Influence of SnO$_2$, ZnO and TiO$_2$ layer on the performance of CIGS and CdTe solar cells

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Abstract. As a type electron transmission layer, SnO$_2$, ZnO and TiO$_2$ layer were applied as a buffer between transparent conductive oxide and n-CdS layer in CIGS and CdTe solar cells. J-V curve of device with three different buffer layer were simulated theoretically through Poisson equation and electron-hole continuity equation. Open-circuit voltage, short-circuit current, fill factor and conversion efficiency were derived. It’s shown that for CdTe solar cells, performance of device with three kind of buffer layers SnO$_2$, ZnO and TiO$_2$ did not differ two much. While for the CIGS solar cells, device with TiO$_2$ showed a small fill factor, then leading to a lower conversion efficiency. Transparent oxide SnO$_2$ and ZnO were suggested for the buffer layer for optimization CIGS and CdTe solar structure depending on the art of manufacturing.

1. Introduction

Both the CuIn$_{1-x}$Ga$_x$Se$_2$ (CIGS) based solar cells to with an adjustable semiconductor band gap in the range of 1.04-1.65 eV and CdTe with a band gap of 1.45 eV were most promising commercial thin film solar cells. They both were constructed with a p-type absorption layer (CIGS, CdTe) and an -CdS layer, with back electrode on absorption layer and top electrode on n-CdS layer [1-7].

Thanks to its their energy levels, including both valence band maximum (VBM) and conduction band minimum (CBM), transparent oxide SnO$_2$, ZnO and TiO$_2$ are the three most commonly electron transport layer (ETL) material in thin film solar cells [7-9]. They can transport electrons while block holes efficiently. Then the ETL materials can be applied between the n-CdS and top (transparent conductive oxide) TCO electrode layer (ITO or AZO), which can be a buffer of n-CdS and TCO layer. The SnO$_2$, ZnO and TiO$_2$ can be prepared through chemical method, which is compatible with the CdS deposition.

In this work, by introducing three kinds of buffer SnO$_2$, ZnO and TiO$_2$ between the n-CdS and TCO layer, thin film solar cells with a structure of CIGS/CdS/buffer and CdTe/CdS/buffer were simulated through solving poisson equation and electron-hole continuity equation of semiconductors, the J-V curves of CIGS and CdTe solar cells with three buffers were presented, and four key parameters: open-circuit voltage, short-circuit current, fill factor and conversion efficiency were derived from the plots.

2. Calculations

Parameters of CIGS and CdTe solar cell were obtained from the current-voltage characteristic curve of the battery, which based on the solution of Poisson equation and electron-hole continuity equation. The Possion equation is as following [10]:

\[ \nabla^2 \phi + \frac{1}{\epsilon_e} \frac{Q_{tot}}{\epsilon_e} = \frac{\dot{j}}{\epsilon_e} \]

where \( \phi \) is the electric potential, \( \epsilon_e \) is the permittivity of the material, \( Q_{tot} \) is the total charge, and \( \dot{j} \) is the current density.
\[
\frac{d}{dx} \left( -\varepsilon(x) \frac{d\psi}{dx} \right) = q \left[ p(x) - n(x) + N_d^+(x) - N_a^+(x) + p_i(x) - n_i(x) \right]
\]

And the continuity equations of electron and hole are expressed as following equation (2) and equation (3):

\[
\frac{dp_n}{dx} = G_n - \frac{p_n - p_{n0}}{\tau_n} + p_n \mu_n \frac{d\xi}{dx} - \mu_n \xi \frac{dp_n}{dx} + D_n \frac{d^2 p_n}{dx^2} \tag{2}
\]

\[
\frac{dn_p}{dx} = G_p - \frac{n_p - n_{p0}}{\tau_p} + n_p \mu_p \frac{d\xi}{dx} + \mu_p \xi \frac{dn_p}{dx} + D_n \frac{d^2 n_p}{dx^2} \tag{3}
\]

Where \( \psi \) is the electrostatic potential, \( p_i \) and \( n_i \) are the composite center electron and hole concentration respectively; \( N_d^+ \) is the acceptor like doping concentration of ionization; \( N_a^+ \) is the donor like doping concentration of ionization; \( \xi \) is the electric field; \( p_n \) is the minority carrier (hole) concentration in n-type semiconductor; \( \tau \) is the minority carrier (electron) concentration in p-type semiconducting body. The above parameters are all related to the coordinate position \( x \) of CIGS solar cells. G denotes carrier generation rate, \( \tau \) denotes carrier lifetime, \( \mu \) is carrier mobility, \( \varepsilon \) denotes dielectric constant, \( D \) denotes carrier diffusion coefficient, and \( q \) denotes electron charge.

In this work, both CIGS and CdTe solar cells with an-CdS layer and a p-absorption layer, three kinds of ETL buffer layer SnO\(_2\), ZnO, TiO\(_2\) were introduced between the n-CdS and TCO (transparent conductive oxide) layer. For both CIGS and CdTe solar cells, CdS is n type electron transmission window layer, absorption layer is p type hole transmission layer, transparent oxide SnO\(_2\), ZnO and TiO\(_2\) were applied to as the buffer the. The parameters of CIGS, CdTe and CdS materials in batteries simulations were presented in Table 1.

