ISSN 2347-3487
Volume 12 Number 2
Journal of Advances in Physics

Band Gap Optimization of CdTeSe Thin-Film Solar Cells

Sean Meng[a], Yanfa Yan[b]
a. Lynbrook High School, San Jose, California USA
b. Department of Physics, University of Toledo, Toledo, Ohio USA

ABSTRACT

Device modeling and simulation studies of a CdTeSe thin film solar cell have been carried out. A variety of band-gap profiles, including ungraded, front graded, back graded, and double graded profiles of the CdTeSe absorber layer are examined and their performance characteristics have been analyzed. The calculation reveals that single junction cells with band-gap at the optimum value of 1.38 eV exhibit the maximum performance; alloys of CdTe and CdSe with a ratio of 1:1 forming CdTe0.5Se0.5 achieve the band-gap of 1.38 eV due to the bowing effect. The benefits of the band-gap grading are evaluated when the minimum band-gap is set at the optimum band-gap of 1.38 eV. It is shown that only few graded band-gap profiles exhibit an increase in efficiency, while most of graded profiles reduce performances.

Indexing terms/Keywords

CdTe,CdTeSe, Thin Film, Solar cell, Band gap structures, Band-gap grading

Academic Discipline And Sub-Disciplines

Materials Science, Electrical Engineering

SUBJECT CLASSIFICATION

Physics

TYPE (METHOD/APPROACH)

Simulation and Modeling

INTRODUCTION

Cadmium Telluride (CdTe) has been shown to be one of the most promising absorber materials for producing high-efficiency and low cost thin-film solar cells because of its high absorption coefficient ($\alpha > 10^4$ cm^{-1}) and direct band gap of 1.45 eV, which is well matched to the solar spectrum[1-2]. The recent record efficiency of laboratory size CdTe thin-film solar cells ties the best laboratory size CIGS thin-film solar cells, sparking interest in investigating new materials to work with CdTe[3]. Much information is available in the literature regarding single-junction CdTe solar cells; one common limitation for single band gap CdTe cell is the inability of matching its band-gap to the solar spectrum since one third of photons that have energy lower than its band gap was not utilized, as shown in Figure 1[4].

Change of the absorber band-gap profile to a narrower band gap (< 1.45 eV) materials could improve the spectral response in the long wavelength region, thus enhancing photocurrent. Zdanowicz et al has done the theoretical analysis comparing the maximum efficiency of single junction solar cell with the absorber energy band-gap of semiconductors, and results indicated that the optimum absorber's energy band gap for single junction solar cells is around 1.39 eV[5]. In addition, studies of band-gap grading in Cu(In,Ga)Se2 solar cells have shown that using a non-uniform band-gap grading profile of the absorber, additional fields can be built into p-type based solar cells, which could also enhance performance[6]. Alloying the CdTe with CdSe to form a CdTeSe absorber layer can change the band-gap to the lower band gap due to the bowing effect. Thus, band-gap engineering geared to controlling the composition profiles and spatial distribution of the CdSe content in the absorber layer can lead to enhancing the overall performance of CdTeSe cells. However, despite the promise that CdTeSe holds as a solar cell structure, there has been few research done into the use of CdTeSe as an absorber material of solar cells thus far.

In this study, device modeling and numerical simulations of CdTeSe cells are conducted to analyze the impacts of various band-gap profiles for the absorber layers on the performance characteristics of the cells. Such modeling works provide insight into which band-gap structures may be desired. The study first focuses on the determination of the optimum band-gap corresponding to the maximum efficiency for the uniform band-gap CdTeSe absorber, which is used to establish reference performance. The effect of various graded band-gap profiles on performance are then analyzed and compared against the ungraded reference performance, including the front graded, the back graded, and the double graded.

MATERIALS AND METHODS

Cell structures and simulation parameters

The schematic energy-band diagram for a typical CdS/CdTe solar cell with a uniform band-gap profile is illustrated in Figure 2[7,8]. The CdTe cell structure consists of the following material layers: n-SnO$_2$ (TCO), n-CdS, p-CdTe absorber, and the back contact. This structure is the simplified device structure; it can be modified by taking into account of the possible inter-diffusion layers arising from the cell processing. The cell simulation tool SCAPS (Solar Capacitance

Simulator), developed by the University of Gent, is used by specifying input values as the parameters in each layer of the cell structure[9]. The band-gap of the CdTe absorber is engineered through alloying with other II-VI compounds (CdS and CdSe) to adjust its band gap. The band-gap of these alloys varies with the composition according to this equation:

$$\mathrm{Eg_{alloy}}\,(\mathrm{x}) = \mathrm{xEg_{CdTe}} + (1-\mathrm{x})\mathrm{Eg_{add}} - \mathrm{bx}(1-\mathrm{x}),$$

where b is the bowing factor. In this study, the bowing factors for CdS/CdTe and CdTe/CdSe are 1.8 and 0.75 respectively.

