Exploring the Potential for High-Quality Epitaxial CdTe Solar Cells

Tao Song\textsuperscript{1}, Ana Kanevce\textsuperscript{2}, and James R. Sites\textsuperscript{1}

\textsuperscript{1}Department of Physics, Colorado State University, Fort Collins, CO, 80523, USA
\textsuperscript{2}National Renewable Energy Laboratory, Golden, CO, 80401, USA

Abstract — Traditional polycrystalline CdTe solar cell performance is limited by recombination at the grain boundaries, low carrier density (\(p\)), compensation from impurities, and a low minority carrier lifetime (\(\tau\)). The maximum values for these critical parameters in polycrystalline devices are \(p < 10^{15} \text{ cm}^{-3}\) and \(\tau \sim 10 \text{ ns}\) with open-circuit voltage (\(V_{\text{oc}}\)) \sim 900 \text{ mV}\) and \(\eta \sim 20\%\). Epitaxial CdTe with high-quality, low defect-density, and high carrier density could yield a higher-efficiency PV device. Using numerical simulation, we investigate the combined effects of minority carrier lifetime \(\tau\) (0.1 – 500 ns) and carrier density \(p\) (\(1 \times 10^{14} – 5 \times 10^{18} \text{ cm}^{-3}\)) on device performance, predicting obtainable performance of \(V_{\text{oc}} > 1100 \text{ mV}\) and \(\eta > 25\%\) for high \(\tau\) and high \(p\). While the \(V_{\text{oc}}\) is strongly affected by both \(p\) and \(\tau\), the short-circuit current (\(J_{\text{sc}}\)) is mainly dependent on the lifetime \(\tau\) and absorption losses in the front contact stack. In addition, increasing the thickness of p-CdTe (varied from 0.5 – 20 \(\mu\text{m}\)) at different \(\tau\) (1 – 100 ns) shows an improvement in \(J_{\text{sc}}\) due to increased long-wavelength photon collection and then saturates for thicker p-CdTe. In some cases, the cell performance is compromised by the presence of a significant back-contact barrier \(\phi_b\). The simulated results show that the cell performance is not strongly affected until \(\phi_b\) exceeds 0.4 eV.

Index Terms — device modeling, solar cells, epitaxial CdTe.

I. INTRODUCTION

Although existing device models [1], [2] provide general support for the need to increase values of the carrier density \(p\) and minority carrier lifetime \(\tau\), they have not provided specific parameter requirements for efficiencies > 20\% in CdTe. In this paper, an expanded range of both \(p\) and \(\tau\) is included in numerical simulation to estimate the maximum device performance achievable with a high-quality epitaxial CdTe structure with improved material characteristics. The effects of absorber thickness and back-contact barrier are also taken into account. The primary goal of the device modeling here is to provide guidance for optimizing the device design for MBE-grown CdTe and to help interpret experimental data from non-ideal materials.

II. DEVICE STRUCTURE AND MODELING

The baseline structure used in this model is shown in Fig. 1(a). It differs from the traditional superstrate structure of polycrystalline CdTe solar cells, and it consists of 50-nm-thick ZnO window layer, 50-nm-thick n-type CdTe buffer, and 3-\(\mu\text{m}\)-thick p-type CdTe absorber.

![Fig. 1. (a) Device structure for epitaxial CdTe solar cell used as a baseline in the model. (b) Simulated energy band diagram at equilibrium with \(p = 5 \times 10^{16} \text{ cm}^{-3}\).](image)

Numerical simulations were performed with the software package AFORS-HET v2.4.1 (Helmholtz Zentrum Berlin, Berlin, Germany) [3]. Most of the electronic parameters are based on [4], and Table I lists the specific parameters crucial to the simulations presented here. Fig. 1(b) shows the energy band diagram at equilibrium with the absorber carrier density \(p = 5 \times 10^{16} \text{ cm}^{-3}\) for the baseline case. The n-type CdTe layer has a high minority carrier lifetime of 100 ns and, since it is a homojunction device, there is no conduction-band offset at the n-/p-type CdTe interface. The back contact barrier is assumed to be as low as 0.2 eV and 5\% of incident light is assumed to be reflected at the front contact. The primary variations among the cases analyzed happen in the absorber layer. The carrier density in the absorber is varied for over 4 orders of magnitude, from \(10^{14}\) to \(5 \times 10^{18} \text{ cm}^{-3}\). The minority carrier

