Comprehensive study on CdSe thin film as potential window layer on CdTe solar cell by SCAPD-1D

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Photovoltaics significantly contributes towards the emerging renewable energy drive. Amongst the available thin film solar cell technologies, presently CdTe is leading at commercial state. CdS is being widely used as window layer in CdTe solar cell but challenged with toxicity. Therefore, this project explores the feasibility of CdSe as alternative window layer in CdTe solar cell. The CdSe is optimized to determine the best complete CdTe based solar cell. The study also compares the device performance of proposed CdSe/CdTeSe/CdTe solar cell with other reported CdSe/CdTe and CdS/CdSe solar cells. While degenerating the optimized thickness of CdSe solar cell with respect to different prospective window layer materials, the simulation results reveal that CdTe thickness can significantly reduce, at least by 500 nm, with only 1% reduction in PCE by replacing conventional CdS window layer with CdSe layer. Furthermore, while determining the appropriate Se composition on CdSe\textsubscript{x}Te\textsubscript{1-x} as this layer forms between CdTe and CdSe layer during the fabrication, it has been found that 18% efficiency can be obtained in CdTe solar cell if the stoichiometry of CdSe\textsubscript{x}Te\textsubscript{1-x} can be maintained as CdSe\textsubscript{0.3}Te\textsubscript{0.7} during the device fabrication.

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1. Introduction

With a global drive towards renewable energies, photovoltaics is an increasing part of global energy supply. CdTe is the leading technology amongst thin film solar cells for cost effective solar electricity production, due to its high photovoltaic conversion efficiency (PCE), long-term performance stability, low fabrication costs and short energy-payback time (Green et al. 2017). The current efficiency record for CdTe cells is 22.1%, held by First Solar (Swanson et al. 2017, Green et al. 2015) but still PCE is far from the Shockley-Queisser Limit which is 33%. In state-of-the-art CdTe solar cells, the J\textsubscript{SC} is already close to its theoretical limit (Green et al. 2012).
Increasing the short-circuit current density ($J_{sc}$) is one of the key methods to elevate the performances of photovoltaic devices (Green et al. 2015, Green et al. 2012). Over the past few years, it is suggested that bandgap engineering of CdTe using Se diffusion results higher efficiency than conventional one. Besides that, by increasing the cell photo-response for short and longer wavelength photons will also increases the $J_{sc}$ as well. It is quite obvious that solar cell is a combination of few buildings component apart from the main absorber layer. Tuning those supportive martials’ characteristic properties in achieving better performance than its primitive version is a common practice in photovoltaic technology. Generally, a CdTe solar cell device is composed with glass substrate, charge transferring conductive oxide (TCO), n-type CdS buffer layer, CdTe absorber layer, font and back contact evidently. It is noteworthy to mention that CdS has been nominated as one of the preferable buffer layer from the very beginning of CdTe device architecture. So, improvement of device performance by manipulation of CdS layer seems be an alternative approach. It is already reported that PCE of CdTe solar cell increases when traditional CdS window layer is being replaced by CdS/CdSe window layer stack (Yang et al. 2016a, Yang et al. 2016b).

But window layer like the n-type CdS are used in high-efficiency CdTe solar cells which has a large lattice mismatch of 11% compared to CdTe layer and a bandgap ($E_g$) of 2.4eV. Moreover, interdiffusion occurs at CdS/CdTe interfaces during heat treatment resulting the formation of CdS$_{1-y}$Te$_y$ layer and CdTe$_{1-x}$S$_x$ layer. This results in a shortfall of current density ($J_{sc}$) and open circuit voltage (Voc) compared with conceptual predictions. To overcome this problem, CdSe is used as window layer to replace CdS.

