Impact of Interface Recombination on Time Resolved Photoluminescence (TRPL) Decays in CdTe Solar Cells (Numerical Simulation Analysis)

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Impact of Interface Recombination on Time Resolved Photoluminescence (TRPL) Decays in CdTe solar cells (Numerical Simulation Analysis)

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***Abstract* — Using Sentaurus Device Software, we analyze how bulk and interface recombination affect time-resolved photoluminescence (TRPL) decays in CdTe solar cells. This modeling analysis could improve the interpretation of TRPL data and increase the possibility of rapid defect characterization in thin-film solar cells.**

By illuminating the samples with photons of two different wavelengths, we try to deduce the spatial origin of the dominant recombination loss. Shorter-wavelength photons will be more affected by the interface recombination and drift compared to the longer ones. Using the two-wavelength TRPL characterization method, it may be possible to determine whether a specific change in deposition process has affected the properties of interface or the bulk of the absorber.

***Index Terms* — carrier lifetime, CdTe, interface recombination, numerical simulations.**

I. INTRODUCTION

Increase in CdTe production requires rapid characterization of the absorber layers and devices. TRPL measurement is a contactless and quick method to determine the carrier lifetime in the CdTe absorbers. However, when TRPL is measured on devices, the complex carrier dynamics, including drift, diffusion, and recombination, affects the decay shape [1-3]. Which of these processes dominates the decay depends on the device properties (doping, mobility, defect density in the CdTe absorber and at the heterointerface) and on the measurement conditions (illumination wavelength and intensity), making its interpretation challenging. Despite the complex carrier dynamics, several studies have shown a correlation between the slope measured in TRPL decay and the device's V_{oc} [4, 5]. Here we concentrate on distinction between interface and bulk recombination from a TRPL measurement.

Figure 1 shows a simulated band diagram of a CdTe device and generation profiles due to light pulses with wavelengths of 635 nm and 808 nm. For typical doping levels of CdTe cells, 10^{13} cm^{-3} to 10^{15} cm^{-3}, most of the light is absorbed within the depletion region. According to the CdTe absorption coefficients measured at the National Renewable Energy Laboratory (NREL) [6], the 635 nm wavelength illumination generates 3.3 times more carriers next to the CdS/CdTe interface. Thus, the TRPL decay generated from this illumination is expected to be more influenced by interface recombination compared with 808 nm decay.

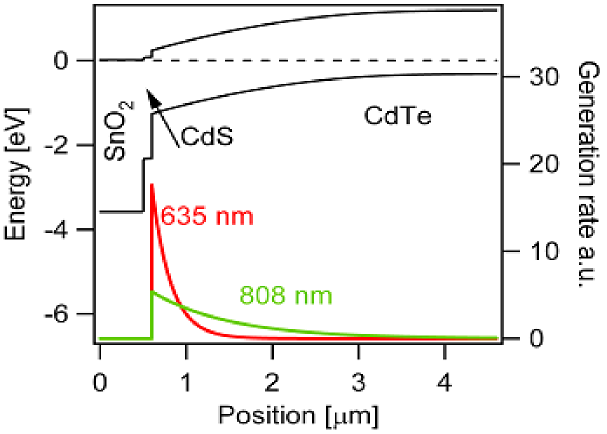

Fig. 1. Simulated band diagram and generation profiles for λ = 635 nm and 808 nm.

Figure 2 shows an example of measured and simulated carrier decays for the two excitation wavelengths. The bi-exponential decays have been observed experimentally and reported in the literature [4, 7, 8].

The lifetime values determined from the slope of the decay curve will be marked with a subscript m (the faster part of the decay will be marked with τ_{1m} and the slower with τ_{2m}), and usually have values different from τ_i determined from the defect density. The bi-exponential nature of the decay is pronounced for λ_1 = 635 nm (red line in Fig. 2), where the difference between the lifetimes derived from the faster (τ_{1m}) and slower part of the decay (τ_{2m}) is large.

