_V(\text{cm}^{-3})$ ($\times 10^{19}$)	1.8	1.8	2.4	1.8
Electron thermal velocity(cm/s)	10^7	10^7	10^7	10^7

Hole thermal velocity(cm/s)	10^7	10^7	10^7	10^7
Electron/hole mobility(cm^2/Vs)	40	75	80	30
Donor/ Acceptor density, N_D/N_A (cm^{-3})	10^{15}	10^{16}	10^{17}	10^{18}
Absorption coefficient(cm^{-1})($\times 10^4$)	5	5	SCAPS value	SCAPS value

Figures

Figure 1

(a) Schematic of the mechanically stacked Tandem solar cell, CZTS is top cell and CZTSSe is the bottom cell, (b) Individual IV of the CZTS cell and CZTSSe cell, (c) Individually simulated Quantum efficiency of the CZTS solar cell and the CZTSSe solar cell. (d) The derivative of the quantum efficiency with respect to wavelength ($dQE/d\lambda$) for the two cells. $dQE/d\lambda$ bring out the cutoff wavelength of the two device below which the solar cell absorb light.

Figure 2

(a) The J-V for the CZTS, CZTSSe and tandem solar cell. The current is highly mismatched; SCAPS does not plot Tandem JV for the mismatched region. (b) shows the short circuit current with the thickness of bottom cell.

Figure 3

The optimized J-V of the tandem cell. The individual J-V of the CZTS and CZTSSe is also shown, at optimum thickness for current matching condition.