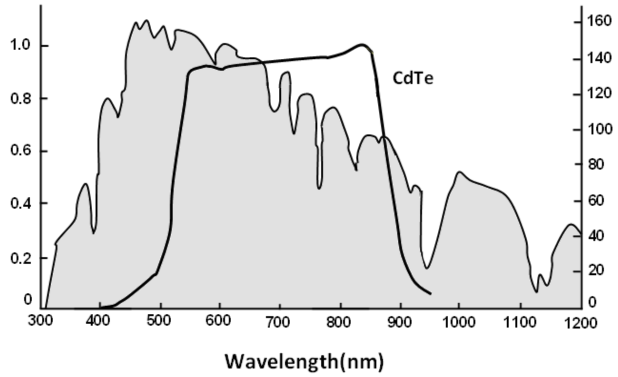


Figure 1 Solar irradiance spectra and spectral response of CdTe

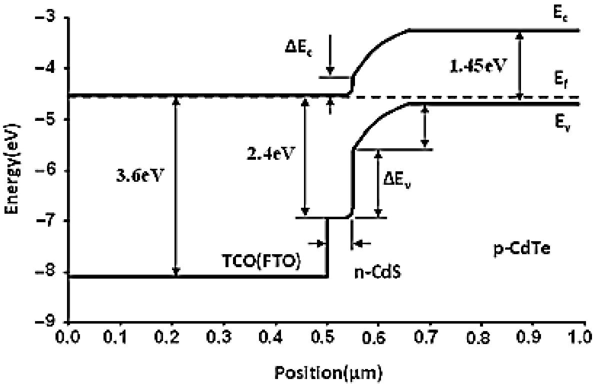


Figure 2 Band diagram of TCO/CdS/CdTe cell

For all simulations in this study, the parameters of FTO (SnO_2) layer and CdS window layer are maintained unchanged. The total thickness of the absorber is maintained at 3µm for all cases. In order to model an effective recombination center, a deep level defect is placed in the middle of the band-gap. The distribution of the energy levels for the defects was set as Gaussian with a characteristic energy of 0.1eV. Table 1 summarizes the basic parameters for the simulation in this study[10-12]. The anticipated changes in the physical properties of the absorber layer include changes in the band-gap, changes in the doping concentration, bulk defect densities, absorption coefficients, and electron affinities.

Table 1 Simulation parameters in this study

	SnO2	CdS	CdTe	CdSe
Thickness (nm)	500	50	varies	varies
Band gap (eV)	3.6	2.4	1.45	1.7
N(donor)	10^{18}	1.1 x10^{18}	N/A	N/A
N(acceptor)	N/A	N/A	10^{12}-10^{15}	10^{12}-10^{15}
Electron Affinity (eV)	4	4	3.9	3.9
Dielectric Permittivity	10	10	9.4	9.4
Defect Density	10^{15}	10^{15}	10^{12}-10^{14}	10^{12}-10^{14}

RESULTS

CdSe has very similar characteristics like CdTe, and CdTe-CdSe forms a series of solid solution alloy $CdTe_{1-X}Se_X$, since selenium has a higher solubility in CdTe[13-19]. Experimental results indicate that the minimum band gap of $CdTe_{1-X}Se_X$ can be as low as 1.32 eV with x ~0.38. The energy band gap of these alloys varies as a parabola with the composition according to this following equation: Eg(x) = 1.70x + 1.45(1 − x) − bx(1 – x), with a bowing parameter b~0.75.

When using wide band materials as absorbers, the light absorption becomes limited only to high energy photons while for those low energy photons (E< Eg) the solar cell practically remains "transparent". This loss of photocurrent collection results in a lower photocurrent of such cell, but wide band gap solar cells do have a higher value of the output voltage of the cell. In contrast, solar cells made of narrow band materials - though capable of absorbing a larger part of solar spectrum - exhibit lower output voltage. This leads to the obvious conclusion that to achieve maximum efficiency for a specified solar spectrum, the absorber material with optimum band gap structure should be realized. Below is the approach of selecting the optimum absorber band-gap for a single junction cell. The current of the illuminated ideal solar cell can be described by a simplified equation:

$$I = I_{sc} - I_{dark} = I_{sc} - I_o\left(e^{\frac{qV}{kT}} - 1\right) \qquad (1)$$

