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Investigation of some materials as buffer layer in copper zinc tin sulphide (Cu_2ZnSnS_4) solar cells by SCAPS-1D

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ABSTRACT

In this work, we have simulated Cu_2ZnSnS_4 solar cells with different buffer materials in order to propose an alternative to Cadmium Sulphide (CdS) as a solar cell buffer material. The goal was to reduce the toxic effect of cadmium containing solar cells on the environment. Materials like Zinc Sulphide(ZnS), Zinc Selenide(ZnSe) and Indium Sulphide(InS) were tested along with CdS. Results obtained with ZnSe and ZnS compare favourably well with that of CdS. We therefore propose ZnSe and ZnS as viable alternatives to the toxic CdS as buffer material for Cu_2ZnSnS_4 solar cells.

Keywords: CZTS, SCAPS-1D, CdS, In_2S_3, ZnSe

INTRODUCTION

Thin film Cu_2ZnSnS_4 (CZTS) solar cell is a potential source of low-cost, high efficiency solar electricity. Cu_2ZnSnS_4 is a high efficiency thin film absorber which makes a promising solar cell material. Seol et al. prepared CZTS thin films by RF magnetron sputtering [1]. They reported that the optical band gap energy and absorption coefficient of CZTS were about 1.5eV and $1.0x10^4cm^{-1}$, respectively. Tanaka et al. prepared CZTS thin film films by co-evaporation of elemental sources [2]. Katagiri et al. reported the preparation of CZTS thin films by RF sources co-sputtering followed by vapor phase sulfurization or by sulphurizing electron-beam-evaporated precursors [3–11]. Efficiency as high as 6.77% from the Al/ZnO:Al/CdS/CZTS/Mo/soda lime glass(SLG)substrate structure was reported [12].

Cadmium Sulphide (CdS), Zinc Sulphide (ZnS), Zinc selenide (ZnSe) are used as buffer materials and Zinc oxide (ZnO) as window layer.

2. DEVICE MODELLING

The modelling calculations discussed in the following section uses the software Solar Cells Capacitance Simulator in one dimension (SCAPS-1D), developed at the university of Ghent, Belgium under Professor Marc Burgelman in the Department of electronics and information system. It estimates the steady-state band diagram, recombination profile, carrier transport in one dimension based on the Poisson equation and the hole and electron continuity equations. Recombination currents are calculated with the Shockley-Read-Hall (SRH) model for bulk defects and an extension of the SRH model for the interface defects. The SRH interface approach allows carriers from both conduction and valence bands to participate in the interface recombination process.

The CZTS cell structure that is made up of a p-CZTS absorber layer, the buffer layer and a window layer made of n-ZnO:Al. The entire structure is placed on a soda- lime glass substrate through a Molybdenum (Mo) back contact.

CdS is normally used as the buffer layer but other materials- ZnS, ZnSe, InS were used for the simulation. The schematic diagram of the CZTS cell is shown in fig.1 while the semiconductor parameters of each layer used for the simulation are shown in Table 1.

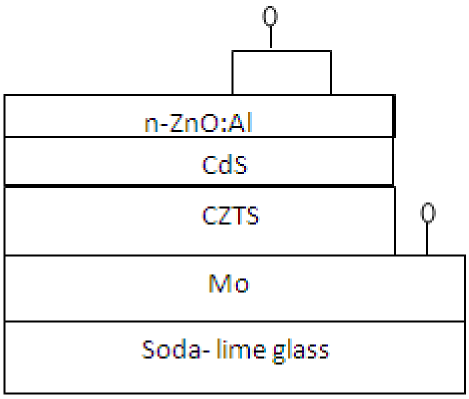

Fig.1 Schematic of one dimensional substrate CZTS solar cells

Table 1: Semiconductor parameters used for the simulation

	CZTS	CdS	ZnS	ZnSe	InS	ZnO
Thickness(μm)	2.500	0.080	0.060	0.080	0.050	0.080
Band gap(eV)	1.450	2.400	3.500	2.900	2.800	3.300
Electron affinity (eV)	4.500	4.500	4.500	4.090	4.700	4.600
Dielectric permittivity (relative)	10.000	10.000	10.000	10.000	13.500	9.000
CB density of state (cm-^{3})	$2.0X10^{18}$	$1.5X10^{18}$	$1.5X10^{18}$	$1.5X10^{18}$	$1.8X10^{19}$	$2.2X10^{18}$
VB density of state (cm-^{3})	$2.0X10^{18}$	$1.8X10^{18}$	$1.8X10^{18}$	$1.8X10^{19}$	$4.0X10^{13}$	$1.8X10^{19}$
μ_e (cm /Vs)	50	50	50	50	400	100
μ_{hole} (cm^2/Vs)	50	20	20	20	210	25
Donor density N_D (cm-^{3})	0	0	0	0	10	$1X10^{17}$
Acceptor density(N_A)	$2.0X10^{15}$	$1X10^{17}$	$1X10^{17}$	$5.5X10^{7}$	$1.0X10^{18}$	0
Electron thermal velocity (cm/s)	$1.0X10^{7}$	$1.0X10^{7}$	$1X10^{7}$	$1.0X10^{7}$	$1.0X10^{7}$	$1X10^{17}$
Hole thermal velocity (cm/s)	$1.0X10^{7}$	$1.0X10^{7}$	$1X10^{7}$	$1.0X10^{7}$	$1.0X10^{7}$	$1X10^{17}$