<table>
<thead>
<tr>
<th>Layers</th>
<th>Thickness [nm]</th>
<th>(n, p \text{ [cm}^{-3})]</th>
<th>(N_{\text{DG}}, N_{\text{AC}} \text{ [cm}^{-3})]</th>
<th>(\sigma_e \text{ [cm}^2)]</th>
<th>(\sigma_h \text{ [cm}^2)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnO</td>
<td>50</td>
<td>(n: 1 \times 10^{18})</td>
<td>(D: 1 \times 10^{19})</td>
<td>(1 \times 10^{-16})</td>
<td>(1 \times 10^{-14})</td>
</tr>
<tr>
<td>n-type CdTe</td>
<td>50</td>
<td>(n: 1 \times 10^{17})</td>
<td>(A: 1 \times 10^{12})</td>
<td>(4 \times 10^{-13})</td>
<td>(1 \times 10^{-12})</td>
</tr>
<tr>
<td>p-type CdTe</td>
<td>varies</td>
<td>(p: \text{varies})</td>
<td>(D: \text{varies})</td>
<td>(1 \times 10^{-13})</td>
<td>(1 \times 10^{-14})</td>
</tr>
</tbody>
</table>
lifetime $\tau$ is also varied over a wide range, from 0.1 to 500 ns, which is achieved by the variation of the defect density in the absorber. In addition, when analyzing the impact of the absorber thickness, the thickness is varied from 0.5 to 20 $\mu$m while setting $p$ to $5 \times 10^{16}$ cm$^{-3}$. And assuming the back-contact barrier is adjusted through varying the work function of the metal contact.

III. RESULTS AND DISCUSSIONS

Since the carrier density $p$ and minority carrier lifetime $\tau$ for a poly-crystalline CdTe device are in a relatively low range, here we expand the range to include parameters reasonable for epitaxial single-crystal CdTe to investigate the combined effect of $p$ and $\tau$. In addition, by varying the thickness of $p$-type CdTe absorber, we can estimate how thick an absorber is needed to achieve optimal performance. It is also common to obtain a significant back-contact barrier in practical CdTe cells. Therefore, the effect of back-contact barrier is considered as well.

A. Combined Effect of Carrier Density and Lifetime

The combined effects of a wide range of minority carrier lifetime $\tau$ and carrier density $p$ on device performance are first calculated with numerical simulation. Fig. 2 shows the results with contour plots for the primary performance parameters as a function of $p$ and $\tau$.

![Contour plots of $V_{oc}$, $J_{sc}$, FF, and $\eta$ for simulated device parameters as a function of carrier density $p$ and lifetime $\tau$ in the absorber. Note that the blue-colored diamond and circle represent the efficiency of the First Solar, Inc. (FSLR) 2013 record CdTe cell [5] and a target efficiency for epitaxial CdTe.](image)

In Fig. 2(a), the open-circuit voltage $V_{oc}$ is expected to increase with higher carrier density and longer minority carrier lifetime. In the region where a low carrier density and minority carrier lifetime exist, the high defect density will increase the recombination rate in the space-charge region (SCR) and quasi-neutral region if the absorber is not fully depleted. The short-circuit current $J_{sc}$ in Fig. 2(b) shows a different trend: $J_{sc}$ suffers a loss at high carrier density when lifetime is short. This is true at high carrier density, but for $p < 5 \times 10^{15}$ cm$^{-3}$, $J_{sc}$ is almost independent of lifetime. Fig. 2(c) shows that FF is higher in the region with high $p$ and $\tau$. Therefore, the overall device efficiency will also be highest for high carrier density and long lifetime.

As shown in Fig 2(b), there is $J_{sc}$ loss at high carrier lifetime in the low lifetime region (0.1-10 ns). From the simulated QE with varying $p$ at two fixed low lifetimes ($\tau = 1$ and 10 ns), it is observed that $J_{sc}$ loss for high $p$ is primarily from the loss of long-wavelength photo-generated carriers. Because of a longer path length, there is more long-wavelength QE loss with increasing $p$ at $\tau = 1$ ns. Since the space-charge region (SCR) narrows while the carrier density $p$ in the absorber is comparable to the n-type buffer ($p = 1 \times 10^{17}$ cm$^{-3}$), the more photo-generated carriers with short lifetime will recombine in the quasi-neutral region where there is not an electric field to assist carriers collection.

