ZnO thickness and ZnTe back contact effect of CdTe thin film solar cell Voc and efficiency progression

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Abstract
CdTe thin film (TF) solar cells are most promising photovoltaic (PV) technology in commercial platform. Back contacts and interface defects related opto-electrical losses are still vital to limit its further technological benefit. TF PV cells shallow recombination and parasitic loss lessening purpose carrier selective back contact with band matching window layers are essential. Beside that back and front contact thickness choice is vital for field associated selective carrier collection and generous optical transmission into the active junction of the cell. It can make variation of cell efficiency. Window and front contact layers band edge variation and back contact thickness effect is analyzed by SCAPS-1D simulation software. ZnO and SnO2 front contact for CdS and CdSe window layers effect are numerically studied for 1 μm CdTe thin film PV cell. Significance of materials for front contact and its thickness effect on current density while ZnTe back surface field contact thickness effect on open circuit voltage and efficiency are demonstrated. Finally, ZnO/CdS/CdTe/ZnTe cell of 0.925 V open circuit voltage and 19.06% efficiency has been achieved for 90 nm of ZnTe with Molybdenum (Mo) back contact.

1. Introduction

Renewable energies massive implementation is substantial to promote renewable energy (RE) mix and lessening of climate change effect as it has been urged in latest COP-26. Research achievements and industrially developed solar photovoltaic (SPV) cell efficiency progression is still demanding to make it more client and industrial favor as RE. SPV development pathway currently selective contact (CS) design for less opto-electrical losses is pondered [1]. Industrial affluence Si and CdTe cells least energy payback time was revealed in the study. At present worldwide well-known Si and CdTe PV technologies and their global advancement are also reported by Fraunhofer ISE research institute in 2020 [2]. Affording performance benefits of CdTe cell well-designed back contacts by replacing metal direct contact is robust to lessen minority carrier recombination by enhancing field effect thus open circuit voltage (Voc) is improved. Optical loss lessening purpose transparent conductive oxide (TCO) materials and it thickness selection is potential that can maximize the acceptor–donor carrier accumulation at the junction [3]. However, it was shown to achieve the efficiency level < 16%. Shallow recombination loss lessening drive an electron barrier for CdTe thin film solar cell (TFSC) and proper work function of metal doping is impending for higher fill factor (FF). Moreover, interface shallow depletion area for CdTe is enhanced recombination as a result Voc and FF is minimized. To overcome these difficulties research is going on to adept new design technologies for improvement of back contact electron barrier and majority carrier lifetime to achieve the highest efficiency [4, 5]. Though this design was shown uppermost efficiency but practical efficiency progression is still a challenge. The back ZnTe layer architecture and rapid thermal annealing degraded the CdTe/ZnTe interface in the presence of Cu [6]. Majority carrier lifetime domain CdTe cell back ZnTe barrier effect and doped metal selection is promising. However, CdTe/ZnTe/Cu/Au cell Voc is decreased linearly with increase of annealing temperature to recrystallize interface layer. Cu inter-diffusion towards ZnTe/CdTe interface and lessening of efficiency nearly 16% at Voc = 0.82 V is reported in the topical study [7]. Thus,
ZnTe barrier proper thickness and annealing temperature selection is very essential \[8, 9\]. It may possibly improve device open circuit voltage, interface stability and efficiency. The interface CdZnTe composition is very potential that is typically depending on Zn and Te fraction \[9\] and Cu diffusion impact toward ZnTe \[10\]. Though several researchers are reported on ZnTe diverse sensitivity matters \[8–12\]; typically thin ZnTe buffer is promising once alternative of Cu can be implemented that can avoid diffusion. For this purpose both Copper (Cu) and Molybdenum (Mo) of nearly similar work function metals contact effect is studied. ZnO and SnO\textsubscript{2} as TCOs while CdSe and CdS window layers impact is numerically investigated by SCAPS-1D simulator. The optimized PV cell \(V_{oc} = 0.925\) V and 19.06% efficiency has been achieved.

2. Methodology

Opto-electric design purpose SCAPS-1D simulator based CdTe TF hetero-junction (HJ) developed on solar glass. Initially front TCO, emitter, active absorber, back surface field (BSF) and finally metal contacts were developed. ZnO or SnO\textsubscript{2} as TCOs of thickness 10–50 nm and CdS or CdSe window of thickness 50–100 nm for 1 \(\mu\)m CdTe TF was established. Aim to improvement of electrical performance the ZnTe as BSF with Cu or Mo contact effect was analyzed for diverse ZnTe thickness.

2.1. CdTe HJ model

CdTe PV cell design and development was executed by SCAPS-1D modeling software. It is commonly used for TF solar cells designed. The configuration is fixed for superstrate type cell was arranged by six layers. The transmission of solar light through solar glass then it passes through higher band gap ZnO or SnO\textsubscript{2} as TCO layer, subsequently light interacts with CdS or CdSe window and CdTe absorber layer junction. Finally the majority p-type carrier is collected through ZnTe as back barrier contact layer that also acts as electron reflector. It layout with metal contact layer as it is shown in figure 1.