where V denotes cell voltage, and I_{dark} denotes the current flowing through cell without illumination, and I_o is the dark saturation current described by $K_c\, e^{-\frac{Eg}{kT}}$, where Eg denotes the band-gap of cell absorber. I_{sc}, the short circuit current of a cell, is described by the following equation: $I_{sc} = Qq\int_{Eg}^{\infty} N(E)dE$, where N(E) denotes the number of incident photons that have energy in the range of (E+dE), and Q denotes the overall cell quantum efficiency. The maximum output power of the illuminated solar cell corresponds to the point on the current–voltage curve where product of voltage and current reaches maximum value, meaning that d(IV)/dV, must be equal to zero, i.e.:

$$\frac{dP}{dV} = \frac{d(IV)}{dV} = \frac{d\left[\left(I_{sc} - e^{\frac{qV}{kT}} - 1\right)V\right]}{dV} = 0 \qquad (2)$$

which gives an implicit relation from which value of voltage V_m responding to maximum power point may be derived:

$$e^{\frac{qVm}{kT}} = \frac{I_{sc}}{I_o\left(\frac{qVm}{kT} + 1\right)} \qquad (3)$$

By definition, the efficiency of the solar cell is

$$\eta = \frac{P_m}{G_o} = \left(\frac{1}{Go}\right)\left(I_{sc} - I_o\left(e^{\left(\frac{qVm}{kT}\right)} - 1\right)\right)Vm \qquad (4)$$

where P_m denotes the maximum power of the cell and *Go*, defined by $\int_0^{\infty} N(E)EdE$, denotes the value of the total power-solar global irradiance-of the incident photon flux. For q V_m >> kT, Eqs (3) and (4) can be simplified as

$$\frac{qVm}{kT} e^{\frac{qVm}{kT}} = Q\frac{q}{Kc}\, e^{\frac{Eg}{kT}} \int_{Eg}^{\infty} N(E)dE \qquad (5)$$

$$\eta \cong Q\frac{q^2 \int_{Eg}^{\infty} N(E)dE}{\int_0^{\infty} N(E)EdE} Vm \qquad (6)$$

Thus, conversion efficiency η can be calculated in Eq. (6) by taking V_m from numerical solution of the Eq. (5). It is found that under the conditions of AM 1.5, the optimum band-gap of the absorber of a single junction cell is around 1.38 eV. Therefore, for maximized efficiency of CdTeSe solar cells, the optimum absorber's band gap of 1.38eV should be used for the band-gap of the $CdTe_{1-X}Se_X$ uniform absorber, which corresponds to x=0.5, i.e., $CdTe_{0.5}Se_{0.5}$. Figure 3 exhibits the calculated quantum efficiency characteristics for CdTe and CdTeSe cells, showing a significant increase of CdTeSe in the long wavelength regions (>855 nm). The simulated characteristics of CdTe and CdTeSe cells are listed in Table 2. The increase in $J_{SC,}$ due to increasing response at the long wavelength region, combined with the slight decrease of Voc, yields an ~8.5% increase in overall cell efficiency.

Table 2 Simulated performance characteristics of CdTe and CdTeSe thin film cells

	Eg(eV)	η (%)	Voc (mV)	Jsc(mA/cm2)	FF (%)
CdTe (3μm)	1.45	18.54	876	25.5	82.92
CdTeSe (3μm)	1.38	20.12	858	28.46	82.40

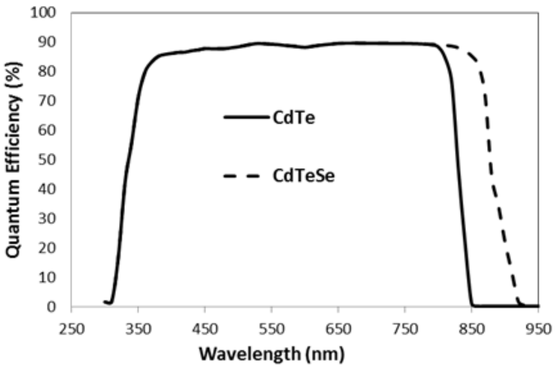


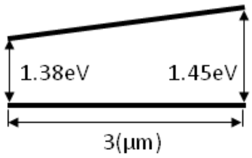
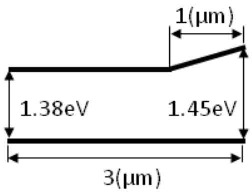
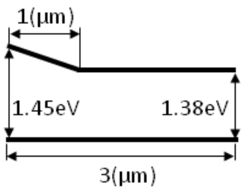
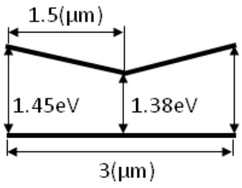
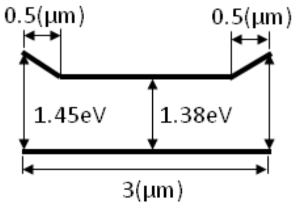
Figure 3 Quantum efficiency of CdTe and CdTeSe cell

