Numerical Simulation of Time-Resolved Photoluminescence to Improve Solar Cell Performance

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ABSTRACT

- Recombination of electron-hole pairs is one of the primary mechanisms that limit solar cell performance.
- Time-Resolved Photoluminescence (TRPL) is a useful technique for studying recombination.
- Cd(Se,Te) solar cells are a leading thin-film, commercial technology that can be improved by understanding where recombination is occurring in the devices
- Here we explore how well analytical models can account for TRPL data.
- We employ numerical simulation to analyze TRPL at various light intensities, material thicknesses, and charge carrier mobilities.
- Comparison of numerical and analytical models indicates that simple analytical models are more effective at higher mobility.
- Analytical models should be improved to reduce the discrepancies at low mobility.

INTRODUCTION

- Climate change and the worlds violent addiction to non-renewable forms of energy require solutions.
- Non-renewable resources are predicted to be obsolete with in this century.[1]
- Solar energy has increased in efficiency[3] (see Fig. 1) and affordability allowing the USA to go from just 0.34 Gigawatts in 2008 to 97.2 Gigawatts today.
- As of today, only 3% of the United States electricity comes from solar photovoltaics and concentrating solar thermal power.[2]
- Our focus is on solar technology and how theoretical calculations can help improve the efficiency of these energy solutions.
- Numerical simulation of TRPL help us determine the electron-hole pair lifetime (τ) at various light intensities and material properties.
- A challenge with TRPL data is determining where in the device most of the recombination is occurring and a lack of accurate analytical models.[4]
- Analytical models are more accessible to experimentalists, so we compared our numerical model results to the analytical estimates to see how well they matched.
- If the predictions match the numerical calculations, then experimentalist can deduce material quality through simpler means.

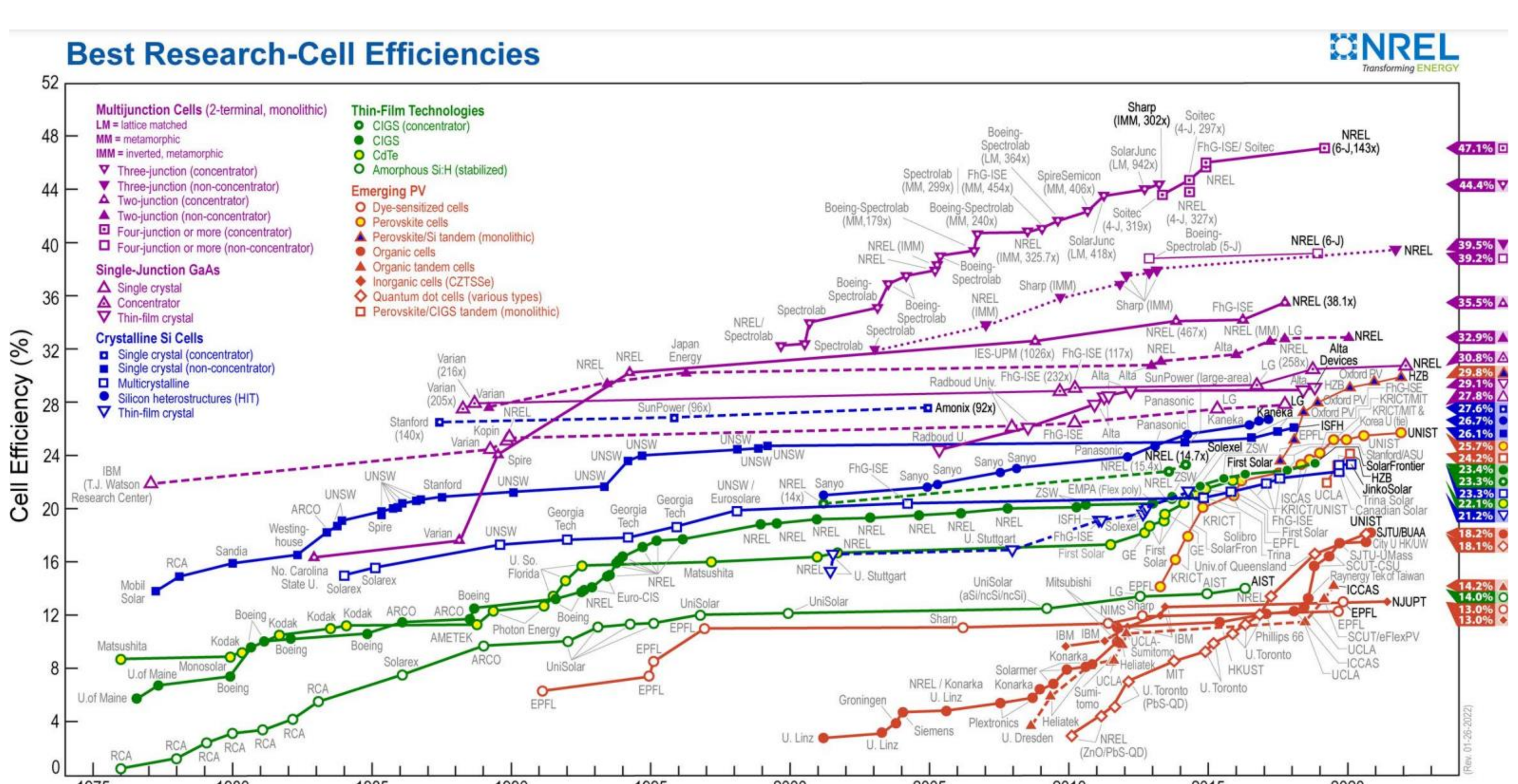


Fig. 1. chart of the highest confirmed conversion efficiencies for research cells for a range of photovoltaic technologies, plotted from 1976 to the present.

