Numerical evaluation of grading benefits in CdS/CdZnTe band-gap back graded solar cells

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Recently, incorporation of band-gap graded structure into CdTe absorption layer has been proposed for CdTe based solar cells. In the present work, we numerically investigate the effects of band-gap gradation on photovoltaic characteristics for CdS/CdZnTe band-gap back graded solar cells. Dependences of short circuit current density, open circuit voltage, and conversion efficiency on the grading strength are obtained and analyzed. Moreover, impacts of minority carrier diffusion length of band-gap graded CdZnTe layer on the grading benefits for CdS/CdZnTe back graded solar cells are discussed in detail.

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Keywords: CdS/CdZnTe thin film solar cell, Graded band gap, SCAPS, Photovoltaic characteristics, Minority carrier diffusion length

1. Introduction

Cadmium telluride (CdTe) based thin film solar cells are among the best candidates to achieve higher efficiency and lower cost in photovoltaic application [1, 2]. To have better solar cell efficiency, introducing band-gap graded structure into CdTe absorption layer has recently been proposed for CdTe solar cells [3, 4]. In band-gap back graded case, the additional quasi-electric field due to band gap variation has the potential to increase carrier collection probability and to reduce back surface recombination velocity. An analytical model is then developed to estimate the grading benefit on the photocurrent density in band-gap back graded CdZnTe thin films [4].

Numerical solution of carrier transport equations allows a better control of parameters and a more exact estimation of solar cell performances, as comparing to the analytical method, In the present work, we numerically investigate the effects of band-gap gradation on photovoltaic characteristics for CdS/CdZnTe band-gap back grading solar cells by software SCAPS [5]. Variations of short circuit current density, open circuit voltage, and conversion efficiency with the grading strength are calculated and analyzed. Minority diffusion length L_n is a major transport parameter influencing the carrier collection in the optical absorption layer. Especially in polycrystalline thin films, the values of L_n vary in a wide range, relying on the grain size and material quality. Therefore, influences of minority carrier diffusion length in band-gap graded CdZnTe layer on the grading benefits for CdS/CdZnTe back graded solar cells will also be discussed.

2. Device structure and parameters

The solar cell structure studied here is an *n*-SnO_2/*n*-CdS/*p*-CdZnTe heterojunction solar cell, with a linearly increased band gap towards the back contact in CdZnTe absorption layer. The band-gap grading strength is defined as the maximum band gap at the rear surface of the cell (E_{gmax}). Surface recombination velocities for electrons and holes at the contacts (S_n and S_p) are assumed to be 10^7 cm/s. The other parameters with their baseline values for the CdS/CdZnTe solar cells are summarized in Table 1. All the cells in our simulation are operated at the temperature of 300 K. Fig. 1 depicts the energy band diagram for the CdS/CdZnTe back graded solar cell under equilibrium condition with E_{gmax} = 1.8 eV, corresponding the maximum Zn mole fraction X_{Zn} of 0.2 at the rear surface of the cell. In general, *p*-CdTe and normal metal form deleterious Schottky junction with the barrier height for holes $\Phi_b = \chi + E_g + \Phi_m$ [8], where Φ_m is the work function of the metal. For the case of *p*-$Cd_{1-x}Zn_xTe$, due to the trade-off of decreased electron affinity χ and increased band gap E_g with the Zinc fraction x, the hole barrier height becomes $\Phi_b' = \Phi_b - 0.04x$, which is obtained according to the data in Table 1. In our simulation, the front and back contacts are assumed to be ohmic to examine the pure effects of band gap gradation on the solar cell performances.