![QE for two fixed lifetimes $\tau = 1$ ns and 10 ns, and varying carrier density $p$: $1 \times 10^{14}$ - $1 \times 10^{18}$ cm$^{-3}$.](image)

The absorber carrier density $p$ and minority carrier lifetime $\tau$ of the First Solar, Inc. (FSLR) 2013 record poly-crystalline CdTe cell were published by Gloeckler et al. [5]. We have included the FSLR parameters in the model and compared the performance of the modeled device with the experimental record cell. Here we assumed that the other material properties for the FSLR CdTe cell are the same as our simulated cells and did not include interfacial recombination. Reasonable parasitic effects were included ($\phi_b = 0.4 \text{ eV}$, $r = 1.5 \Omega$, $R_{sh} = 1000 \Omega$, and 2% reflection to match FSLR’s $J_{sc}$). Table II lists the performance parameters for the FSLR record cell, simulation of a similar cell, and a projected epitaxial CdTe cell.

<table>
<thead>
<tr>
<th>Cells</th>
<th>$p$ (cm$^{-3}$)</th>
<th>$\tau$ (ns)</th>
<th>$V_{oc}$ (mV)</th>
<th>$J_{sc}$ (mA/cm$^2$)</th>
<th>FF (%)</th>
<th>$\eta$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FSLR</td>
<td>$6 \times 10^{14}$</td>
<td>10-15</td>
<td>872</td>
<td>28.0</td>
<td>78.0</td>
<td>19.0</td>
</tr>
<tr>
<td>Simulated</td>
<td>$6 \times 10^{14}$</td>
<td>10</td>
<td>880</td>
<td>27.6</td>
<td>78.0</td>
<td>18.9</td>
</tr>
<tr>
<td>Projection</td>
<td>$5 \times 10^{16}$</td>
<td>100</td>
<td>1010</td>
<td>26.0</td>
<td>87.2</td>
<td>22.9</td>
</tr>
</tbody>
</table>

* $\phi_b = 0.4 \text{ eV}$, $r = 1.5 \Omega$, $R_{sh} = 1000 \Omega$, and Refl. reduced to 2%.
After taking parasitic effects into account, the simulation shows a very similar performance to the FSLR record cell. The epitaxial CdTe with low defect density should be able to achieve a higher range of carrier density (~5×10^{16} cm^{-3}) and lifetime (~100 ns) and thus obtain a conversion efficiency of 23%.

B. Thickness Effect of p-type CdTe Absorber

CdTe has a large absorption coefficient, and most of the light generation occurs in the first micron of the CdTe absorber. In practice, thin polycrystalline CdTe devices (1–2 µm) have been made with relatively little compromise in efficiency at the University of Toledo [6]. However, the question is whether a high-quality epitaxial thin CdTe device could achieve higher performance with modest V_{OC} and/or J_{SC} loss. In this section, Fig. 4 shows simulated device performance of varying the absorber thickness (0.5 – 20 µm) at four different minority carrier lifetime (1, 10, 100 ns) while setting p fixed at 5×10^{16} cm^{-3} for high carrier concentration.

![Fig. 4. Simulated device performance of varying the absorber thickness from 0.5 to 20 µm with τ = 1, 10, and 100 ns and p = 5×10^{16} cm^{-3}.](image)

For short lifetimes and low diffusion lengths, V_{OC} improves only slightly with increasing absorber thickness. For τ = 1 ns, V_{OC} improves slightly as the thickness increases over a few microns and then saturates. For higher lifetimes, there is a greater increase in V_{OC} up to 3 µm. This increase is due to a lower Shockley-Read-Hall (SRH) recombination rate in the quasi-neutral region rather than in the SCR. The SCR width for p = 5×10^{16} cm^{-3} is narrow, ~200 nm, and thus has less effect on the V_{OC} loss compared to the much thicker quasi-neutral region. Fig. 4(b) shows that J_{SC} for short lifetime increases significantly for the first 2 microns where most photon collection takes place, and then becomes saturated. For longer lifetime cases (10 and 100 ns), however, J_{SC} shows greater improvement with thicker CdTe absorbers, primarily due to a longer diffusion length and lower defect recombination in both the SCR and bulk regions. In Fig. 4(c), FF for all lifetime cases shows a modest increase with absorber thickness. The efficiency η in Fig 4(d) increases as the absorber thickness increases to 3 µm, then shows little change except for the very high lifetime case. The analysis here indicates that there is in general little benefit from increasing the absorber thickness above 5 µm unless the lifetime is significantly greater than 10 ns.