In this case (635 nm illumination), more carriers are generated close to the junction where the electric field is the strongest, and many of them are separated very quickly. Since for most devices the drift is faster than diffusion and recombination, one can expect electron-hole pairs generated by short wavelengths to be quickly swept by the electric field and not give accurate information on recombination rate. We have shown elsewhere how different components of carrier dynamics affect the TRPL decay of a typical CdTe cell [2]. For λ_2 = 808 nm, the difference between τ_{1m} and τ_{2m} is much smaller, and the decay appears more single-exponential.

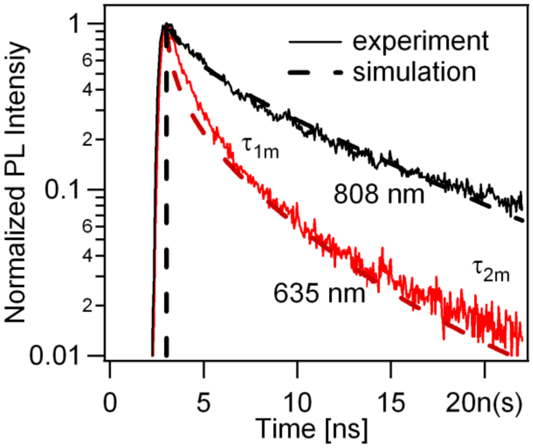

Fig. 2. Experimental and numerically simulated TRPL decay for two excitation wavelengths. The decay is measured at 840 nm with excitation through junction.

II. MODEL

The modeling was performed with Sentaurus Device software [9]. The parameters used in the simulation are described in detail elsewhere [2]. The model consists of three layers: CdTe, CdS, and SnO_2. CdTe layer is 4 µm thick, CdS layer is 100 nm, and SnO_2 layer is 500 nm. The doping in CdTe layer is taken to be 10^{14} cm^{-3}. The Shockley-Read-Hall recombination in the absorber is defined through Gaussian distribution of defects centered on the middle of the bandgap. The carrier lifetime is derived from the defect density and equals to $\tau_i = (N_t \sigma v_{th})^{-1} = 2.5$ ns, unless stated otherwise. Here N_t is the trap density, σ is the capture cross section, and v_{th} is the carrier thermal velocity.

The sample is illuminated with a short monochromatic light pulse (0.2 ps and 250 kHz), and the electron and hole densities are calculated after the light pulse is turned off. The illumination intensity is $P_l = 0.25$ mW, generating $n_l = 3x10^{15}$ cm^{-3} electron/hole pairs in CdTe next to the heterointerface. The radiative recombination rate, proportional to the product of electron and hole densities (n*p), is calculated. It is assumed that the TRPL intensity is proportional to this rate.

To compare how the slope from the TRPL decays is connected to the device's V_{oc}, the current-density voltage (J-V) curves with same variation of parameters were simulated, where the monochromatic illumination was replaced with an AM1.5 spectrum illumination [10].

III. RESULTS AND DISCUSSION

In the TRPL analysis, the actual decay is often approximated with a double exponential. Although most of the decrease in the PL signal occurs in the first, faster part of the decay, we have shown that this part of the decay is dominated by charge separation in the CdTe [2] and not by recombination.

Now we will analyze how the nonradiative recombination rate in the CdTe layer, at the CdTe/CdS interface, and their combination affect both the TRPL decay and devices V_{oc}. Figure 3 shows simulated TRPL decays for illumination wavelengths of a) 635 nm and b) 808 nm for 3 different defect densities in CdTe layer, creating lifetimes τ_i of 1.25 ns, 2.5 ns, and 6.25 ns. In Fig. 3a, both parts of the bi-exponential decay for the 635 nm illumination are affected by the recombination in the CdTe, although the slower part, τ_{2m}, varies significantly more with variation of CdTe defect density. The variation in τ_{2m} from the simulated TRPL decay for both wavelengths 635 nm and 808 nm is comparable, because the defect density is assumed to be uniform throughout the absorber. To compare the TRPL decays with device performance, the J-V curves of devices with equivalent parameters were simulated. As an illustration, the impact of τ_i on the V_{oc} is shown in Figure 3c. The lifetime variation between $\tau_i = 1.25$ ns and $\tau_i = 6.25$ ns is expected to increase the V_{oc} by 70 mV.

