



Theoretical analysis of ZnO and ZnO based alloys as front electrode in CdS/CdTe solar cells



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ABSTRACT

ITO has unique properties to be used as front electrode in CdS/CdTe solar cells, however ITO is expensive not abundant and consequently this type of solar cells is still relatively expensive. This work studies the using of ZnO and ZnO based alloys such as ZnO:Sn, ZnO:Al and ZnO:In as alternative materials of ITO in order to develop the efficiency of CdS/CdTe solar cells. Both optical and recombination losses have been taken into consideration. The calculation of optical losses is carried out based on the multiple reflections effect as well as absorption in TCO and CdS layers. Both the front and back surfaces recombination of the CdTe layer are used to describe the recombination losses. It was found that ZnO and its alloys are considered good alternative materials of ITO that used as a front contact in CdS/CdTe cells. The best results were obtained for ZnO:Al, where the calculated short-circuit current density is 22.64 mA/cm² at width of depletion layer of 0.11 μm, the optical and recombination losses are about 27% and the CdS/CdTe efficiency is about 17.9%.

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1. Introduction

For the last decades CdS/CdTe heterojunction based solar cells have been considered as one of the main candidates for large-scale production and application for terrestrial energy production [1,2]. Recently, the highest efficiency for CdTe thin-film solar cells is about 18.3% which also achieved large area module efficiency of 15.3% [3]. Although, this value is still far from the calculated efficiency 28–30% [4,5]. After the optical losses result from reflection at different interference layers in cell, absorption in ITO and CdS layers and recombination losses (front and back) were taken into account, a good agreement between practical and theoretical results were achieved [6–8].

Development the efficiency of CdS/CdTe solar cells is a great goal of scientists in all decades. Despite decades of these developments, solar cells are still relatively expensive. Using indium tin oxide as a front contact in CdS/CdTe solar cell is considered one of the reasons that make solar cells technology is expensive. It is known that, the front contact in CdS/CdTe solar cell is made of transparent conducting oxides (TCO) materials that must be have transmission more than 85% in visible region and sheet resistance

less than 10 Ω/square at room temperature as well as good adhesion to glass substrate [8,9]. Although indium tin oxide (ITO) is considered one of these promising materials, but it is expensive and not abundant. Therefore, ZnO has been actively investigated as an alternative material to ITO because ZnO is non-toxic, inexpensive and abundant material. It is also chemically stable so it is used for the production of solar cells [10–12].

The main objective of this paper is to assess the effects of using ZnO and its alloys such as ZnO:Sn, ZnO:Al and ZnO:In as front electrode on the calculation of CdS/CdTe solar cell efficiency. Both optical and recombination losses will be taken into consideration. The calculation of optical losses is carried out based on the multiple reflections effect and absorption in TCO and CdS layers. Both the front and back surfaces recombination of the CdTe layer are used to describe the recombination losses.

2. Calculation of transmittance using multi-reflections effects

As the photons are incident upon a boundary between materials of different refractive indices, a reflection occurs, known as the Fresnel reflection. For near-normal incidence angles at the boundary, Fresnel Power Reflection Coefficient can be expressed as:

$$R_f = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2} \quad (1)$$

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or in terms of transmittance it may be written as the Fresnel Power Transmission coefficient:

$$T_f = 1 - R_f = \frac{4n_1 n_2}{(n_1 + n_2)^2} \quad (2)$$

where n_1 and n_2 are the refractive indices of the two media.

The total transmittance for L number of layers can be calculated from:

$$T_{\text{tot}} = T_{12} \prod_{j=2}^{L-1} \frac{T_{j,j+1}}{(1 - R_{j,j-1} R_{j,j+1})} \quad (3)$$

which expands to

$$T_{\text{tot}} = 4 \frac{n_1 n_2}{(n_1 + n_2)^2} \prod_{j=2}^{L-1} \frac{4(n_j n_{j+1}/(n_j + n_{j+1})^2)}{\left(1 - \left(\left((n_j - n_{j-1})^2(n_j - n_{j+1})^2\right) / \left((n_j + n_{j-1})^2(n_j + n_{j+1})^2\right)\right)\right)} \quad (4)$$

These calculations can be found elsewhere [13,14]. Fig. 1 shows a four layers structure and a more layers can be assumed by the same way.