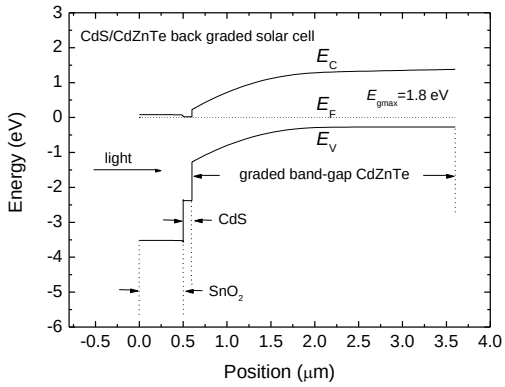

Fig. 1. Energy band diagram of CdS/CdZnTe back graded solar cell under equilibrium condition with the maximum band gap E_{gmax}=1.8 eV at the back contact for CdZnTe.

Table 1. Main parameters with their baseline values in simulating CdS/CdZnTe back graded solar cells at T = 300 K.

Properties	SnO_2 [6]	CdS [6]	$Cd_{1-x}Zn_xTe$
Thickness (μm)	0.5	0.1	3
Energy gap E_g (eV)	3.6	2.4	1.5+0.76x [7]
Dielectric constant ε_r	9	10	9.4+0.3x [6,7]
Electron affinity, χ (eV)	4.5	4.5	4.3-0.8x [7]
Electron mobility μ_n (cm^2/V s)	100	100	320
Hole mobility μ_n (cm^2/V s)	25	25	40
Effective density of states in conduction band N_c (cm^{-3})	2.2×10^{18}	2.2×10^{18}	8×10^{17}
Effective density of states in valence band N_v (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Shallow doping density N_D or N_A (cm^{-3})	N_D, 10^{17}	N_D, 10^{18}	N_A, 5×10^{14}

3. Results and discussion

In this work, band gap E_g, electron affinity χ, and dielectric constant ε_r for band-gap graded CdZnTe layer are position dependent, and other input parameters are assumed to be spatially homogenous, as given in Table 1. The absorption coefficients for CdTe and ZnTe are calculated by using $\alpha = A(h\nu - E_g)$, where $A = 10^5$ $cm^{-1}eV^{-1/2}$. As for $Cd_{1-x}Zn_xTe$, the absorption coefficients are obtained through interpolation method [9], as depicted in Fig. 2. The default illumination condition is AM1.5 spectrum with the light power of 100 mW/cm^2. The carrier generation rate is calculated by using $G(x) = \alpha\Phi_0\exp(-\alpha x)$, where Φ_0 is the incident photon flux from AM1.5 spectrum.

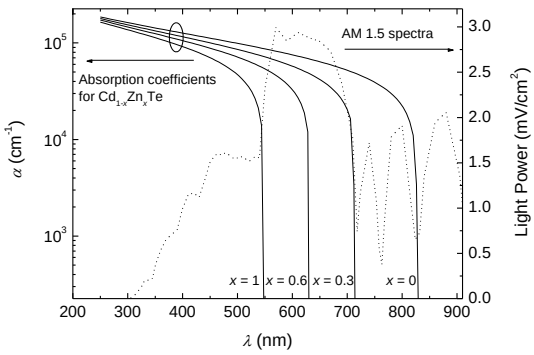

Fig. 2. Absorption coefficients for $Cd_{1-x}Zn_xTe$ with the Zn fraction x equalling 0, 0.3, 0.6, and 1. The dot curve is AM1.5 spectrum profile.

Fig. 3(a) shows the calculated short circuit current density J_{sc} as a function of E_{gmax} for CdS/CdZnTe back graded solar cells with four different values of electron diffusion length L_n in CdZnTe absorption layer. The monotonic decreases of J_{sc} with the increment of grading strength are ascribed to the reductions of optical absorption and subsequent carrier generation rate in the cell due to the lifted band-gap grading in CdZnTe absorption layer [10, 11].