Next we will analyze how the interface recombination affects the TRPL decay and the V_{oc}. Figure 4a shows TRPL decay for illumination with both wavelengths (635 nm and 808 nm) for two interface recombination velocities, S = 100 cm/s and S = 10^5 cm/s. The bulk lifetime is kept at $\tau_i = 2.5$ ns. In a case of 635 nm illumination, more carriers are generated next to the heterointerface, and thus the decay in this case is significantly more affected by the recombination at the interface. In addition, one can see that interface recombination has a stronger influence on the slower part of the decay, where τ_{2m} is deduced. The V_{oc} dependence on the interface recombination velocity is shown in Figure 4b. The change of interface recombination velocity from 10^5 cm/s to 100 cm/s increased the V_{oc} for 40 mV.

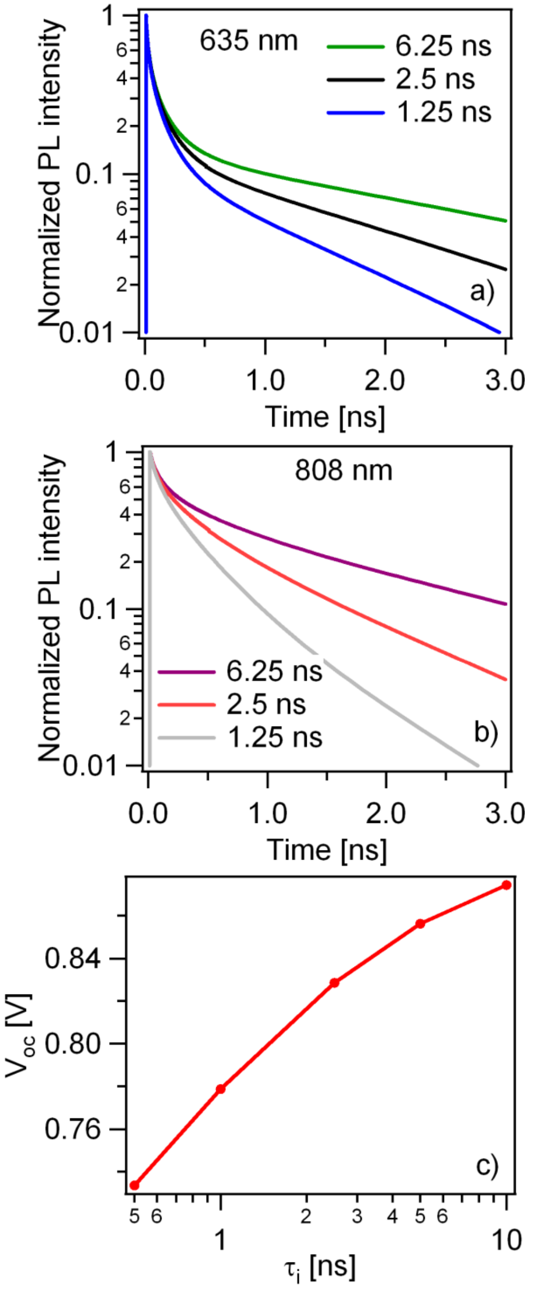

Fig. 3. Simulated carrier decays for three values of τ_i: 1.25 ns, 2.5 ns, and 6.25 ns, for a) 635 nm, b) 808 nm, and c) simulated V_{oc} as a function of τ_i.