When the absorption effect which takes place into TCO and CdS layers is taken into account, the transmission coefficient $T(\lambda)$ can be written in the form:

$$T(\lambda) = T_{\text{tot}} (e^{-\alpha_1 d_1}) (e^{-\alpha_2 d_2}) \quad (5)$$

where $\alpha_1, \alpha_2, d_1, d_2$ is the absorption coefficient and thickness of ITO and CdS layers, respectively. The absorption coefficient is calculated from the following equation:

$$\alpha(\lambda) = \frac{4\pi}{\lambda} k(\lambda) \quad (6)$$

where k is the extinction coefficient of the used materials (TCO, CdS and CdTe). Using the values of optical constant (n, k), the transmission coefficient can be calculated for different TCO materials. The data of n and k of ITO, ZnO, ZnO:Sn, ZnO:Al, ZnO:In, CdS and CdTe are taken from Refs. [15–21], respectively. The extinction coefficient (k) value of glass substrate was taken as $k = 0$, while, the Sellmeier dispersion equation has been applied for calculating the refractive index of glass substrate [22].

Fig. 2a shows the comparison between the calculated transmission of ITO using the present equations (Eqs. (1)–(4)) which take into account the multi-reflections effect (curves 1, 3) and those calculated from Ref. [8] (curves 2, 4). In this figure, curves 1,2 represent the calculated transmission resulting from the reflection from all interfaces (air–glass, glass–ITO, ITO–CdS and CdS–CdTe). While, curves 3,4 represent the calculated transmission due to

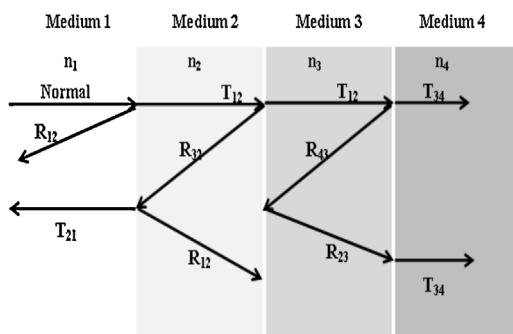


Fig. 1. Diagram of the total transmission of four layers structure due to multi-reflections effect.

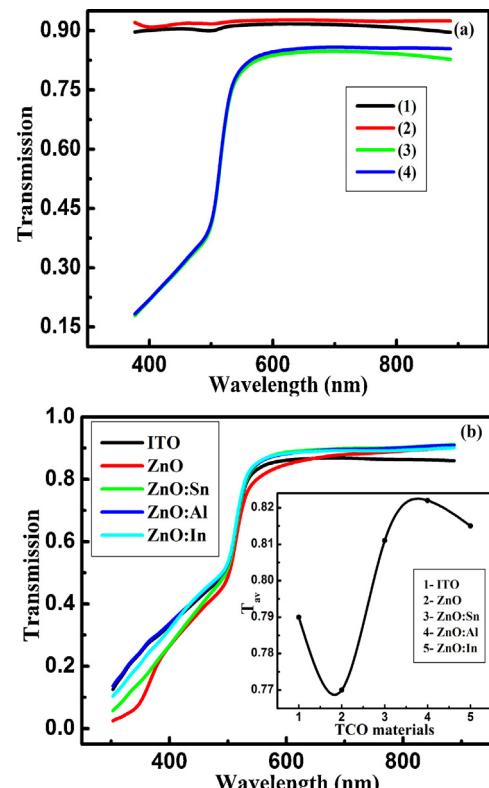


Fig. 2. Calculated transmission of ITO (a) considering only reflection (curves 1,2) as well as absorption (curves 3,4). Curves (1,3) and (2,4) represent the calculated transmission according to Ref. [8] and the current work, respectively. Calculated transmission of different TCOs (b) using the current calculations. The inset figure shows the average transmission (T_{av}) in the wavelength range 500–700 nm for different TCOs.

reflection from all interfaces and absorption into ITO and CdS layers. It is clear that the variation of transmission coefficient with wavelength has the same behavior of both causes. The multi reflections effect leads to slight increase in transmission by a ratio of 1%. Where the average transmission of the current cause is about 81% in the wave length range 500–700 nm, while the transmission coefficient which was calculated in Ref. [8] is about 80%. These values are based on the losses due to reflection and absorption (optical losses).