3. Result and discussion

The SnO\textsubscript{2} and ZnO as front TCO layers thickness effect has been analyzed for CdTe TFPV current density, \(J_{sc}\) and open circuit voltage, \(V_{oc}\) as efficiency parameters. No significant variation of fill factor is realized for SnO\textsubscript{2} and ZnO. However, \(J_{sc}\) is shown to vary in opposite trend with thickness increases and details of it are reported later. However, increasing CdSe and CdS window layer thickness both efficiency parameters like \(J_{sc}\) and FF are shown to reduce. The CdSe and CdS layer 50 nm thickness is optimized and then the variation of TCO layer thickness effect on electrical properties has been studied. The effect of CdSe or CdS is shown trivial though their thickness variation effect is presented vital. The real fabrication process chemical bath deposition (CBD) technique is very promising for CdS \[13, 14\]. Therefore, our study we have mostly investigated the CdS window effects. The band gap of SnO\textsubscript{2} is greater than ZnO and the electron extraction for ZnO is more preferable than SnO\textsubscript{2} due to barrier effect \[15\]. Thickness of back contact layer is vital for field effect, carrier selectivity and conductivity. The external quantum efficiency, current density and \(V_{oc}\) are highly related to the barrier matching contact between metal and CdTe absorber layer. Thus, BSF contact design for electrical performance.
and back metal contact significance is widely explored in this study. P-type ZnTe as buffer for electron reflector and p-type conductive property is most potential to determine the open circuit voltage and efficiency. ZnTe layer of thickness is varied and it effect on CdTe cell Voc and efficiency is studied. The majority carrier collection possibly increases Voc for thinner ZnTe electron barrier. The details of the research are reported below.

3.1. CdTe HJ electrical analysis

The variation of current density of ZnO and SnO2 layers diverse thickness for CdS/CdTe HJ cell is reported. ZnO greater thickness is shown to decrease short current density whereas it is increased with SnO2 layer thickness as it is shown in figure 2. The thinner SnO2 layer lowest Jsc is realized but increasing of thickness it is increasing whereas current density is decreased with increasing ZnO layer thickness. The band gap of SnO2 is higher than ZnO so the transparency of greater thickness of SnO2 comparison to ZnO is obvious. However, Jsc is shown relatively lower for SnO2 layer. The Voc for CdSe in contrast to CdS window for both ZnO and SnO2 TCOs are revealed lower. Due to the band gap and growth associated technological advantage of CdS over CdSe, the study was carrier out using CdS window. The TCOs, diverse windows band gap and Voc of CdS/CdTe HJ is shown below figures 3(a) and (b).

The trend of increasing Voc with increasing ZnO nano layer thickness is shown in figure 3(b). The PN junction device open circuit voltage and short circuit current is related to the below equation (1). Due to ZnO layer the trend of decreasing Jsc is shown

\[
V_{oc} = \left( \frac{E_{g}}{q} \right) - \left( \frac{kT}{q} \right) \left( \frac{J_{omax}}{J_{sc}} \right)
\]

Figure 2. Variation of current density, Jsc with increases of ZnO (a) and SnO2 thickness (b).

Figure 3. Eg versus lattice constant (a) and Voc of CdS/CdTe HJ for ZnO (b).
earlier in figure 2(a) and it is presented to decrease with increasing ZnO thickness. For the consideration of other parameters as fixed, the effect of Jsc can be explained. However, the ZnTe buffer also influences on Voc. It is revealed that the back barrier thickness < 100 nm is better to sensibly increased Voc. It may possibly due to the buffer to adjust the barrier between CdTe and metal back contact as a results increases conduction thus, Voc is increased. But optimized ZnTe layer with diverse metals back contact the Voc and FF is reported from simulator result. The Jsc = 26.87 mA cm$^{-2}$, Voc = 0.924 V, and FF = 76.7% has been shown in figures 2(a), 3(b) and 4(a) respectively. The efficiency of this designed cell is also shown in figure 4 from SCAPS data. Henceforth, the highest 19.06% efficiency is achieved for 90 nm of ZnTe BSF layer. The fill factor and open circuit voltage for diverse thickness of ZnO layer of CdS/CdTe/ZnTe cell is represented to increase with ZnO thickness while the current density is decreased with thickness. Though similar cell configuration the Jsc increasing trend was shown for SnO$_2$ but it was lower than the Jsc of ZnO optimum equivalent thickness as it has been displayed in figure 2.