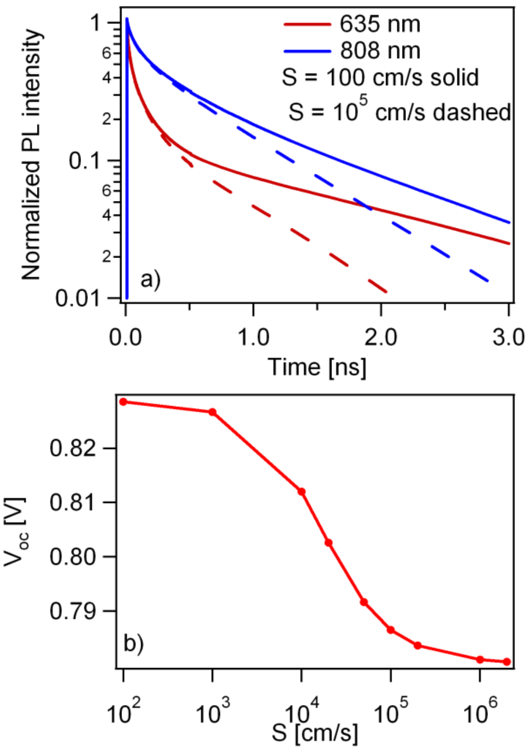

Fig. 4. a) Simulated TRPL decays for an interface recombination velocity equal to 100 cm/s (solid) and S = 10^5 cm/s (dashed) and wavelengths of 635 nm (red) and 808 nm (blue); b) The impact of interface recombination velocity on V_{oc}.

To visualize the carrier dynamics we have plotted the calculated product of electron and hole density as a function of position at 11 different times during the carrier decay (Figure 5). In the 635 nm illumination case (Fig. 5a and b), during the fast part of the decay (the first 0.5 ns or the first 6 curves in the plots) the n*p product is reduced only slightly due to interface recombination. (For example, at t = 0.1 ns, n*p at x = 0.6 μm, is 4.14 x 10^{29} cm^{-6} for S = 100 cm/s and 3.63 x 10^{29} cm^{-6} for S = 10^5 cm/s.)