Fig. 2b shows the calculated transmission spectra (considering Eqs. (1)–(5)) that reach to the absorber layer after passing through glass substrate, TCOs and CdS layers. The transmission of various transparent conducting oxides such as ITO, ZnO, ZnO:Sn, ZnO:Al and ZnO:In is plotted in this figure. It is clear that, apart from the transmission of ZnO all other TSOs have values of transmission greater than the transmission of ITO. This result mainly depends on the optical constants of the used material and hence the conditions of preparation. Therefore any material of them can be used as alternative of ITO material, particularly ZnO:Al that has the maximum average transmission of 82% in wavelength range 500–700 nm as shown in the inset figure.

3. Spectral distribution of quantum efficiency

The total internal quantum efficiency η_{int} of solar cell is the sum of the drift (η_{drift}) and diffusion (η_{diff}) components of quantum efficiency. This quantity is used in calculating the short-circuit current density. The drift component (η_{drift}), which takes into account

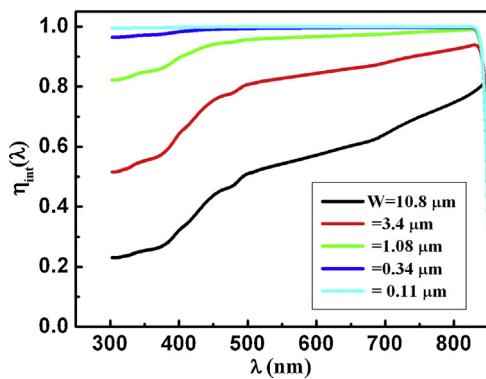


Fig. 3. Total internal quantum efficiency spectra (η_{int}) for different values of space-charge width (W).

recombination at the CdS–CdTe interface (front recombination), is governed by the following expression [5]:

$$\eta_{drift} = \frac{1 + S/D_p \left(\alpha + (2/W) \left((\phi_0 - qv)/kT \right) \right)^{-1}}{1 + S/D_p \left((2/W) \left((\phi_0 - qv)/kT \right) \right)^{-1}} - \exp(-\alpha W) \quad (7)$$

where S is the recombination velocity at the heterojunction interface, D_p is the diffusion coefficient of holes, α is the absorption coefficient of CdTe at a given wavelength, ϕ_0 is the barrier height at the semiconductor side, v is the applied voltage, q is the electron charge and k is the Boltzmann constant.

The dependence of width W of space-charge region (depletion layer) on the concentration of uncompensated acceptors ($N_a - N_d$) is given by

$$W = \sqrt{\frac{2\varepsilon\varepsilon_0(\phi_0 - qv)}{q^2(N_a - N_d)}} \quad (8)$$

where ε is the relative permittivity of the semiconductor and ε_0 is the permittivity of free space. In current calculations, $(\phi_0 - qv)$ is taken as 1 eV, $D_p = 2.5 \text{ cm}^2/\text{s}$, ε is taken as 10.6 and $S = 10^7 \text{ cm/s}$, these values are taken from Ref. [23]. The diffusion component η_{dif} of the internal quantum efficiency, which takes into account recombination at the back surface of the solar cell, is given by the following expression [24,25]:

$$\eta_{dif} = \frac{\alpha L_n}{\alpha^2 L_n^2 - 1} \exp(-\alpha W) \times \left\{ \alpha L_n - \frac{S_b L_n / D_n [\cos((d-W)/L_n) - \exp(-\alpha(d-W))] + \sinh((d-W)/L_n) + \alpha L_n \exp(-\alpha(d-W))}{S_b L_n / D_n \sinh((d-W)/L_n) + \cos((d-W)/L_n)} \right\} \quad (9)$$