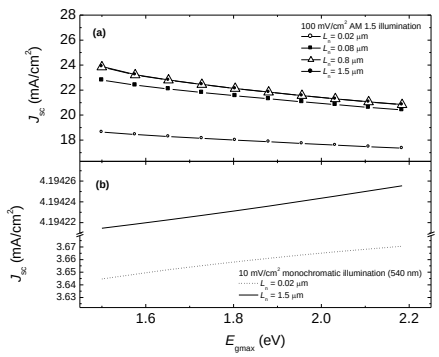

Fig. 3. Dependences of the short circuit current density J_{sc} on the grading strength defined as E_{gmax} in CdS/CdZnTe back graded solar cells. Fig. 3(a) is solar cells with L_n = 0.02 μm, 0.08 μm, 0.8 μm, and 1.5 μm under default illumination. Fig. 3(b) is solar cells with L_n = 0.02 and 1.5 μm under 'constant G(x)' condition.

To verify the above prediction, we introduce a 'constant $G(x)$' condition, in which the loss of $G(x)$ due to the band-gap gradation is eliminated. We assume Φ_0 comes from a monochromatic light centered at 540 nm and ranging from 534 nm to 546 nm, with the light power of 10 mW/cm^2. The photon energy in this spectrum is lower than band gaps of SnO_2 and CdS, but larger than that of CdTe. Meanwhile, α is set to be a constant of 10^5 cm^{-1} for photon energy above CdTe band gap. Thus, the carrier generation rate $G(x)$ keeps the same level when CdZnTe graded cells with different values of E_{gmax} are illuminated. Through the above strategy, the calculated J_{sc} as a function of E_{gmax} for two CdZnTe graded solar cells is given in Fig. 3(b). The gradually increasing of J_{sc} with E_{gmax} in Fig. 3(b) is only provided by enhanced carrier collection by the additional quasi-field associated to band-gap gradation, whereas the increment of J_{sc} as increased E_{gmax} is very weak. Comparing Figs. 3(a) with 3(b), it is seen that the variations of J_{sc} with E_{gmax} depend on a trade-off between the loss of $G(x)$ and the gain in carrier collection. In practice, the reduction of $G(x)$ from band to band absorption exceeds carrier collection increment with increased grading strength if without an effective light trapping, resulting in a lower current output in the solar cell.

As shown in Fig. 3, there is an overall increase of J_{sc} for solar cells with larger values of L_n, The improvement of J_{sc} is marginal when L_n increases from 0.8 μm to 1.5 μm. Moreover, solar cell with lower L_n shows the slower decrease of J_{sc} with E_{gmax}, that is, the increased band-gap grading strength has less negative effect on J_{sc} for solar cells with smaller L_n. In Fig. 3(b), the increase of J_{sc} with E_{gmax} for the cell with L_n = 0.02 μm is more significant than that in the cell with L_n = 1.5 μm, indicating band-gap grading tends to give larger improvement in J_{sc} to the cell with smaller L_n for the 'constant $G(x)$' case.

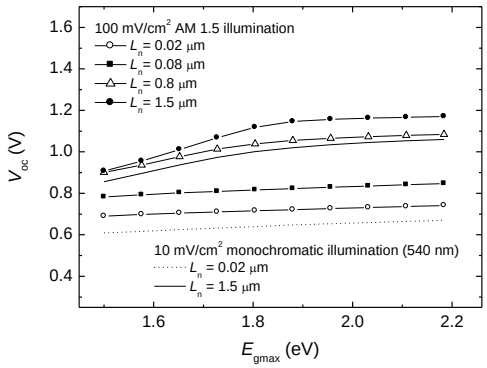

Fig. 4. Dependences of the open circuit voltage V_{oc} on the grading strength defined as E_{gmax} in CdS/CdZnTe back graded solar cells as described in Fig. 3.

With the increased grading strength, the values of V_{oc} increase for all the studied solar cells, as give in Fig. 4. The improvement of V_{oc} with increasing E_{gmax} is ascribed to the enlarged band gap and reduced carrier recombination in the absorption layer due to band-gap grading. In Fig. 4, solar cells with larger L_n exhibit higher V_{oc} for all the values of E_{gmax}. Meanwhile, when E_{gmax} increases from 1.5 eV to 1.8 eV, the improvement of V_{oc} for the largest L_n of 1.5 μm is about 0.2 V, as shown by the solid circles in Fig. 4, and for the smallest L_n of 0.02 μm the rise of V_{oc} is only about 0.02 eV, as depicted by the open circles in Fig. 4. It can be seen the drift field from band-gap variation exerts positive impacts on V_{oc}, particularly for solar cells with larger L_n.