Diffusing CdSe layer in to the CdTe is easier compared to CdS during the CdTe growth and post-processing treatment because of higher solubility of Se into CdTe (Yang et al. 2016a, Yang et al. 2016b, Wei et al. 2000, McCandless et al. 2002, Ohata et al. 1973, Nunoue et al. 1990). Adding a CdSe window layer may absorb photons without contributing to the photocurrent (Paudel, & Yan 2014, Paudel et al. 2015, Tit et al. 2009, Lane 2006). However, it is reported that a graded CdSe$_x$Te$_{1-x}$ layer form during the Se diffusion process in CdTe. This CdSe$_x$Te$_{1-x}$ alloy becomes cubic zincblende structure when 0.6 ≤ $x$ ≤ 1 and changes to wurtzite structure when 0 ≥ $x$ ≥ 0.3 (Belyaev & Kalinkin 1988, Strauss & Steininger 1970, Steininger & Strauss 1972, Bauta 1982). Bandgap tuning occur when there is a change in the Se content. Thus, to improve CdTe solar cells by using Se diffusion, the CdSe$_x$Te$_{1-x}$ alloy need to be understood in term of structure, composition and photoactivity.

This work numerically models the ideal incorporation of CdSe in the CdTe solar cell and validates the improvement of $J_{sc}$ which has been experimentally proven. The study also identifies the ideal stoichiometry of intermediate buffer layer CdSe$_x$Te$_{1-x}$. Finally, the study also compares the device performance of proposed CdSe/CdSeTe/CdTe solar cell with other reported CdSe/CdTe and CdS/CdSe solar cells.

2. Methodology

SCAPS is a one-dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. Marc Burgelman and several researchers have contributed to developing this software. This program simulates the AC and DC electrical characteristics of thin film heterojunction solar cells. Initially, SCAPS focus on developing for CuInSe$_2$ and CdTe family cell structure [24]. However, several extensions have improved its capabilities so that it is also applicable to amorphous (a-Si and microporous Si and crystalline solar cells (Si and GaAs family). This simulation program provides a broad scope of photovoltaic performance parameters and charge carrier such as charge carrier generation and recombination profile, spectral response, $V_{oc}$, $J_{sc}$, FF and PCE can be accurately acquire upon numerical converges.

By using Poisson’s equation, SCAPS can solve the fundamental semiconductor equation for electrons and hole
\[
\frac{d^2 \Psi(x)}{dx^2} = -\frac{e}{\varepsilon_0 \varepsilon_r} \left( p(x) - n(x) + N_D - N_A + \rho_p - \rho_n \right)
\]

(1)

\[
\frac{d \ln n}{dx} = G - R
\]

(2)

\[
\frac{d \ln p}{dx} = G - R
\]

(3)

\[
J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\phi}{dx}
\]

(4)

\[
J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\phi}{dx}
\]

(5)

Here, \( \Psi \), \( e \), \( \varepsilon_r \), \( \varepsilon_0 \), \( N_D \) & \( N_A \) are electrostatic potential, electrical charge, relative permittivity, vacuum permittivity, donor charged impurities and acceptor charged impurities respectively. \( \rho_p \) and \( \rho_n \) are the hole distribution and electron distribution.

Fig. 1 shows three different schematic of CdTe solar cells. The first is a conventional CdTe solar cell structure comprises of a Tin Oxide (SnO) coated glass substrate where a n-type window layer CdS is deposit on top of it and afterwards a p-type absorber layer CdTe. The second and third window layer is change to the n-type CdSe and CdSe\(_{1-x}\)Te\(_{x}\) are emphasized in this simulation to see the effects on \( V_{oc} \), \( J_{sc} \), FF, and efficiency of CdTe solar cell. Table 1 summarized the simulation parameters which are being used.

![Fig. 1. Schematic diagram of CdTe solar cell with CdS, CdSe and CdSe/CdSe\(_{1-x}\) window.](Image)

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<td>2.2x10(^{18} )</td>
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<td>2.2x10(^{18} )</td>
<td>2.2x10(^{18} )</td>
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<td>( NV (1/cm^2) )</td>
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<td>1.8x10(^{19} )</td>
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3. Results

3.1. Optimization CdTe Carrier Concentration and Thickness with CdS Window Layer

In this simulation, we have studied the effect of both absorber layer thickness and carrier concentration on the performance of CdS/CdTe solar cell. This structure has been considered in terms of CdTe absorber and CdS window layer. The carrier concentration of CdS is kept constant at $1 \times 10^{18}$ while for CdTe is varied from $1 \times 10^{13}$ to $1 \times 10^{18}$. The CdS thickness is also kept constant at 50 nm while for CdTe varies from 500 nm to 4000 nm.