where $L_n = (\tau_n D_n)^{1/2}$ is the electron diffusion length, τ_n is electron lifetime, D_n is the electron diffusion coefficient, S_b is the recombination velocity at the back surface of CdTe layer, d is the thickness of CdTe. In the present calculations, $\tau_n = 10^{-9} \text{ s}$, $D_n = 25 \text{ cm}^2/\text{s}$, $S_b = 10^7 \text{ cm/s}$ and $d = 5 \mu\text{m}$. Fig. 3 shows the total internal quantum efficiency spectra (η_{int}) for different values of space-charge width (W). It is clear that η_{int} is strongly dependence on the width of space-charge region and hence on the uncompensated acceptors ($N_a - N_d$). When the space-charge region width is wide, the internal quantum efficiency records low values due to the electric field in the space charge region is weak and then the front recombination is strongly takes place. At narrowing width of space charge region, the internal quantum efficiency represents higher values than the above case. Where the strong electric field prevents recombination of carriers generated near the CdTe surface [26]. Therefore, the values of short-circuit current will be high at small values of the width of space charge region as will be seen in the following section.

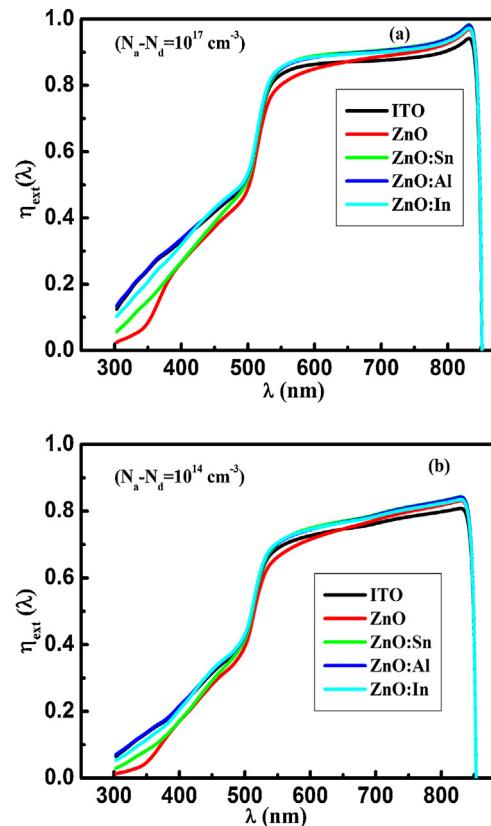


Fig. 4. External quantum efficiency spectra (η_{ext}) for different TCOs at $N_a - N_d = 10^{17} \text{ cm}^{-3}$ (a) and $N_a - N_d = 10^{14} \text{ cm}^{-3}$ (b).

The external quantum efficiency η_{ext} of a solar cell is defined as the ratio of the number of charge carriers that form the photocurrent I_{ph} to the number of photons of a given energy impinging on the solar cell [23]:

$$\eta_{ext} = \frac{I_{ph}/q}{P_{opt}/h\nu} \quad (10)$$

where P_{opt} is the optical power at a given wavelength. Besides, η_{ext} is related to η_{int} according to the following formula [23]:

$$\eta_{ext} = F \cdot T \cdot \eta_{int} \quad (11)$$

where F is the shade factor of the frontal contact and it is taken by unity in these calculations.

Using Eqs. (7)–(9) and (11), the external quantum efficiency η_{ext} of CdS/CdTe cell is calculated and plotted in Fig. 4 for different TCO materials. This figure shows that the response observed below 500 nm is due to the small thickness of CdS (70 nm). This thin layer allows a fraction of photons with energy above its band-gap (2.42 eV) to be transmitted to the CdTe absorber layer, contributing to an increased photocurrent [27]. With further increase in wavelength an increase in η_{ext} is observed. The cutoff wavelength observed at 855 nm corresponds to the cadmium telluride band-gap. One observes that the external quantum efficiency curves for all TCO material are similar in shape and ZnO:Al has the highest value of η_{ext} comparing with other TCO materials in most

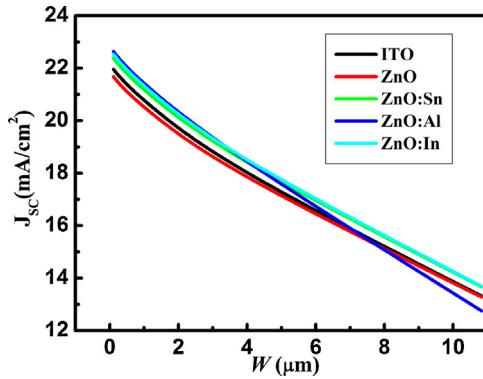


Fig. 5. Short-circuit current density J_{SC} as a function of space-charge width (W) for different TCOs.

