Development of a novel CdTe/ZnS/ZnTe heterojunction thin-film solar cells: a numerical approach

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Abstract

A novel heterojunction structure of cadmium telluride (CdTe)/zinc sulfide (ZnS)/zinc telluride (ZnTe) for thin-film solar cell (TFSC) applications was investigated numerically by Solar Cell Capacitance Simulator in One Dimension (SCAPS-1D). We made a comparative study on the performance of single-layer of Si/CdTe and multi-layers of Si/CdTe/ZnS/ZnTe structures. The optimum values for the thicknesses of CdTe absorber, ZnS, and ZnTe layers in the cell were found to be 2500, 40, and 80 nm, respectively. In the present work, the conversion efficiency ($\eta$) of 21.38% was obtained with open-circuit voltage, $V_{oc} = 1.01$ V, short-circuit current density, $J_{sc} = 29.32$ mA cm$^{-2}$, and fill-factor, $FF = 72.06\%$ in case of multi-layer structure with antireflection coatings (ARCs). The simulation results suggest that the ARC layers presented in this study would be effective to fabricate the high-efficiency solar cells.

1. Introduction

One of the most promising candidates for photovoltaic device applications is the crystalline silicon heterojunction solar cell due to its high efficiency and low cost [1, 2]. In the silicon solar cells, photons in the Sunlight hit the solar panel and are absorbed by silicon substrates. However, the reflection of the incident photons by the silicon surface is a major source of energy loss during photovoltaic conversion [3]. Therefore, there are some challenging issues regarding the performance and reliability of silicon solar cells. To overcome the challenges in the conventional silicon-based solar cells, several researchers have reported semiconductor TFSCs with optical absorber layer and ARC layers [4–7]. Unfortunately, the expansion of manufacturing production has been restricted due to the use of toxic, scarce, and expensive elements in the proposed semiconductor TFSCs [5, 6].

In recent years, CdTe based TFSCs has received much attraction for photovoltaic energy conversion [7–9]. The energy conversion efficiency of the CdTe-based TFSCs was reported to be about 19% [7]. Therefore, it is necessary to understand the optical losses for the reduced conversion efficiency of the CdTe-based solar cells. It has been reported that the optical losses can be minimized by using ARCs in the heterojunction solar cell [10, 11]. In the previous works, ZnS with a wide band gap has been extensively carried out as ARCs in the heterojunction solar cells [12]. It has also been reported that the energy conversion efficiency can be increased by using ZnTe as the ARC layer by 44% [13].

In order to realize the CdTe-based photovoltaic devices, it is necessary to understand the effect of ARC layers on the absorber layer in the heterojunction structures. In the present study, a comparative study on the performance of TFSCs using single-layer and multi-layer with ARCs was made. The heterojunction structure of CdTe/ZnS/ZnTe for solar cell applications was designed, and the performances of the solar cells were studied numerically by SCAPS-1D.

2. Device modelling and simulation

Figure 1 shows the schematic diagrams of heterojunction TFSCs. The SCAPS-1D program was used to simulate the behavior of the solar cell. In this study, the simulation works on single-layer (Si/CdTe) and multi-layer...
structures (Si/CdTe/ZnS/ZnTe) are conducted. In the heterojunction structure, ARC layers with high refractive index materials of ZnS and ZnTe [14] are used for the simulation. In order to measure the reflectance, in this work, the transfer matrix method was also used [15]. The reflectance has been simulated with a single-layer and multi-layer with ARCs on the silicon substrate. In addition, the influences of thickness, working temperature, and defect density on $V_{oc}$, $J_{sc}$, $FF$, and $\eta$ were investigated. The thickness of absorber layer was varied from 50 to 2500 nm, while keeping other material parameters of different layers unchanged. The thicknesses of the ARCs were 40 and 80 nm, respectively. The measurements were simulated in light under the solar spectrum with an incident solar power at a temperature of 300 K. The values of the physical parameters used in this study are summarized in table 1.