Fig 2 (a) represents the impact of carrier concentration and thickness of CdTe layer on Voc. It is evident from the figure that the resulting Voc does not give much impact from increasing the CdTe absorber layer thickness. However, the Voc increases when the carrier concentration increases from its lowest values of $10^{13}$ cm$^{-3}$ to the highest of $10^{18}$ cm$^{-3}$. Equation (4) and (5), establishes the typical relationship between reverse saturation current ($I_0$) and open circuit voltage (Voc) [29-30].

$$I_0 = A n_i^2 \left( \frac{D_e}{L_e N_A} + \frac{D_h}{L_h N_D} \right)$$

(4)

here, $A$ is cross-sectional area of p-n heterojunction, $n_i$ intrinsic carrier concentration, $L_e$ minority carrier diffusion length (electron) in the p-side, $L_h$ minority carriers diffusion length (hole) in the n-side, $D_e$ diffusion coefficient of electron, $D_h$ diffusion coefficient of hole, $N_A$ donor concentration, and $N_D$ acceptor concentration, respectively.

$$V_{oc} = \frac{kT}{q} \ln \left( \frac{I_L}{I_0} + 1 \right)$$

(5)

here, $k$ is Boltzmann constant, $T$ temperature, $q$ electron electric charge, $I_L$ photo-generated current, and $I_0$ reverse saturated current. From the above two equations it is evident that Voc and $I_0$ are inversely related. $I_0$ decreases with the increase of carrier concentration which causes Voc to increase. In this study, the increment in Voc is 50% more when the carrier concentration is increased from $10^{13}$ cm$^{-3}$ to $10^{18}$ cm$^{-3}$. Fig 2(b) shows the effect of carrier concentration absorber layer and thickness on the Jsc for CdS/CdTe solar cell. As the carrier concentration increases, the lifetime of photo-generated electrons is reduced, which results in the decreasing probability of carrier collection and thus, lower Jsc. It can be observed from the figure that, the Jsc keeps decreasing continuously with cumulative increment of carrier concentration and thickness. The highest Jsc is 24 mA/cm$^2$ at $1 \times 10^{14}$ increases from 17 mA/cm$^2$ which is 42% incremental of Jsc at lower carrier concentration and 2500 nm thickness. Carrier concentration of CdTe absorber layer mainly affects the space charge region width, also known as the depletion width, which in turn plays a crucial role in determining the maximum photocurrent density. Depletion width, $W_d$ of a p-n heterojunction diode and theoretically maximum photo-generated current and $I_{plh}$ are given as in equations (6) and (7), respectively [31].

$$W_d = \left[ \frac{2\varepsilon_1\varepsilon_2(V_{bi} - V)(N_A^2 + N_D^2)}{q(\varepsilon_1 N_D + \varepsilon_2 N_A)N_D N_A} \right]^{1/2}$$

(6)

where, $\varepsilon_1$ is the dielectric permittivity of CdS, $\varepsilon_2$ dielectric permittivity of CdTe, $V_{bi}$ built-in voltage, $V$ applied voltage, $N_A$ acceptor concentration, $N_D$ donor concentration, and $q$ electric charge of electron.

$$I_{ph} = qAG(L_e + W_d + L_h)$$

(7)

where, $q$ is the electric charge of electron, $A$ is p-n junction cross-section area, $G$ electron hole pair generation rate, $L_e$ minority carrier diffusion length (electron) in the p-side and $L_h$ minority carrier diffusion length (hole) in the n-side.
The normal thickness of the CdTe layer is about 4000nm. If the performance of solar cell does not decrease with reduced thickness, the deposition time of CdTe layer can also be reduced. Thus, saving the production and material cost, which adds up in large scale manufacturing. Producing a certain material with high carrier concentration requires expensive sophisticated deposition system which reduces defect. However, if the performance of the solar cell does not affect by high carrier concentration, cheaper deposition system can be used. Both material thickness and carrier concentration are important cost reducing factor in PV industry.