wavelength range. When the $N_a - N_d = 10^{17} \text{ cm}^{-3}$ which corresponds to $W = 0.11 \mu\text{m}$ (Fig. 4a), η_{ext} represent higher values than for $N_a - N_d = 10^{14} \text{ cm}^{-3}$ which corresponds to $W = 10.83 \mu\text{m}$ (Fig. 4b).

4. Short-circuit current and cell efficiency

Using Eqs. (5) and (7)–(9) the short-circuit current density can be calculated from the following formula:

$$J_{SC} = q \sum_i T(\lambda_i) \frac{\varphi_i(\lambda_i)}{h\nu_i} \eta_{int}(\lambda_i) \Delta\lambda_i \quad (12)$$

where φ_i is the spectral power density (mW/cm²/μm) and $\Delta\lambda_i$ is the interval between the two neighboring values λ_i . The calculations will be done for AM1.5 solar radiation using Tables ISO 9845-1:1992 (Standard ISO, 1992) [28]. In order to study the effect of reflection losses that are calculated from this work (considering the multi-reflections effect) and those are calculated from Ref. [8], the values of J_{SC} are calculated under the same conditions. According to Ref. [8], J_{SC} records a value of 28.61 indicating that the losses due to this type of reflection are about 8%. When the multi-reflections method is taken into account, the contribution of reflection loss is about 7% where $J_{SC} = 28.86 \text{ mA/cm}^2$. This indicates there is no big difference between the two methods, however the multi-reflections method is more accurate and it will affect on the efficiency of CdS/CdTe solar cell. Fig. 5 represents the short-circuit current density J_{SC} as a function of space-charge width (W) for different TCO materials. It can be seen that J_{SC} strongly depends on the width of space-charge region. At low width, J_{SC} attains its maximum value for all TCO materials. In case of ZnO:Al, the value of J_{SC} is greater than the others TCO materials and this value is about 22.64 mA/cm^2 for $W = 0.11 \mu\text{m}$. Moreover, these results show that the optical and recombination losses are about 27% at the lowest value of the width space-charge region and this ratio is increased to more than 59% at $W = 10.83 \mu\text{m}$ since the calculated current density is 12.75 mA/cm^2 .

5. Current-voltage curve

The I - V characteristic under illumination of CdS/CdTe solar cells can be presented as:

$$J(V) = J_d - J_{ph} \quad (13)$$

where $J_d(V)$ is the dark current density and J_{ph} is the photocurrent density. The dark current density is the sum of the

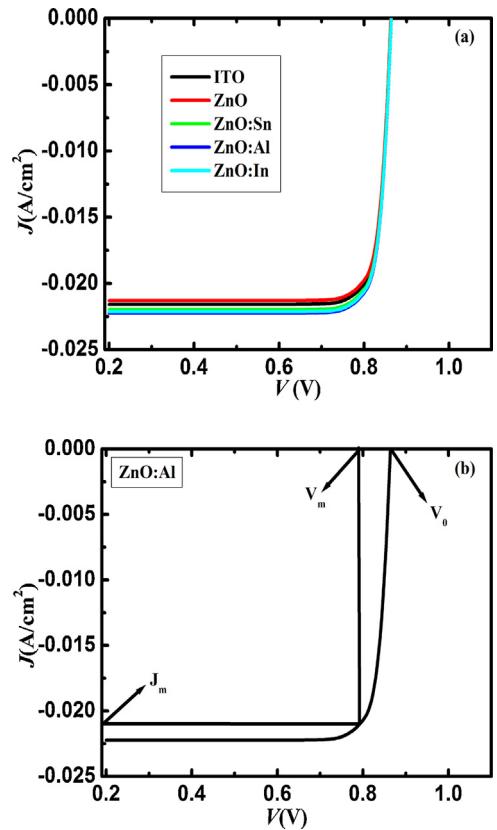


Fig. 6. I - V characteristic for different TCOs (a) and for ZnO:Al (b). Where V_m , J_m and V_0 represents the maximum voltage, the maximum current density and the open circuit voltage, respectively.

generation-recombination current density J_{gr} and the over-barrier current density J_n and can be written in the form.

$$J_d(V) = J_{gr}(V) + J_n(V) \quad (14)$$

More details of calculation J_{gr} and J_n can be found elsewhere [4,5,29,30].