### 3. Results and discussion

The simulated reflectance spectra as a function of wavelength of the single-layer and multi-layer with ARCs structures for the solar cells designed in this study are shown in figure 2. The reflection losses were calculated to be 21.15% and 7.60% for the single-layer and multi-layer with ARCs structures, respectively. It is suggested that the optical loss in the heterojunction TFSCs can be minimized by using the ARCs [10, 11].

#### 3.1. Single layer structure (Si/CdTe)

##### 3.1.1. Effect of CdTe layer thickness

Figure 3 shows $V_{oc}$, $J_{sc}$, $FF$, and $\eta$ as a function of the thickness of CdTe absorber layer. The thickness of CdTe layer was varied from 50 to 500 nm. In figure 3(a), $V_{oc}$ was increased as a function of the thickness of CdTe layer. We can see that $V_{oc}$ was almost constant after 200 nm. On the other hand, $J_{sc}$ was increased until 300 nm, and then decreased, as shown in figure 3(b). It can also be seen in figure 3(c) that $FF$ decreased rapidly until 400 nm, and then again increased with increasing the thickness of CdTe. $FF$ of 80.13% was found at 50 nm. We can see in figure 3(d) that $\eta$ increased until 200 nm, and then decreased with increasing the thickness of CdTe. The value of

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**Table 1. Summary of simulation parameters used for SCAPS-1D simulation.**

| Parameters          | Si         | CdTe [16] | ZnS [17] | ZnTe [18] |
|---------------------|------------|-----------|----------|-----------|
| Thickness (nm)      | 100        | 2500      | 40       | 80        |
| Band gap (eV)       | 1.12       | 1.45      | 3.54 [19]| 2.26      |
| Dielectric constant | 11.9       | 9.4       | 8.9 [19] | 10.1      |
| Conduction band-DOS | 1.3E + 19  | 7.5E + 17 | 1.5E + 18| 1.5E + 18 |
| Valence band-DOS    | 7.6E + 17  | 1.8E + 19 | 1.8E + 18| 1.16E + 19|
| Electron mobility   | 5.00E + 1  | 5.00E + 2 | 1.80E + 2| 4.00E + 2 |
| Hole mobility       | 3.00E + 1  | 6.00E + 1 | 5.00E + 1| 5.00E + 1 |
| Donor density       | 0.00       | 1.00E + 16| 1.00E + 19| 1.50E + 20|

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**Figure 1.** Schematic diagrams of heterojunction solar cell structures: (a) single-layer and (b) multi-layers (with ARCs).
\[ \eta \text{ was obtained to be 4.72\% at 50 nm. The thickness of CdTe was optimized to be 200 nm for single-layer structure.} \]

3.2. Multi-layer structure (Si/CdTe/ZnS/ZnTe)

3.2.1. Effect of CdTe layer thickness

Figure 4 shows \( V_{\text{oc}}, J_{\text{sc}}, FF, \text{ and } \eta \) with an increase in CdTe thickness. In figures 4(a), (b), and (d), it was observed that \( V_{\text{oc}}, J_{\text{sc}}, \text{ and } \eta \) are low at lower thickness. These results are due to high recombination of the photo-generated carriers \([20]\). \( \eta \) of 18.77\% was obtained at the absorber thickness of 500 nm, which is greater as compared to that of the single-layer structure. This larger efficiency of the solar cell with ARCs is due to minimization of the optical loss in the solar cell \([10, 11]\). As was described in figure 2, the low reflection loss for the multi-layer structure with ARCs will contribute to the high absorption in solar cells and thus provide high efficiency. It is suggested that the absorption, as well as the efficiency, can be improved by employing the ARCs on absorber layer. The maximum value of \( \eta \) was found to be 21.38\% at thickness of 2500 nm (\( V_{\text{oc}} = 1.01 \text{ V} \),
3.2.2. Effect of working temperature