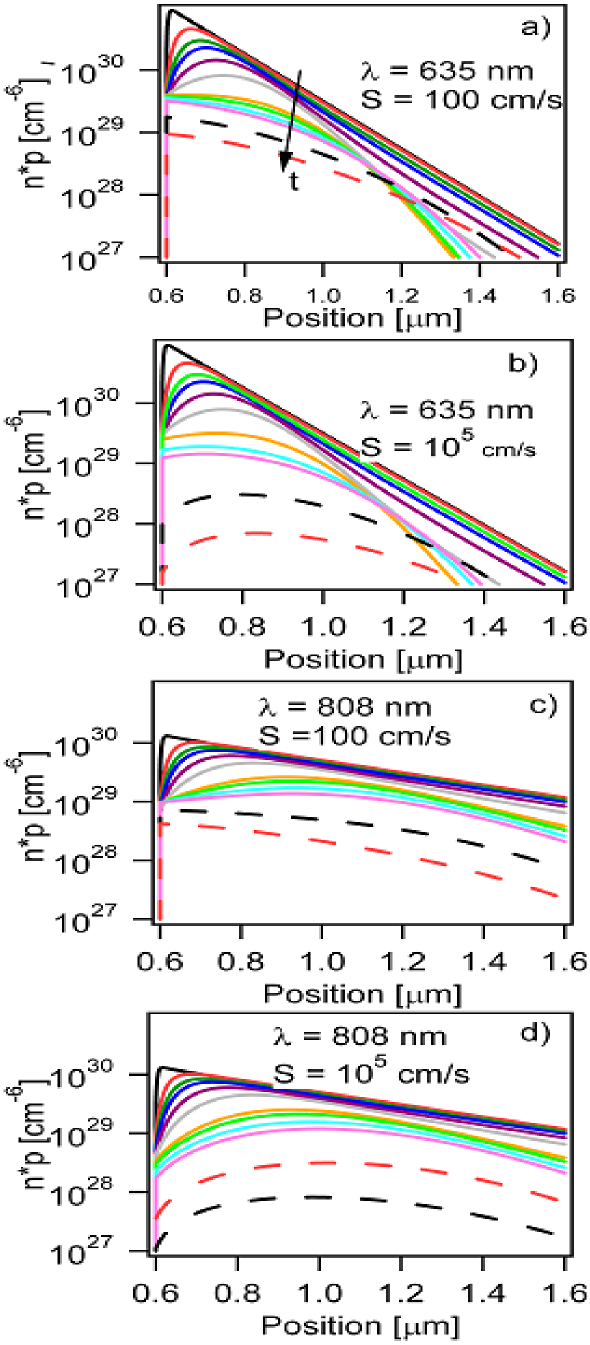

Fig.5. Calculated n*p product for a) λ = 635 nm and S = 100 cm/s; b) λ = 635 nm and S = 10^5 cm/s; c) λ = 808 nm and S = 100 cm/s; and d) λ = 808 nm and S = 10^5 cm/s. The different curves correspond to times: 0, 10 ps, 30 ps, 50 ps, 0.1 ns, 0.2 ns, 0.5 ns, 0.6 ns, 0.8 ns, 1 ns, 2 ns, and 3 ns. The CdTe/CdS heterointerface is located at x = 0.6 μm.

At later times, these differences become larger: at t = 2 ns, for example, n*p at the same point decreases by an order of magnitude due to increase of interface recombination velocity. For 808 nm, one can see the broader distribution of carriers within the absorber, and thus the smaller impact of interface recombination. Note that in a case of nonuniform defect density in the absorber, in a case of higher defect density in CdTe absorber within 200 nm to the heterointerface, the 635 nm decay is again affected more than 808 nm decay, and in this case distinguishing between interface and absorber quality close to the interface would require additional analysis.

Figure 6 shows simulated carrier decays for two devices. One device has a lifetime of τ_i = 0.5 ns and low interface recombination velocity (solid lines) and the other has five times higher lifetime τ_i, but higher recombination velocity, (10^5 cm/s). If the slope from the second part of the decay is measured at 635 nm, both of the samples would give similar τ_{2m}. From this measurement, it is not possible to determine the dominant loss mechanism in the device. However, if the measurement is also performed at 808 nm, there is a large difference between the decay times.

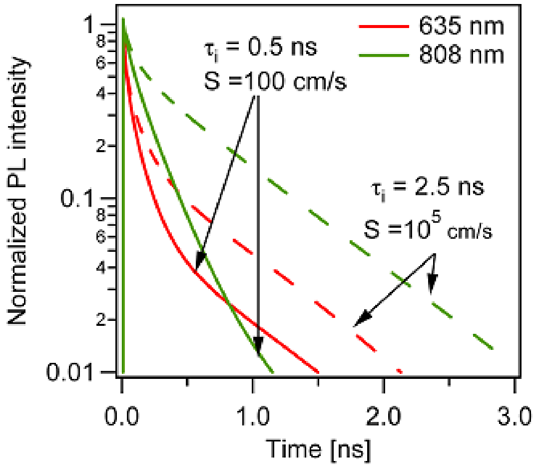

Fig. 6. Comparison of TRPL decays for two devices, where in one device the lifetime is lowered (solid lines) and in the other the interface recombination velocity is increased (dashed lines). The decays are simulated for a wavelength of 635 nm (red) and 808 nm (green).

Next, we consider how both the τ_i and interface recombination velocity would affect the second component (τ_{2m}) of TRPL decays. Figure 7 shows contour plots of simulated decay times (τ_{2m}) as a function of input carrier lifetime and interface recombination velocity. As expected, both interface and bulk recombination accelerate the carrier decay. But if the measurements are performed with two different wavelengths, one can see a difference in decay times. In a case of 635 nm illumination (Fig. 7a) the decays are affected by interface recombination stronger than for the longer wavelengths (Fig. 7b). For example, when the bulk lifetime is τ_i = 10 ns, interface recombination velocity increase from 100 cm/s to 10^6 cm/s decreases the decay time to τ_{2m} = 1.60 ns when the excitation wavelength is 635 nm, but only to τ_{2m} = 3.20 ns for 808 nm illumination. In addition, if S < 10^4 cm/s, its impact on the TRPL decay is not significant.

By measuring the carrier decays for two different wavelengths, another observation can be made. When S is low, τ_{2m} for 635 nm excitation is higher than τ_{2m} for 808 nm excitation. This seems counterintuitive, as one would expect the 635 nm decay to be faster due to the generation in the stronger electric field. But, as one can see from Figs. 2-4, the 635 nm decay is double exponential. The generated carriers separate faster, but that is evident in τ_{1m}. As the S increases, the decay due to 635 nm excitation is faster, and for S >10^5 cm/s the $\tau_{2m(808nm)} > \tau_{2m(635nm)}$.