Dependences of conversion efficiency η on E_{gmax} for CdS/CdZnTe back graded solar cells with different values of L_n are shown in Fig. 5. It can be seen solar cells with larger L_n have overall higher η for all the possible E_{gmax}. As given in Fig. 5(a) for L_n = 0.02 μm, η shows a nearly linear increase as a function of E_{gmax}, with the maximum rise of about 0.27% in η. As for the solar cells with L_n = 0.08 μm, 0.8 μm, and 1.5 μm, the optimum E_{gmax} corresponding to the maximum η is not the largest E_{gmax} in simulation, as shown in Figs. (b) to (d). The maximum improvements in η for the just mentioned three solar cells are about 0.12%, 0.5%, and 1% respectively. The decreases of η when E_{gmax} is above the optimum values are ascribed to the loss of optical generation overweighting the carrier collection increment, indicating the improvement of a quasi-drift field on the carrier collection comes to saturation when L_n is large enough. In the 'constant $G(x)$' case, η shows a rise of about 2.2% under maximum grading profile for solar cell with L_n = 0.02 μm. As for the solar cell with L_n = 1.5 μm, the increment of η is around 5.1% when the largest E_{gmax} is applied.

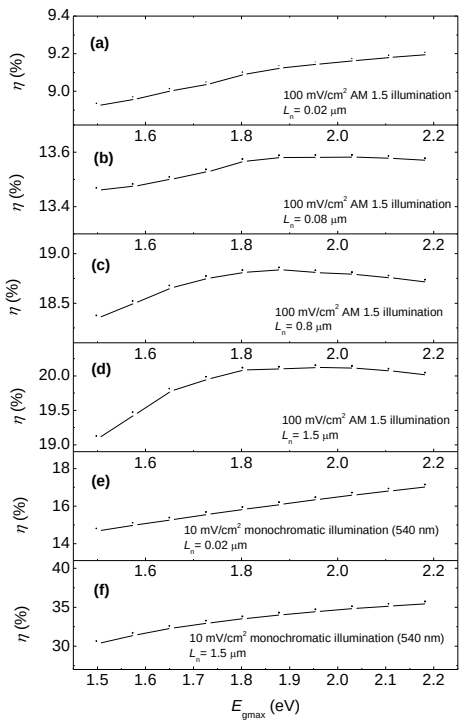

Fig. 5. Dependences of the conversion efficiency η on the grading strength defined as E_{gmax} in CdS/CdZnTe back graded solar cells as described in Fig. 3.

From above results, it is predicted that band-gap grading can improve the conversion efficiency of the cell, and solar cells with larger minority diffusion length in the

absorption layer are expected to have higher efficiency for all the values of grading strength. Whereas, the optimum E_{gmax} is no longer the largest E_{gmax} that can be used, when L_n is large enough that carrier collection ability from the quasi-field by band-gap grading is less significant than the loss of optical absorption due to graded band gap.

4. Conclusion

To evaluate the band-gap grading benefits on the performances of CdS/CdZnTe band-gap back graded thin film solar cells, a numerical investigation is carried out by using SCAPS. Photovoltaic characteristics as a function of the grading strength, including short circuit current density, open circuit voltage, and conversion efficiency, are studied. It can be seen that band-gap gradation can improve the open circuit voltage and power conversion efficiency, whereas causes a reduction of short circuit current density due to the loss of optical absorption from band-gap gradation. As expected, solar cells with larger minority carrier diffusion length in the CdZnTe absorption layer have overall better performances. In this work, solar cell with smallest minority diffusion length shows a slower decrease of short circuit current density and a monotonic increase of efficiency with increased grading strength, which is attributed to the effectively enhanced carrier collection ability by the quasi-field from band-gap gradation.

Acknowledgements

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