The increase thickness of the absorber layer increases both of Jsc and Voc. Thicker p-type region of solar cell which is the absorber, contributes to the electron-hole pair (EHP) generation because it allows the longer wavelengths of the illumination to be collected. Thus, improving the value of Jsc and Voc. It is also understood that if the absorber layer is reduced, both the Jsc and Voc value is reduced. Thin absorber layer makes the back contact nearer to the to the depletion region causing recombination process at the back contact of solar cell. Making the electrons captured easily by the back contact. Thus, the values for Jsc and Voc becomes low because fewer electrons will contribute to the quantum efficiency of solar cell. Fig 2 (c) reveals the FF in carrier concentration from 1x10^{13} to 1x10^{18}. It has been observed that FF has not shown significant improvement with consecutive increment of carrier concentration. The FF lays within the range of 77% to 82% and remains almost constant at higher absorber layer thickness and lower carrier concentration of 1x10^{14} cm^{-3}. It is quite interesting to see that lower thickness and carrier concentration could offer highest FF of 82%. Finally, as shown in Fig. 2 (d), it has been found an unpredictable trend in the PCE as a result of Jsc, Voc, and FF. The PCE happens to be the highest 17% for 2500 nm thickness and 1x10^{15} cm^{-3} carrier concentration. Meanwhile, a 16% PCE is shown at 1000 nm thickness and 1x10^{15} cm^{-3} carrier concentration. So, there is a trade-off between absorber layer thickness and carrier concentration. However, focusing on PCE of the cell, the optimized carrier concentration and thickness of CdTe with respect to CdS window layer are 1x10^{15} cm^{-3} and 2500 nm respectively.
3.2. Optimization CdTe Carrier Concentration and Thickness against CdSe Window Layer

In this fragment of replication, the consequence of together absorber layer thickness and carrier concentration on the photovoltaic presentation of CdSe/CdTe solar cell have been considered for improved judgement. This assembly has been measured in terms of CdTe as absorber and CdSe as window layer in lieu of CdS. The charge carrier volume of CdSe is reserved unchanged at $1 \times 10^{18}$ though CdTe is diverse from $1 \times 10^{13}$ cm$^{-3}$ to $1 \times 10^{18}$ cm$^{-3}$. The CdSe thickness is likewise retained constants at 50 nm when varying from 500nm to 4000nm for CdTe. Fig 3 (a) represents the influence of carrier concentration (CC) and thickness of CdTe layer on Voc with CdSe window layer. It is observed from the figure that the consequential Voc retains growing undeviatingly with growing carrier concentration of CdTe. It is thought-provoking to witness that the highest Voc for any carrier concentration positions around 2000 nm thick CdTe except for the carrier concentration $1 \times 10^{13}$ cm$^{-3}$. Yet, Voc increases when the carrier concentration increases from its lowest values (0.75 V) of $10^{13}$ cm$^{-3}$ to the highest value (1.05%) of $10^{18}$ cm$^{-3}$. The accomplish highest Voc is 50% higher than the lowest value. Fig 3(b) displays the consequence of carrier concentration and thickness of absorber layer on the Jsc for CdSe/CdTe solar cell. For example, as the carrier concentration increases, lower Jsc might be due shorter carrier life time at higher carrier concentration. That’s why the lowest carrier concentration is responsible for the highest Jsc of 23 mA cm$^{-2}$ though the thickness is around 3500 nm. It can be observed from the figure that, the Jsc keeps dipping uninterruptedly with increasing augmentation of carrier concentration. Most of the higher Jsc arise at 2000 nm thickness of CdTe while considering CdSe as buffer layer.

![Graphs showing Voc and Jsc vs. CdTe thickness and carrier concentration](image)