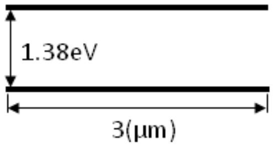
DISCUSSION

In the band-gap profile study of CIGS, the general expectation has been that (a) back grading increases minority carrier collection from the bulk, due to additional drift fields for electrons established in the quasi-neutral region, and (b) front grading leads to higher open-circuit voltage as the band gap in the space-charge region (SCR) expands, while similar current-densities can be maintained. Both approaches are predicted to allow for combinations of Voc and Jsc that are better than those that can be achieved with uniform absorber layers with constant Eg. However, some results reveal that the back, front, and double grading have also been observed to reduce efficiency when simulation parameters or experimental conditions were varied[20]. A simulation study is conducted to evaluate the effect of graded band-gap profiles of the CdTeSe absorber on the performance of the cells. Six graded band-gap profile cases are considered in Table 3. The simulation results for each case yield these performance characteristics: efficiency η(%), Voc, Jsc, and FF, which are reported in columns 3–6 of the table.

The band-gap profiles of Cases 1 and 2 are two back graded cases, where the band-gap increased monotonically toward the back contact (1.38 eV to 1.45 eV). Cases 3 and 4 represent the front graded cases, where the band-gap increased monotonically toward the front junction. In Cases 5 and 6, a double graded band-gap structure is introduced, where the band-gap increased toward both the front and the back of the absorber. The simulated results for uniform $CdTe_{0.5}Se_{0.5}$ is also listed in Table 3, as Case 7, for a reference performance. Comparing with the uniform band-gap reference case, the performance characteristics of all graded profiles in Table 3 (with the notable exception of Case 2) did not demonstrate the better performances that were expected, unlike what most CIGS studies revealed. This lack of improvement is because in

Table 3 Simulated performance characteristics of CdTeSe cells with various absorber band-gap profiles

	Structure	Band-gap profile	η(%)	Voc (mV)	Jsc (mA/cm2)	FF (%)
1	Low Gradient Back Graded		18.59	877	26.38	80.33
2	High Gradient Back Graded		20.57	888	28.15	82.27
3	Low Gradient Front Graded		17.11	906	23.94	78.92
4	High Gradient Front Graded		16.38	879	24.62	75.68
5	Low Gradient Double Graded		16.80	894	24.23	77.56
6	High Gradient Double Graded		18.73	882	27.55	77.02

7	Uniform (CdTeSe Baseline)		20.12	858	28.46	82.40

most CIGS studies, the reference uniform band-gap was generally set to be the band-gap of CIS, 1.04 eV. Since this band gap of 1.04eV is quite narrow compared with the optimum absorber's band gap of 1.38 eV, the cell efficiency is relatively low. Thus, any increases of the band-gap (due to either graded or ungraded band-gap increases) may lead to significant increase in efficiency. The generally expected grading benefits actually come from two parts: the true grading benefits and the contribution of the band-gap increase. In fact, Dullweber *et al.* observed a close correlation in CIGS solar cells between the average Ga-content (the band-gap) and the device performance, independent of the Ga distribution (the graded band-gap)[21]. M Gloeckler *et al.* further indicated that if uniform band-gaps being equal to the graded band-gap minimum are used for comparison to determine the grading benefit, this selection of the reference performance would result in overestimates of efficiency gains attributed to the grading benefit, especially for front and double graded structures where the band gap increases in high recombination regions. Therefore in this study, the optimum band-gap of 1.38 eV is used for the uniform band-gap reference to minimize the contribution from ungraded band-gap increase, as to identify the true grading benefits. As seen in Table 3, only Case 2, the high slope back graded profile provides the true grading benefits to CdTeSe cells.

CONCLUSION

Comprehensive device modeling and numerical simulation studies for CdTe based thin film solar cells have been carried out using the SCAPS simulation program. It is shown that the better performance for CdTe based solar cells can be achieved by alloying CdTe with CdSe forming $CdTe_{0.5}Se_{0.5}$ of which the band-gap approaches to the optimum absorber band-gap of single junction, 1.38 eV. The effect of graded band-gap profiles of absorbers on the performance of CdTeSe cells has been investigated. An approach of selecting and optimizing the graded band-gap profiles corresponding to the maximum performance has been presented.