These simulations assumed a very high recombination velocity S_n = 10^7 cm/s at the back contact. Note that at τ = 100 ns, both V_{OC} and J_{SC} still increase slightly even with 20-µm-thick CdTe absorber. However, if the back surface recombination is lower, V_{OC} and J_{SC} will vary less with thickness, especially for thinner devices. Fig. 5(a) & (b) show how V_{OC} and J_{SC} change when S_n is varied from 10 to 10^7 cm/s for τ = 100 ns. In Fig. 5(a), the impact of the first few microns (<3 µm) on V_{OC} is much greater with lower S_n (= 10 cm/s) than with high S_n. This is due to fewer photo-generated carriers diffusing to the back surface and recombining when S_n is lower. V_{OC} at S_n = 10 cm/s decreases with increasing absorber thickness, because carriers recombine to a greater extent in the thicker bulk region. At high S_n, however, V_{OC} increases with the absorber thickness, as the back contact becomes less of a factor. For thick CdTe, V_{OC} converges to the same value for all values of S_n.

![Fig. 5. Simulated V_{OC} and J_{SC} for varying p-CdTe thickness with the back surface recombination velocity S_n = 10, 10^3, 10^5, 10^7 cm/s at τ = 100 ns.](image)

In Fig. 5(b), J_{SC} increases over the first few microns (<3 µm) due to greater photon absorption. At high S_n (= 10^7 cm/s) and thin CdTe, a significant fraction of the electrons reach the back surface and recombine. There is less electron recombination loss for thicker CdTe (>10 µm) at the back surface and high S_n, thus an increase in J_{SC}. J_{SC} with low S_n has greater variation over the first few microns compared to the J_{SC} with high S_n, but also saturates for thicker cells as the effect of back surface recombination diminishes.

C. Back-contact Barrier Effect

CdTe is a p-type semiconductor with a high electron affinity (χ = 4.3 eV) and high band gap (E_g = 1.5 eV). Most metals do not have a sufficiently high work function and the CdTe/metal
contact can form a blocking Schottky back-contact barrier $\phi_b$ that may affect both the FF and the $V_{OC}$ [7]. To investigate its effect on the epitaxial CdTe cells, the back-contact barrier is varied from 0.2 to 0.8 eV (see Fig. 6), the thickness and carrier density of the CdTe absorber are taken to be 2 µm and $5 \times 10^{16}$ cm$^{-3}$, respectively, and the back surface recombination velocity $S_n = 10^5$ cm/s.

Fig. 6. Simulated energy-band diagram for varying back-contact barrier $\phi_b$ (0.2 - 0.8 eV) at equilibrium. $\phi_b$ is varied by adjusting the work function of metal.

Fig. 7 shows the simulated device performance for varying back-contact barrier ($\phi_b = 0.2 - 0.8$ eV) at three lifetimes ($\tau = 1, 10, 100$ ns). In Fig. 7(a), $V_{OC}$ is not affected by increasing $\phi_b$ for barrier heights below 0.4 eV. Above 0.4 eV, however, hole blockage and enhancement of electron recombination current begin to dominate the forward diode curve and reduce FF and $V_{OC}$ [7].

Fig. 7. Simulated device performance ($V_{OC}$, $J_{SC}$, FF, and $\eta$) vs. back-contact barrier at three lifetimes ($\tau = 1, 10, 100$ ns).

In Fig. 7(b), there is a slight $J_{SC}$ reduction with increasing barrier for all three lifetimes. Note the $J_{SC}$ gap between 1 ns and 10 ns (or 100 ns) is primarily due to shorter diffusion length and lower defect recombination in the absorber. In Fig. 7(c), FF begins to decrease when $\phi_b$ is greater than 0.4 eV and the voltage is less. Overall, the efficiency shows a strong decreasing trend with back-contact barrier above 0.4 eV.

IV. SUMMARY

In this paper, the device performance for high-quality epitaxial CdTe solar cells has been investigated by expanding the ranges of both carrier density $p$ and minority carrier lifetime $\tau$. High $V_{OC}$ above 1000 mV should be achievable when the absorber has a high carrier density ($> 5 \times 10^{16}$ cm$^{-3}$). However, superior device performance with $\eta > 25\%$ requires both high carrier density and lifetime. Simulated variations in the thickness of CdTe absorber show that the efficiency improvement for thicker absorbers with high $S_n$ is due to enhancement of both $J_{SC}$ and $V_{OC}$. However, the variations above 3 µm are modest when the back-contact recombination is relatively small. In addition, the cell performance is little affected with a modest back-contact barrier (0.2 - 0.4 eV). When it exceeds 0.4 eV, however, there is performance loss in both $V_{OC}$ and FF, due to enhancement of the electron recombination current and limitation to hole current.

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REFERENCES