To understand the performance of the proposed solar cell, the effect of operating temperatures ranging from 300 to 400 K was investigated. Figure 5 shows the cell performance such as \( V_{oc} \), \( J_{sc} \), \( FF \), and \( \eta \) as a function of operating temperature in multi-layer structure. In figures 5(a) and (b), both \( V_{oc} \) and \( J_{sc} \) decreased with increasing temperature. This is due to reverse saturation current which increases with temperature and reduces the saturation current to decrease the open-circuit voltage. It was also found in figure 5(c) that \( FF \) increases linearly with increasing temperature, and then decreases for higher temperature due to light-induced degradation. In figure 5(d), the efficiency was found to be 21.39% at 300 K, and then decreased linearly with increasing temperatures. The effective density of states, electron and hole mobility, and energy band gaps of materials would be affected at a higher temperature. This would result in lower efficiency of solar cells. The energy band gap of materials will be slightly decreased at a higher temperature, thus the electrons would have extensive energy to recombine with holes. As a result, the rate of recombination of electron-hole pairs between the valence and conduction bands is increased. This would enhance the decrease of \( V_{oc} \) and efficiency. On the other hand, at a higher temperature, more free electrons are generated in the conduction band. However, the energy band gap of materials is unsettled at high temperatures. This may lead to an increase in the rate of recombination of electrons and holes during traveling across regions.

3.2.3. Effect of defect density

The simulation results of \( V_{oc} \), \( J_{sc} \), \( FF \), and \( \eta \) as a function defect density of CdTe in multi-layer structure are shown in figure 6. In figure 6(a), the \( V_{oc} \) was almost constant near defect density of \( 1.5 \times 10^{18} \) cm\(^{-3} \), and then decreased with increasing of defect density. In figure 6(b), \( J_{sc} \) was decreased with an increase of the defect density in CdTe. It was also found that the fill-factor was nearly kept constant up to the density of \( 1.5 \times 10^{18} \) cm\(^{-3} \), and then were increased, as shown in figure 6(c). Moreover, in figure 6(d), the efficiency of the solar cell was decreased with increasing defect density. This degradation is due to the localized energy levels created during increasing the defect density. In addition, the defect density would lead to a low number of electron-hole pairs, and hence it reduces the conversion efficiency of solar cells [17]. It is concluded that the performance parameters of the proposed solar cell structures obviously deteriorated with increasing the defect density in CdTe layer, and the corresponding conversion efficiency of the solar cell dropped to 18.69% at \( 1.5 \times 10^{19} \) cm\(^{-3} \).
4. Conclusion

In this work, the heterojunction structure of CdTe/ZnS/ZnTe incorporating the absorber layer of CdTe and ARCs of ZnS and ZnTe for solar cell applications was investigated numerically using SCAPS-1D. It was investigated that the use of ARCs was able to reduce reflection losses of the proposed structure for solar cell applications. It is suggested that ARC layers deposited on the absorber layer would be effective to improve the

Figure 5. Variations of (a) $V_{oc}$, (b) $J_{sc}$, (c) FF, and (d) efficiency as a function of operating temperature in multi-layer structure.

Figure 6. Variations of (a) $V_{oc}$, (b) $J_{sc}$, (c) FF, and (d) efficiency as a function of defect density of CdTe in multi-layer structure.
efficiency. The efficiency of the multi-layer structure with ARCs was found to be 21.38% at the absorber layer thickness of 2500 nm ($V_{oc} = 1.01 \text{ V}$, $J_{sc} = 29.32 \text{ mA cm}^{-2}$, and $FF = 72.06\%$). This result leads us to suggest that the energy conversion efficiency of the heterojunction TFSC can be improved by employing ZnS and ZnTe as alternative promising materials. The optimization of the simulation results investigated in the present study can lead us to suggest that the multi-layer structure with ARCs would be effective to fabricate the high efficiency solar cell applications.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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