**Fig. 3. Effect of CdTe thickness and carrier concentration with CdSe buffer layer.**

3.3. Optimization of CdSe$_x$Te$_{1-x}$ Diffusion Depth with Se Composition

Recently, CdSe$_x$Te$_{1-x}$ draws researchers’ interest as prospective buffer layer in CdTe solar cell. Infact, a thin CdSe$_x$Te$_{1-x}$ layer forms between CdTe and CdSe layer during the fabrication of CdTe solar cell. As Se is highly reactive, hence efforts were made to identify the suitable
composition of Se and replace the CdSe layer with the CdSe\textsubscript{x}Te\textsubscript{1-x}. Hence, it is essential to identify the ideal stoichiometry of CdSe\textsubscript{x}Te\textsubscript{1-x}. The bandgap for pure CdSe and CdTe are 1.74eV and 1.5eV making the absorption peak at 570 nm and 660 nm respectively \cite{24}. For the ternary CdSe\textsubscript{x}Te\textsubscript{1-x} alloy, the variation of bandgap is as certain to be composited differently. The spectral changes are mainly because for a “light bowing” effect which mainly caused by the nonlinear relationship between the composition and the bandgap of CdSe\textsubscript{x}Te\textsubscript{1-x} alloy. The bandgap value between 1.5eV to 1.74eV is attained with different Se content. For CdSe\textsubscript{x}Te\textsubscript{1-x} alloy semiconductors, the bandgap vs composition can be conventionally compatible with a bowing formula \cite{32}:

$$E_g(x) = (1-x) E_g(CdSe) + xE_g(CdTe) - bx(x-1)$$ (8)

where $b = 0.75$ is the bowing coefficient and the vales of $E_g(CdSe)$ and $E_g(CdTe)$ are 1.74eV and 1.5eV, respectively. Lower Se content between $x = 0.1$ to 0.6 can reduce the bandgap compared to the 1.5eV CdTe as shown in the figure 4, producing higher range of absorption spectrum. The absorber layer edge changes from 660 nm up to 780 nm increasing the absorption range. Even though CdSe/CdTe structure contains selenium, only by changing the ratio Se and Te will allow the bandgap to be tuned.

![Graph showing Se content vs Bandgap (eV)](image)

**Fig. 4. Bandgap CdSe\textsubscript{x}Te\textsubscript{1-x} alloy based on Se fractional content.**

It can lower the bandgap for CdSe\textsubscript{x}Te\textsubscript{1-x} alloy with it being also part of the absorber layer at the front interface leading to higher absorption. Fig. 5 shows the simultaneous effect of Se content in CdSe\textsubscript{x}Te\textsubscript{1-x} alloy and its thickness on the Jsc, Voc, FF and PCE for CdTe solar cell where the carrier concentration has been fixed at 1x10\textsuperscript{16} as optimized from the previous discussion. As per the Figure 5(a), a consistent Voc is observed around 0.94 V when the Se content is 0.5 fraction in the 3500 nm absorber thickness range. No trace of Voc occurs at any thickness before 3000 nm. As a comparison this structure with CdS/CdTe and CdSe/CdTe, the Se content results in a higher Jsc as shown in the Figure 5(b). The result shows that the highest Jsc of 27 mA cm\textsuperscript{-2} occur when the Se content x is at 0.3~0.4 and CdSe\textsubscript{x}Te\textsubscript{1-x} alloy diffuse 0.8 um into the CdTe 4 um absorber layer making its CdSe\textsubscript{x}Te\textsubscript{1-x} layer 0.8um thick and CdTe absorber layer 3.2 um thick. The FF also follow in producing consistent value of 86% at 0.3~0.4 fraction of Se (Fig 5(c)) at 500 nm CdTe thickness. The ultimate photovoltaic performance for this section is shown in Figure 5(d). It is quite obvious that the highest PCE is produced at 0.3~0.4 fraction Se in CdSe\textsubscript{x}Te\textsubscript{1-x} alloy which happens to be in the 500 nm to 1500 nm thickness range.
3.4. Determination of ideal stoichiometry of CdSe$_{x}$Te$_{1-x}$

