Impact of Back Surface Field (BSF) Layers in Cadmium Telluride (CdTe) Solar Cells from Numerical Analysis

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Abstract. Numerical simulation has been executed using Solar Cell Capacitance Simulator (SCAPS-1D) to study the possibility of favourable efficiency and stable CdS/CdTe cell in various cell configurations. A basic structure of CdS/CdTe cell is studied in this work with 4 μ m CdTe absorber layer and 100 nm tin oxide (SnO₂) as front contact, 25 nm cadmium sulfide (CdS) as buffer layer, zinc telluride (ZnTe) is used as back surface field (BSF) material compared with ZnTe:Cu, Cu₂Te and MoTe₂ in order to reduce the minority carrier recombination at back surface field (BSF). The cell structure of glass/SnO₂/CdS/CdTe/MoTe₂ has shown the highest conversion efficiency of 17.04% (Voc=0.91V, Jsc=24.79 mA/cm², FF=75.41). These calculations have verified that SnO₂ as buffer layer and MoTe₂ as back contacts are suitable for an efficient CdS/CdTe cell. Also, it is found that a few nanometers (about 40 nm) of back surface layer is enough to achieve high conversion efficiency. When MoTe₂ is used, high conversion efficiency of more than 17% has been achieved compared to other BSF materials.

INTRODUCTION

The investigations for feasible solar cell structure which can be replaced with fossil fuel has admitted CdTe based thin film solar cell as a compatible substitute to reach the desired affordable photovoltaic device. Among the group of semiconductors, CdTe is an utmost favourable material in thin film solar cell technology. Having a great commercial success, CdTe has become a remarkable thin film photovoltaic technology and is drawing a significant attention from both scientific and commercial outlook. CdTe thin cells are noticed to be the superior photovoltaic materials for its affordability, simple deposition, great optical absorption coefficient and high chemical rigidity. CdTe's direct band gap is about 1.5 eV, very near to the desired amount for the efficient photo conversion [1-5]. The basic superstrate design of CdTe/CdS thin film solar cell is commonly consist of four layers: a transparent conducting oxide (TCO) as a front contact, an n-CdS film as the window layer, a p-CdTe absorber layer on CdS window layer, with a back contact on the CdTe layer.

Apparently, one of the first objectives of recent studies is to reduce the price of semiconductor material through making thinner cell. Thinning will reduce the production cost by less materials and less production time. The main difference between thin films and thicker ones is that the back-contact interface will be deposited very close to the CdS/CdTe junction. Thus, the choice of the back-contact material consequently has a high impact on the overall cell functionality. A low contact resistance is vital for better functionality and sustainability [6]. However, it is not easy to realize ohmic contact to p-CdTe partly because it has a high work function of 5.7 eV which is higher compared to other metals [7]. A metal with a work function > 5.7 eV is needed, yet there is no metal available in this range. The common approach to rectify the existing Schottky barrier is to create a heavily p-type doped CdTe surface using chemical etching [8, 9] and apply a buffer layer of high carrier concentration between CdTe and the metal. This can lead to a useful band alignment to fades the barrier width at the back-contact layer.

Zinc telluride (ZnTe) is one of the semiconductors used in optoelectronic devices that attracted a considerable attention in recent years for its direct band gap 2.26 eV at room temperature. It has been used in tandem and flexible panels. Also, doping is done using group V, Cu, Ga and Sb to improve the properties and reduce the resistivity of ZnTe [10]. Moreover, Copper is utilized to reduce degradation and form a low resistance back surface. Normally, efficient back contacts have been attained by applying a thin layer of Cu on the Te rich surface. Hence ZnTe:Cu and Cu₂Te are proposed in this study to be compared with the conventional structure. Molybdenum di-Telluride (MoTe₂) is also leading back contact choice for CdTe thin film solar cell with direct bandgap of 1.1 eV, work function of 4.7 eV. MoTe₂ crystals are recognized to show clean Photoluminescence spectra, without any bound exciton shoulders at low temperatures, high carrier mobility, and negligible number of defects [11].

Numerical simulation is a first step to find out the optimize structure of a solar cells. Currently, there is a need for numerical simulation report about the most logical back contact material and their efficient thickness for CdTe solar cells [12]. As a result, a numerical simulation based on SCAPS-1D is presented in this study to look over the desired thickness of BSF layer and also to find a suitable material as a BSF. Here, high bandgap materials like ZnTe and ZnTe:Cu and lower bandgap materials like Cu₂Te and MoTe₂ are used as BSF to lessen minority carrier recombination loss at the back contact in thin CdTe cell. In this research, the highest conversion efficiency of CdTe based PV cell without BSF is achieved 17%. Moreover, the suggested structures are resulted in a great improved stability in most extents by using MoTe₂ as BSF.

NUMERICAL MODELING

SCAPS is one-dimensional simulation software to simulate alternating current and direct current electrical virtues of thin film heterojunction cells. This application is fostered to analyse mainly CdTe and CIGS based solar cells with a unique way to illustrate simulation yield [13]. It has unique properties such as simulation of current voltage characteristics both in dark or under radiance condition. This simulation system computes results from the basic semiconductor equations in 1-D scale and in stable conditions [14]. In this research, SCAPS is used to dissect the CdTe based solar cells.