Finally, we consider how the interface recombination and bulk recombination affect the V_{oc}, and how V_{oc} is connected with the measured decay. The V_{oc} is plotted in the contour plots in Fig. 7c. It is interesting to note that the shape of V_{oc} contours is very similar to the shape of the decay contours. This confirms that the V_{oc} can be predicted from the decay slope. This is also in agreement with other studies that have established logarithmic dependence of V_{oc} on lifetime [4, 5].

IV. CONCLUSIONS

Carrier decays after a short-light pulse illumination have been simulated to enhance the interpretation of TRPL measurement. The TRPL decays in thin-film devices are influenced by the carrier dynamics, including drift, diffusion, interface, and bulk recombination. We have found that at 635 nm illumination, the decay is affected more by the interface properties compared with the 808 nm decay. We have also calculated the n*p product at different moments during the decay to show that the interface recombination affects the second, slower part of the decay. By comparing the decays at different wavelengths, it may be possible to estimate whether the dominant recombination is located at the interface or in the bulk.

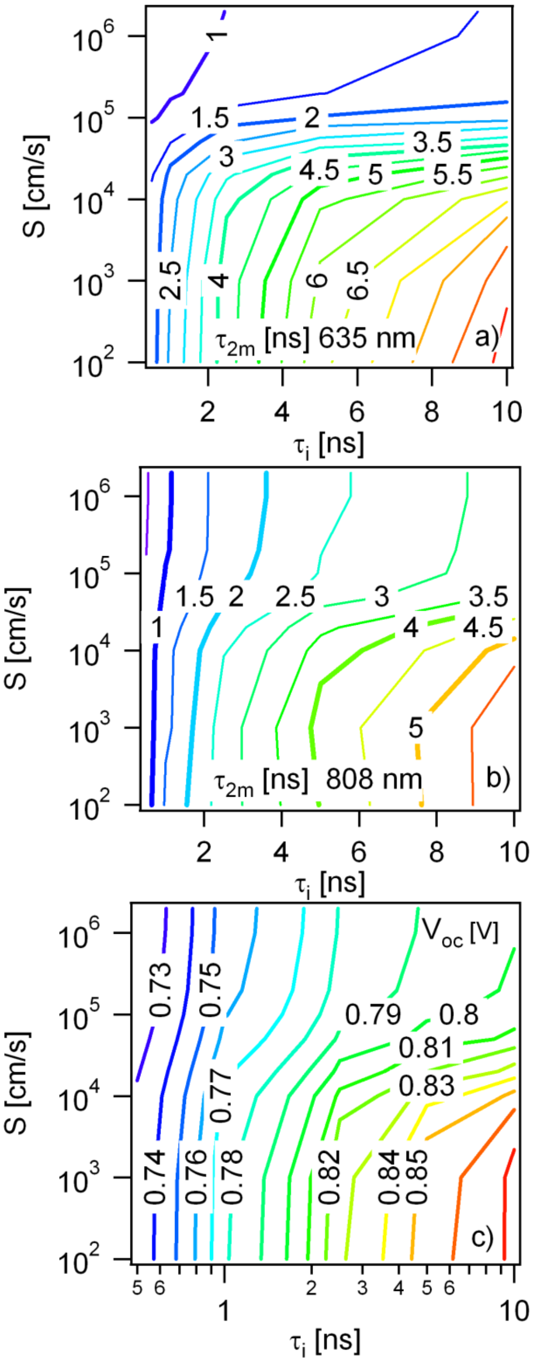

Fig. 7. Contour plot of calculated decay time τ_{2m} as a function of input bulk lifetime τ_i and interface recombination velocity S for two illumination wavelengths: a) 635 nm and b) 808 nm. In c), contour plots for V_{oc} dependence on carrier lifetime and interface recombination velocity.

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