| Parameter                  | CIGS | CdTe | CdS(n) | SnO\(_2\) | ZnO |
|----------------------------|------|------|--------|-----------|-----|
| dielectric constant        | 13.6 | 9.4  | 10     | 9         | 9   |
| Band gap (eV)              | 1.10 | 1.5  | 2.4    | 3.5       | 3.3 |
| Electron affinity (eV)     | 4.5  | 3.9  | 4.2    | 4         | 4.4 |
| \( N_e \) (cm\(^{-3}\))  | 2.2e18 | 8e17 | 2.2e18 | 2.2e18   | 2.2e18 |
| \( N_v \) (cm\(^{-3}\))  | 1.8e19 | 1.8e19 | 1.8e19 | 1.8e19   | 1.8e19 |
| \( \mu_n \) (cm\(^2\).V\(^{-1}\).s\(^{-1}\)) | 100 | 320 | 100 | 20 | 100 |
| \( \mu_p \) (cm\(^2\).V\(^{-1}\).s\(^{-1}\)) | 25 | 40 | 25 | 10 | 25 |
| \( N_d \) (cm\(^{-3}\))  | 2e16 | 2e14 | 0     | 0         | 0   |
| \( N_a \) (cm\(^{-3}\))  | 0    | 0    | 1e18  | 5e17      | 1e18 |

3. Results and discussion
As the commonly used electronic transmission materials, band of SnO\(_2\), ZnO, TiO\(_2\) and CdS layers were presented in Figure 1. All three kind buffer layers SnO\(_2\), ZnO, TiO\(_2\) can block the hole and facilitate the electrons transmission to the TCO layers.
The current-voltage relationship, electric field distribution, generation and recombination of carriers, carrier lifetime, band structure, free electrons and trapped electrons concentration, defect distribution and other device structures are calculated under the irradiation of AM1.5 standard solar energy spectrum at 300 K at room temperature. Current density (J) under different voltage (V) is simulated.

Plots of J-V for CIGS and CdTe solar cells were presented in Figure 2 and Figure 3. According to the current-voltage (J-V) curve of the battery as shown in Figure 2 and Figure 3, four parameters of the battery, open circuit voltage, short circuit current, fill factor and conversion efficiency, can be obtained from the following equations (4) and (5):

\[
\text{FF} = \frac{I_{mp} \cdot V_{mp}}{I_{oc} \cdot I_{sc}}
\]

\[
\eta = \frac{I_{mp} \cdot V_{mp}}{P_{in}}
\]
Where FF and η denote the fill factor and conversion efficiency, respectively. ImP and VmP denote the current and voltage values at the maximum power point, and Pin denotes the incident power.

Jsc is the intersection of J-V curve and J axis, and open circuit voltage (VOC) is the intersection of curve and V axis. VmP is the current and voltage at the maximum power point of the battery. The short circuit current (ISC) and current at the maximum power point of the battery (ImP) are related to Jsc and the Jmp as following equation (6):

\[ I = J \cdot \sigma \]  

(6)

Where I is the current and J is the density of current, σ is the area of solar cell.

![Figure 3. J-V for CdTe solar cells with SnO\textsubscript{2} or ZnO or TiO\textsubscript{2} layers.](image)

The four parameters Voc, Jsc, FF and η of CdTe and CIGS were listed in Table 2.

**Table 2.** Voc, Jsc, FF and η parameters of CdTe and CIGS with SnO\textsubscript{2} or ZnO or TiO\textsubscript{2} layers.

| Parameter | CIGS | CdTe |
|-----------|------|------|
|          | SnO\textsubscript{2} | ZnO | TiO\textsubscript{2} | SnO\textsubscript{2} | ZnO | TiO\textsubscript{2} |
| Voc (V)   | 0.61 | 0.61 | 0.61 | 0.87 | 0.87 | 0.87 |
| Jsc (mA/cm\textsuperscript{2}) | 34.46 | 33.71 | 34.13 | 24.8 | 24.46 | 24.8 |
| FF (%)    | 77.856 | 79.4 | 57.33 | 76.21 | 72.9 | 76.18 |
| η (%)     | 16.44 | 16.39 | 11.95 | 16.46 | 15.57 | 16.46 |

And we can see that for the CIGS solar cell with lower bandgap of 1.1eV, the Voc of cells with three different SnO\textsubscript{2} or ZnO or TiO\textsubscript{2} layers differ litter, the Jsc differ not too much. While for the FF, the solar device with TiO\textsubscript{2} layer is much worse than that of SnO\textsubscript{2} and ZnO. It’s indicated that for the CIGS solar cells, both SnO\textsubscript{2} and ZnO may be good choice for the buffer layer of TCO and n-CdS layer, depending on the compatible art of the manufacturing. The bandgap of absorption layer played a key role on the Voc of solar cells, the band gap 1.1eV is too low, and should be increased through Cu(In\textsubscript{x}Ga\textsubscript{1-x})Se \textsubscript{x} value. For the CdTe based solar cells, parameters of solar cells with SnO\textsubscript{2} or ZnO or TiO\textsubscript{2} layers did not differ too much. Solar cells with SnO\textsubscript{2} and TiO\textsubscript{2} were with the exactly the same properties. Then for the ITO substrates, SnO\textsubscript{2} is the good choice for buffer layers.
4. Conclusions
Based on Poisson equation and electron-hole continuity equation, the current-voltage curve (J-V) characteristics of copper-indium-gallium-selenium (CIGS) and CdTe based solar cells under normal temperature illumination were simulated, and the four key parameters open-circuit voltage, short-circuit current, filling factor and efficiency were analyzed. The simulation is based on buffer layer between TCO and n-CdS layer. Calculations show that for CdTe solar cells, performance of device with three kind of buffer layers SnO$_2$, ZnO and TiO$_2$ did not differ two much. While for the CIGS solar cells, device with TiO$_2$ showed a small fill factor, then leading to a lower conversion efficiency. In summary, transparent oxide SnO$_2$ and ZnO were suggested for the buffer layer of TCO and n-CdS layer for optimization of CIGS and CdTe solar structure depending on the art of manufacturing.

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