FIGURE 1. Schematic diagram of (a)proposed solar cell and (b)simulated structures

A typical CdTe solar cell design comprises a glass substrate, SnO_2 as a transparent conducting oxide layer, CdS a window layer and CdTe absorber layer on top of it is illustrated in Fig. 1(a). Also new structures are proposed by adding BSF to the conventional cell which is shown in Fig. 1(b). Various parameters are studied using SCAPS: efficiency, Voc, Jsc and FF of CdTe cells with different BSF layers and their thickness variation effects are observed. Simulation parameters for a standard CdTe solar cell and new designs are summed up in Table 1.

TABLE 1. The parameters for the simulation in SCAI 5-1D at 500K								
Parameters	SnO_2	CdS	CdTe	ZnTe	ZnTe:Cu	Cu ₂ Te	MoTe ₂	
Thickness(nm)	100	25	4000	20	20	20	20	
Bandgap(ev)	3.6	2.4	1.5	2.26	2.2	1.19	1.1	
Electron Affinity (ev)	4	4	3.9	3.1	3.2	4.1	4.2	
Dielectric Permittivity (relative)	9	10	9.4	14	11	10	13	
CB effective density of states	2.2×10^{18}	2.2×10^{18}	8x10 ¹⁷	7x10 ¹⁷	7.8x10 ¹⁸	7.8x10 ¹⁷	$1x10^{15}$	
(1/cm^3)								
VB effective density of states	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.5×10^{19}	1.7×10^{19}	1.6x10 ¹⁹	$1x10^{18}$	
(1/cm^3)								
Carrier Density (cm ⁻³)	1x10 ¹⁷	1.1×10^{18}	$2x10^{14}$	1.6x10 ¹⁹	1.5×10^{20}	1.6x10 ¹⁹	2x10 ¹⁷	
Electron mobility (cm ² /Vs)	100	100	320	100	400	500	426	
Hole mobility (cm ² /Vs)	25	25	40	50	100	100	110	

TABLE 1. The parameters for the simulation in SCAPS-1D at 300K

RESULTS AND DISCUSSIONS

To validate the simulation, a standard CdTe absorber with CdS buffer layer-based structure has been considered. Here the CdTe thickness of 4000 nm, CdS thickness of 25 nm, SnO_2 thickness of 100 nm have been used. BSF layer thickness are changed from 20 nm to 100 nm to examine the impacts on photovoltaic parameters such as Jsc, VoC, FF and efficiency. From Fig. 2, it is clearly seen that all the output parameters are almost stable after 40 nm of thickness in BSF layers. Hence, the optimum thickness for BSF layers is 40 nm.



FIGURE 2. Changes in back surface layer (nm) thickness and its effect on (a) efficiency (b) Jsc (c) Fill Factor and (d) Voc

Operating temperatures are important in determining the performance of solar cells. In most simulations, the optimum operating temperature used in is 300K. At high temperatures, parameters of a solar cell like electron/hole mobility, carrier concentration and the bandgap will be affected leading to lower efficiency. The

effect of increasing temperature from 300 K to 400 K on the cell performance has been explored. A survey is done on the base and suggested structures to study the effect of changes in temperature on each parameter for every solar cell design. Fig. 3 shows that the efficiency and fill factor declined with the increase in temperature from 300K to 400 K. Furthermore, it has been found that MoTe₂ has higher efficiency rate and stability compared with other BSF layers. As open circuit potential is very sensitive to the changes in temperature, the increase in temperature from 300 to 400 K declines the open circuit voltage. This leads electrons to gain more energy at higher temperature and more recombination will happen before they can reach the depletion region and be collected.



FIGURE 3. Changes in temperature and its effect on (a) efficiency (b) Jsc (c) Fill Factor and (d) Voc

The effect of adding back surface field is also remarkable when the structures are compared with respect to the J-V curve under the AM1.5 illumination condition as presented in Fig. 4. It is visible from Fig. 4 that the short circuit current density J_{SC} is improved with different BSF layers.



FIGURE 4. J-V characteristic curves for CdTe base and structures with different BSF layers

It is obvious from Fig. 5 that while the functioning wavelength is lower than 500 nm the quantum efficiency (QE) is seriously affected, with the decrease in thickness of MoTe₂ layer. Jsc and the conversion efficiency of the cell are mainly influenced. However, Table 2 shows the best simulation results from the cell structure using the

MoTe₂ with 30 nm thickness and it is selected as the best BSF with efficiency of 17.04% (Voc = 0.91 V, Jsc = 24.79 mA/cm², FF = 75.4). It is clear that the enhanced cell efficiency has been attained mostly because of the improvement in Jsc.



FIGURE 5. EQE of CdTe base structure compared to CdTe with BSF (MoTe₂) structure

TABLE 2. Parameters of the best simulated structure and base line CdTe cell

Parameters	Reference cell	Simulated cell
Efficiency, η (%)	16.41	17.04
Fill factor (%)	76.21	75.41
Short circuit current density, Jsc (mA/cm ²)	24.72	24.79
Open circuit voltage, Voc (V)	0.87	0.91

CONCLUSION

In this study, performance of different BSF layers in CdTe based solar cells have been investigated using numerical simulation viewpoints. The main focus was to choose the best BSF material among all the proposed designs with respect to their efficiency. It is revealed that $MoTe_2$ can be a great option as a BSF in CdTe solar cells. By analysing simulation results, it is clear that the solar cell functionality is temperature sensitive for all types of BSF with various rate of temperature coefficient. Based on optimization, the highest efficiency of 17.04% has been achieved for ($MoTe_2/CdTe/CdS/SnO_2$) solar cell with 4000 nm thick absorber and 40 nm thick BSF layer.

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