RESULTS AND DISCUSSION

The performance characteristics of our solar cells in our simulations are as summarized in Table 2 below and their J-V characteristics in figures.2-5 respectively:

Table 2 Summary of the performance characteristics of our simulated solar cells

Buffer layers	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
CdS	0.3240	29.481809	71.48	6.83
ZnS	0.3249	29.259514	68.63	6.52
ZnSe	1.2575	35.694595	15.06	6.76
InS	3.3622	3.960808	3.32	0.44

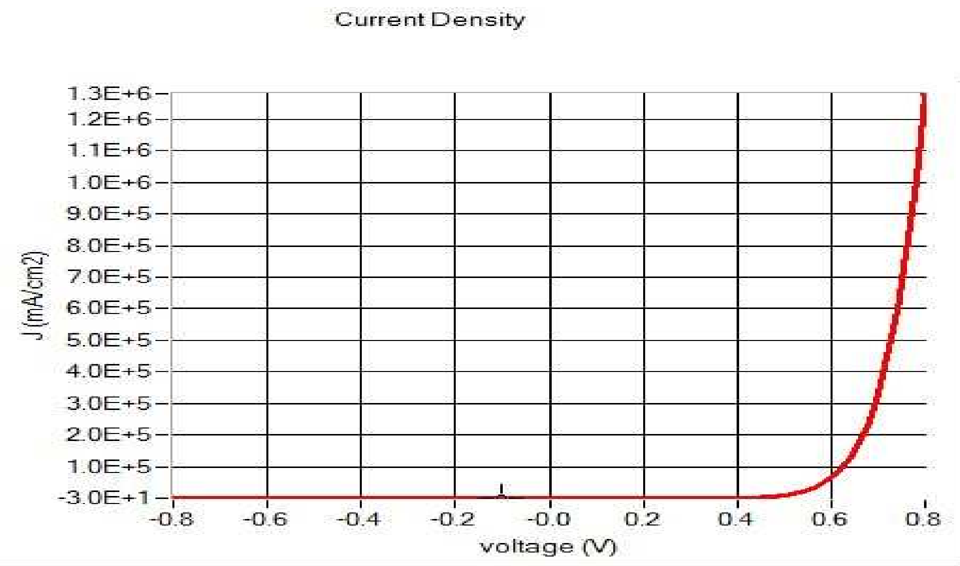

Fig 2: Light characterisitic curve J-V Graph of simulation with CdS Buffers

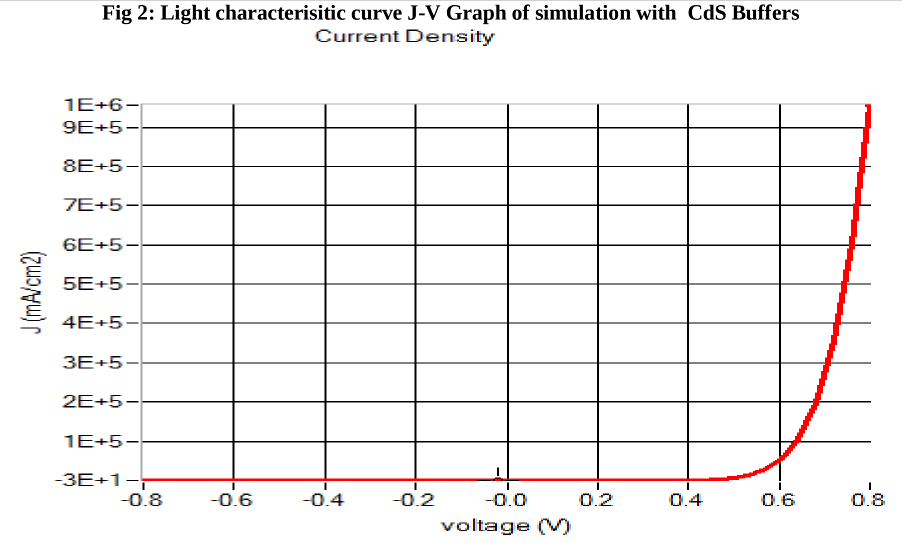

Fig 3: Light characterisitic curve J-V Graph of simulation with ZnS Buffers

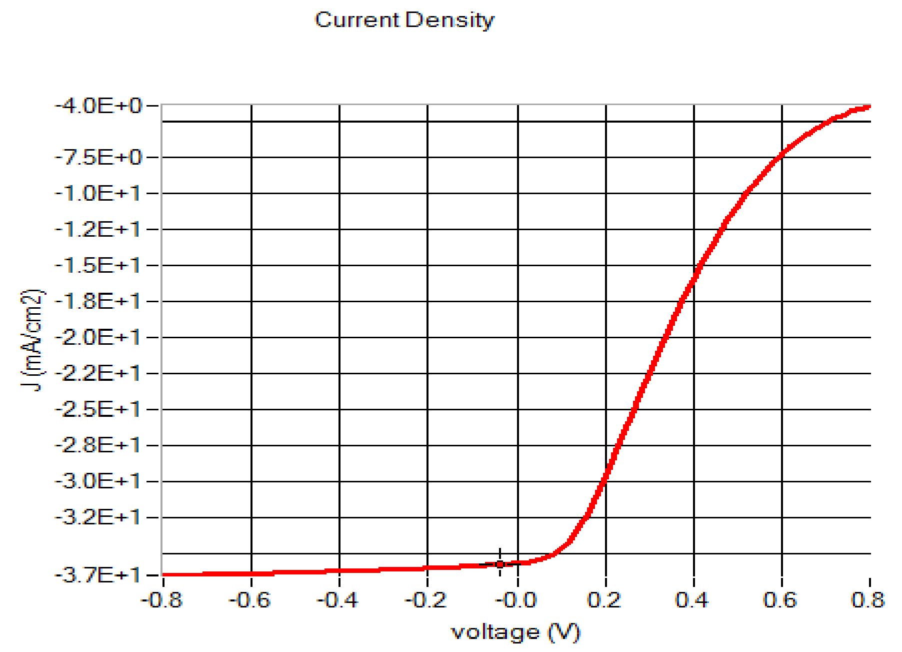

Fig 4: Light characterisitic curve J-V Graph of simulation with ZnSe Buffers

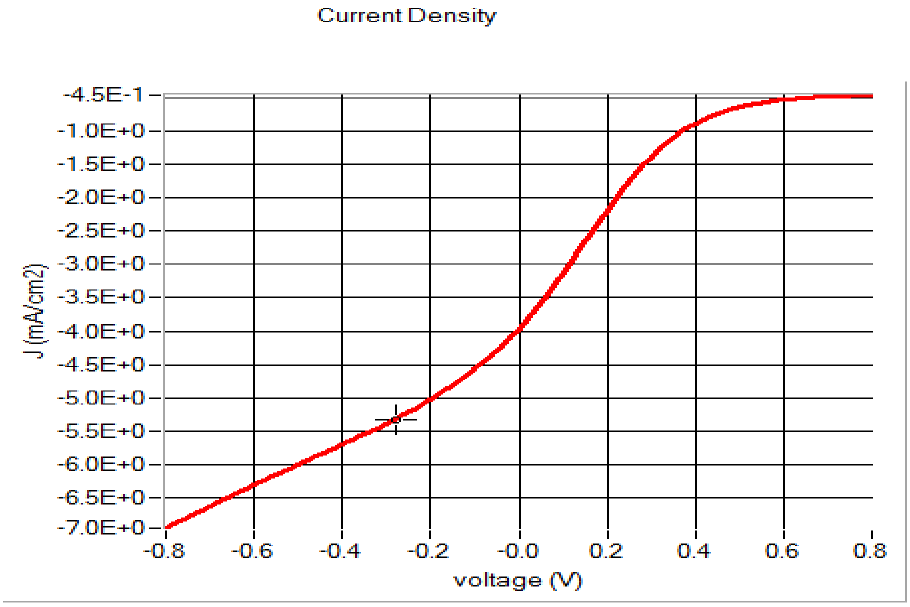

Fig 5 :Light characterisitic curve J-V Graph of simulation with InS Buffers

In the simulation of our solar cells with CdS and other materials (ZnS, ZnSe, InS) as buffer layers, it was observed that solar cells with CdS as buffer layer had the highest efficiency of 6.83% which is an improvement on the reported experimental results of 6.77%. Indium sulphide(InS) had the least efficiency of 0.44%. To this end, ZnS and ZnSe could be alternative buffers to the CdS in the production of CZTS solar cells. This is due to their efficiencies of 6.52% and 6.76% respectively which is closer to the established experimental efficiency. The low efficiency of InS as a buffer material could be as a result of interface defects or lattice mismatch between the InS and other materials of the CZTS thin film solar cell.

CONCLUSION

The results of the simulations with the Solar Cells Capacitance Simulator in One dimension (SCAPS-1D) simulator reveals that CZTS solar cells with alternative buffer layers can be achieved. Photovoltaic parameters obtained with ZnSe and ZnS as buffer materials can be compared to CdS-buffer cell, we concluded that ZnSe and ZnS can be used as alternative material to CdS. As the later presents serious environmental problems.

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