Fig. 6(a) shows the simultaneous effect of Se fraction in CdSe$_{x}$Te$_{1-x}$ alloy and its thickness on the Voc for CdTe solar cell at 1x10$^{14}$ carrier concentration for comparison. The highest Voc of 0.80 V is seen at 0.5 fraction of Se in the 2000-3500 nm absorber thickness range. It has been noticed that all the corresponding Voc is originated at aforementioned Se content.
The Se content results in a higher Jsc (Figure 6(b)) which is 27 mA cm$^{-2}$ which falls in 0.3 to 0.5 Se fraction. The Jsc decreases as thickness of CdSe$_{x}$Te$_{1-x}$ progressively increases. The highest FF of 82% is also generated at 0.5 Se fraction (Fig 6(c)) between 2500 nm to 3000 nm CdSe$_{x}$Te$_{1-x}$ thickness though lower thickness is also capable of producing very competitive FF. As for an example, a 77% of FF is occurred in 0.1 Se content and thickness lower than 500 nm of CdSe$_{x}$Te$_{1-x}$. The final PV output show has been displayed in Figure 6(d). It is fairly clear from the figure that the maximum PCE of 18% is formed at Se fraction of 0.3 and 1000 nm thickness of CdSe$_{x}$Te$_{1-x}$ blend. As CdSe$_{x}$Te$_{1-x}$ gets thicker, PCE also tends to lower sequentially. Hence, the optimized Se content can be fixed as 0.3 with the stoichiometry CdSe$_{0.3}$Te$_{0.7}$.

3.5. Comparison between CdS, CdSe and CdSe$_{x}$Te$_{1-x}$

The collective quantum efficiency (QE) for the CdS, CdSe and CdSe$_{x}$Te$_{1-x}$ buffer layer in CdTe device architecture has been depicted in the Figure 7. The device with CdS and CdSe buffer layers offer around 64% and 80% EQ in the visible spectrum region. On the other hand, CdSe$_{x}$Te$_{1-x}$ buffer layer shows quite improve QE. The QE reaches to almost 90% with extended absorption till 900 nm due to increasing the absorption range with Se insertion in CdSe$_{x}$Te$_{1-x}$. The alloy shows very outstanding promotion red light response due to lowered surface recombination while increasing response longer wavelength high diffusion length. Meanwhile, proposed CdSe shows a noticeable increment lowering reflection loss and improved diffusion length which ever better in case of CdSe$_{x}$Te$_{1-x}$ alloy.

![Fig. 7. Quantum efficiency for the CdS, CdSe and CdSe$_{x}$Te$_{1-x}$ buffer layer in CdTe device architecture.](Fig. 7)

Table 2 shows the summarization of the photovoltaic output for the CdS/CdTe, CdSe/CdTe and CdSe$_{x}$Te$_{1-x}$/CdTe based solar cells. The current highest PCE of CdTe solar cell is leading by First Solar with Jsc, Voc, FF and PCE of 31.69 mA cm$^{-2}$, 0.89 V, 78.5% and 21.6%, respectively. However, the proposed device architecture of glass/TCO/ CdSe$_{x}$Te$_{1-x}$/CdTe/back contact shows a better enhancement of photovoltaic output with Jsc, Voc and PCE of 27.45 mA cm$^{-2}$, 0.95 V, 86.17% and 22.43%, individually which is about 4% higher than First Solar champion one. So, tuning the bandgap though insertion of Se into CdSe buffer layer prove to be an effective way boost up CdTe device performance.

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<th>Solar cell</th>
<th>Carrier conc. (window layer)</th>
<th>Carrier conc. (Absorber layer)</th>
<th>Absorber thickness (µm)</th>
<th>Selenium content (%)</th>
<th>Jsc (mA/cm$^2$)</th>
<th>Voc (V)</th>
<th>FF (%)</th>
<th>PCE (%)</th>
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</table>
4. Conclusion

In this simulation, we have determined the optimized thickness of CdTe solar cell with respect to different prospective window layer materials. The PCE of 17% has been observed for 2500 nm thickness of CdTe with the carrier concentration of 1x10^{15} cm^{-3} when CdS been used as window layer. On the other hand, 16% efficiency has been found for 2000 nm thick CdTe with carrier concentration 1x10^{16} cm^{-3} when CdSe been used as window layer. Hence, it can be concluded that CdTe thickness can significantly reduce at least by 500 nm with only 1% reduction in PCE by replacing conventional CdS window layer with CdSe layer. Moreover, this study also identifies the suitable Se composition on CdSe_{x}Te_{1-x} as this layer forms between CdTe and CdSe layer during the fabrication. It has been revealed that 18% efficiency can be obtained in CdTe solar cell if the stoichiometry of CdSe_{x}Te_{1-x} can be maintained as CdSe_{0.3}Te_{0.7} during the device fabrication.

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