3.2. CdTe back metal and ZnTe contact effect analysis

Metal work function ($\varphi_m$) is usually greater than the work function of semiconductor. Due to metal contact with absorber semiconductor the electrons from the absorber layer can be tunnelled into the metal thus BSF barrier effect is potential for band bending so electrons moving back from to the active absorber semiconductor.

$$\varphi_B = \varphi_m - \chi$$

(2)

$\varphi_B$ is the barrier height is determined by the metal barrier, $\varphi_m$ and the electron affinity, $\chi$. Two different metals Cu and Mo are applied with ZnTe back contact to study the electrical properties of CdTe solar cell in which Mo is employed as alternative to Cu.

Table 1 shows diverse electrical output of CdTe PV for two different metal metals back contact. As it can be seen from the table 1, Mo work function is slightly greater thus its potential to increase of Voc and efficiency is presented. Mo highest melting point whereas copper high thermal conductivity is attractive. Cu is cheaper and more easily obtainable than Mo. However, Cu composition and interface degradation is well known [6–10]. Mo in real fabrication and its significance was reported [13]. The external quantum efficiency is the determining factor of optical to electrical energy conversion point of view. The significance of ZnTe with Mo metal increases the conversion efficiency at longer edge and it is appreciated to ultimately improve the efficiency. The result of the ZnTe:Mo contact is shown in figure 5.

Table 1. Data for two different metals back contact.

| Metal work function ($\varphi_m$) (eV) | Voc (V) | Jsc (mA cm$^{-2}$) | Fill factor | Efficiency  |
|--------------------------------------|---------|--------------------|-------------|------------|
| Copper (Cu)                          | 4.7000  | 0.919              | 26.00       | 77.24%     | 18.48%     |
| Molybdenum (Mo)                      | 4.7600  | 0.925              | 26.87       | 76.70%     | 19.06%     |

The variation of CdS or CdSe window layers effect is realized trivial to change the efficiency parameters. However, among ZnO and SnO$_2$ thickness variation for CdTe HJ thin film solar cell and ZnTe barrier contact layer thickness effect is realized substantial. Analysis of Voc, Jsc and FF as the efficiency parameters of the cell the best model is finally reported. The model of ZnO/CdS/CdTe/ZnTe cell is shown in figure 6. The data resembles that the p-CdTe majority carrier conduction is increased until certain thickness while minority carrier is...
suppressed to recombine. It is possibly due to the effective band barrier of minority carrier by ZnTe material and this barrier may improve stability using Mo contact. The effective barrier at the back for CdTe solar cell is eventually improved the open circuit voltage. Efficiency of solar cell is depending on Voc, Jsc and FF. Since the back contact barrier layer < 100 nm the majority carrier transport and conduction is supposed to increase thus FF is increased. Declining of current density is one of the limitations of this model. It may have relation with the relatively thinner CdTe cell and front surface recombination velocity. In our model we have investigated it at diverse electron and hole carrier density. The lowest value of density is shown to increase Voc and efficiency.

Figure 5. External quantum efficiency for CdTe cell with ZnTe: Mo contacts (blue-outside) and without ZnTe (green-inside).

Figure 6. Final model of CdTe thin film HJ solar cell with layer thickness and function.

Though front ZnO as TCO and back ZnTe buffer thickness impact is investigated however, CdTe TF solar cell Voc and efficiency further upgrading towards its S-Q limit both surfaces advancement of contacts technologies are desired. Both ZnO and ZnTe have contributed to carrier generation and majority carrier conduction respectively whereas low work function of back metal contact Jsc lessening impact is an impediment [16]. The Mo as back contact and its significance for low cost contact design is also reported very recently [17]. Comparing to the latest literature reports our study the greater Voc and efficiency is realized. This is the main achievements of HJ CdTe TF solar cell in the numerical study.
4. Conclusions

SCAPS Software based CdTe HJ solar cells development and its utmost Voc and energy conversion efficiency is numerically realized. The 90 nm ZnTe BSF buffer effect with Mo metal contact is presented. It is understood to progress CdTe open circuit voltage, Voc = 0.925 V and 19.06% efficiency. The increment of BSF layer thickness results in increased Voc, FF and efficiency. Efficiency upsurge till certain thickness of ZnTe isn’t clear yet however, CdTe cell Voc, FF and efficiency are revealed to increase considerably due to ZnTe BSF contact and ZnO TCO along with CdS window appropriate thickness. In contrast to SnO₂ layer the ZnO nanostructured contact cell better Voc and FF is realized. In order to improve efficiency, TCO and back contact profound design is likely to progress device performance. Compared to Cu, Mo is shown better of electrical output however; back metal contact is granted that the barrier adjustment between CdTe and the metal is vital.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

Declaration

There is no conflict of interest of this submission.

Author’s contributions

Authors of this manuscript have contributed in diverse ways to make it success. One collaborative author from other institutes has contributed significantly to provide efforts for improving content whereas the same institute co-authors have contribution in literature search and figures redrawn.

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