The typical I - V characteristic curve for CdS/CdTe solar cell at different TCO materials is shown in Fig. 6. Some important parameters such as the maximum voltage V_m , maximum current density J_m and open circuit voltage V_0 can be determined from this figure as shown in Fig. 6b for ZnO:Al. These parameters and other related parameters such as cell power density P_{max} ($P_{max} = V_m J_m$) are estimated and listed in Table 1. It is clear that most TCO materials have very close values of open circuit voltage. Besides, the maximum voltage and current density of 790 mV and 21.77 mA/cm^2 is observed for ZnO:Al; and consequently the corresponding maximum power density is 17.2 mW/cm^2 .

The CdS/CdTe solar cell efficiency can be expressed by:

$$\eta = \frac{P_{max}}{P_{inc}} \quad (15)$$

Table 1

The maximum voltage V_m , maximum current density J_m , open circuit voltage V_0 and CdS/CdTe solar output power P_{out} for different TCO materials.

TCO material	V_m (mV)	J_m (mA/cm ²)	V_0 (mV)	P_{out} (mW/cm ²)
ITO	783	20.58	863	16.11
ZnO	774	20.34	860	15.74
ZnO:Sn	787	20.99	864	16.52
ZnO:Al	790	21.77	866	17.2
ZnO:In	787	21.07	864	16.58

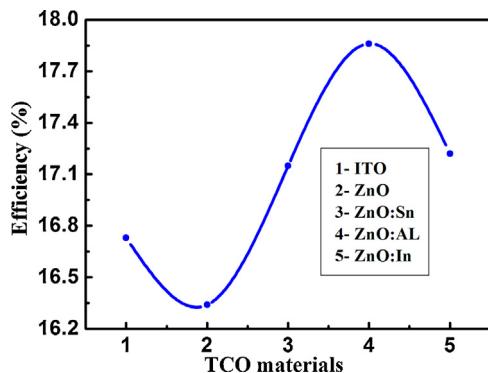


Fig. 7. The efficiency of CdS/CdTe solar cells for different TCO materials as a front contact.

where P_{inc} is the density of the total AM 1.5 solar radiation power over the spectral range $h\nu \geq E_{g\text{CdTe}} = 1.46 \text{ eV}$ equals 96.3 mW/cm^2 [31]. Fig. 7 shows the calculated efficiency of CdS/CdTe solar for different TCO materials. It can be observed, the efficiency of cell is more than 16.5% for all TCO materials that used as front electrodes in these cells. The maximum efficiency of 17.86% is observed for ZnO:AL indicating ZnO or any their alloys can be used as alternative material of ITO.

6. Conclusions

CdS/CdTe heterojunction based solar cells have been considered one of the main candidates for terrestrial energy production. This work represents the theoretical results of using ZnO and its alloys as a front contact in CdS/CdTe solar cell as alternative material to expensive and not abundant ITO. The calculation of optical losses is carried out based on the multi-reflections effect and absorption in TCO and CdS layers. Both the front and back surfaces recombination of the CdTe layer are taken into account to describe the recombination losses. It has been found that using the multi-reflections effect leads to increase the ratio of transmitted light reaching the absorber layer. Both the internal and external quantum efficiency are strongly depending on the width of space-charge region. ZnO and its alloys are considered suitable alternative materials to ITO when used as front electrode in CdS/CdTe cells. ZnO:Al has the maximum short-circuit current density of 22.64 mA/cm^2 at space-charge width of $0.11 \mu\text{m}$ and the corresponding optical (reflection and absorption) and recombination (front and back) losses are about 27%. The efficiency of CdS/CdTe solar cell using ZnO:Al is about 17.9% at certain parameters of absorber layer.

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