ACKNOWLEDGEMENT

This work was supported by the Research In Science & Engineering (RISE) program at the University of Toledo, with financial assistance from UT's College of Natural Science and Mathematics and the National Science Foundation.

REFERENCES

i. N. R. Paudel and Y. Yan, "Enhancing the photo-currents of CdTe thin-film solar cells in both short and long wavelength regions." Appl. Phys. Lett. 105, 183510 (2014).

ii. M. A. Green, K. Emery, Y. Hishikawa, W. Warta, and E. D. Dunlop, "Solar cell efficiency tables (Version 44)." Prog.Photovoltaics 22, 701 (2014)

iii. Press release by First Solar, August 5, 2014. http://investor.firstsolar.com/releasedetail.cfm?ReleaseID=864426

iv. B.E. McCandless and J.R. Sites, "Chapter 14. Cadmium Telluride Solar Cells." Handbook of Photovoltaic Science and Engineering, 2nd Edition 2005.

v. T. Zdanowicza, T. Rodziewiczb, M. Zabkowska-Waclawek, "Theoretical Analysis of the Optimum Energy Band Gap of Semiconductors for Fabrication of Solar Cells for Applications in Higher Latitudes Locations." Solar Energy Materials & Solar Cells 87 (2005) 757–769

vi. O. Lundberg, "Band-Gap Profiling and High Speed Deposition of Cu(In,Ga)Se2 for Thin Film Solar Cells." PhD thesis, Uppsala Univ. (2003).

vii. L. Chen, "Random deposition model of CdS layer in CdSs/CdTe thin-film solar cells." M.Sc. thesis, Colorado State University, 2008.

viii. B. A. Korevaar, A. Halverson, J. Cao, J. Choi, C. Collazo-Davila and W. Huber, "High efficiency CdTe cells using manufacturable window layers and CdTe thickness." Thin Solid Films,vol. 535, pp. 229–232, 2013.

ix. M Burgelman, P Nollet, S Degrave, "Modelling polycrystalline semiconductor solar cells." Thin Solid Films 361-362 (2000) 527-532.

x. K. Hsiao, "Electron-reflector strategy for CdTe thin-film solar cells." Ph.D. dissertation, Colorado State University, 2010.

xi. L. Kosyachenko, "Efficiency of thin-film CdS/CdTe solar cells." Solar Energy, R. D. Rugescu, Ed., pp. 105–130, 2010.

xii. J. Sites and J. Pan, "Strategies to increaseCdTe solar-cell voltage." Thin Solid Films, vol. 515, no. 15, pp. 6099–6102, 2007.

xiii. J. Britt and C. Ferekides, “Thin-film CdS/CdTe solar cell with 15.8% efficiency.” Appl. Phys. Lett. 62, 2851 (1993).

xiv. B. A. Korevaar, J. R. Cournoyer, O. Sulima, A. Yakimov, and J. N. Johnson, “Role of oxygen during CdTe growth for CdTe photovoltaic devices.” Prog. Photovoltaics 22, 1040 (2014).

xv. N. W. Duffy, L. M. Peter, and R. L. Wang, “Characterisation of CdS/CdTe heterojunctions by photocurrent spectroscopy and electrolyte electroreflectance/absorbancespectroscopy (EEA/EER).” J. Electroanal. Chem. 532, 207 (2002).

xvi. W. Lane, “A review of the optical band gap of thin film CdSxTe1−x.” Solor Energy Mater. Sol. Cells 90, 1169 (2006).

xvii. B. E. McCandless, G. M. Hanket, D. G. Jensen, and R. W. Birkmire, “Phase behavior in the CdTe-CdS pseudobinary system.” J. Vac. Sci. Technol., A 20, 1462 (2002).

xviii. J. P. Mangalhara, R. Thangaraj, and O. P. Agnihotri, “Structural, Optical and Photoluminescence Properties of Electron Beam Evaporated CdSe1−xTex Films.” Solar Energy Mater., 19, 157-165 (1989).

xix. P. J. Sebastin, “The transport and optical properties of CdSe-CdTe pseudobinary thin films.” Thin Solid Films 245, 132 (1994).

xx. M. Gloeckler and J. R. Sites, “Band-gap grading in Cu(In, Ga)Se_2 solar cells.” Journal of Physics and Chemistry of Solids, Volume 66, Issue 11, 1891-1894

xxi. T. Dullweber, G. Hanna, W. Shams-Kolahi, A. Schwartzlander, M. A. Contreras, R. Noufi, and H. W. Schock, “Study of the effect of gallium grading in Cu(In,Ga)Se_2.” Thin Solid Films 361-362, 478 (2000).