MATERIALS AND METHODS

TRPL Simulation

Double Heterostructures are when a semiconductor material is grown into a "sandwich" with a larger band gap material on both sides. These structures are very useful for optoelectrical studies due to confinement of charge carriers in the semiconductor. For this reason, a Al_2O_3/Cd(Se,Te)/Al_2O_3 heterostructure were used for TRPL simulations.

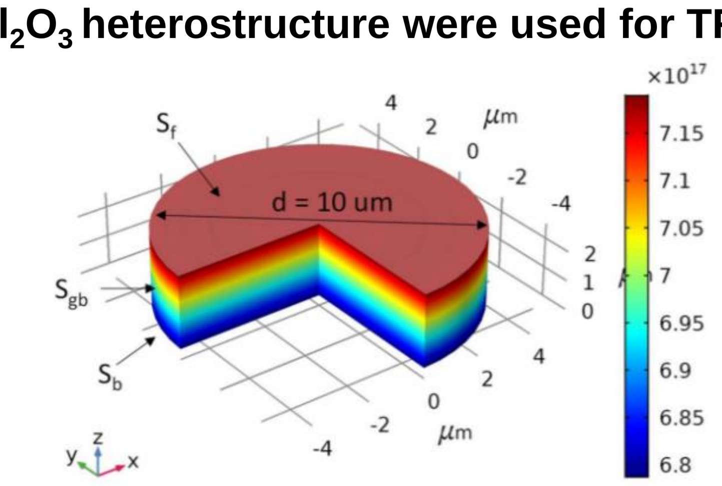
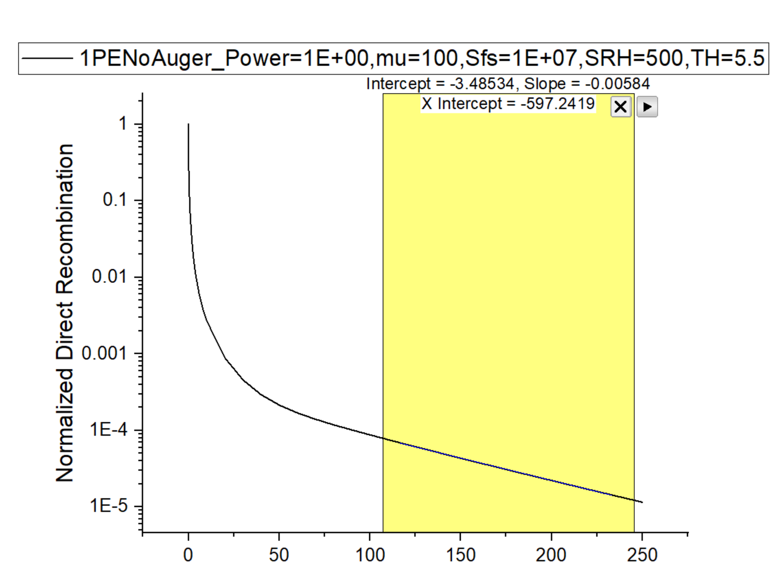


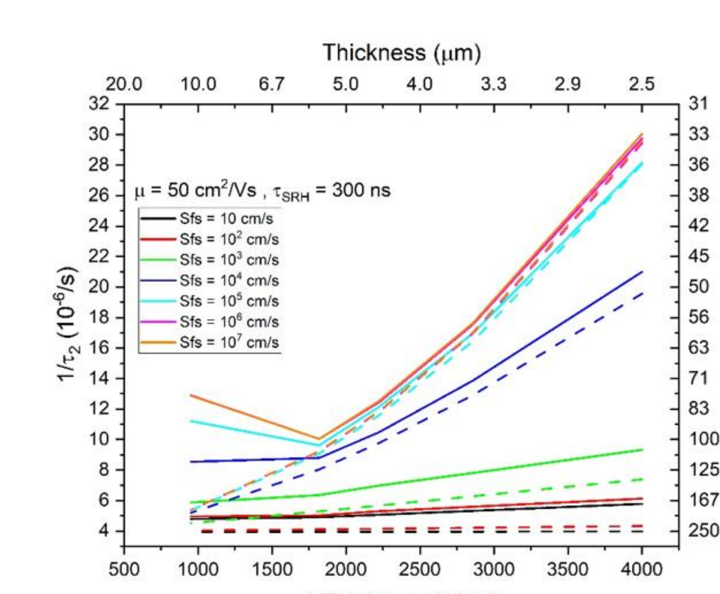
Fig. 2. Simulated electron-hole pair generation rate ($cm^{-3}\ s^{-1}$) for a Al_2O_3/Cd(Se,Te)/Al_2O_3 heterostructure under 1-sun light intensity and 2-photon excitation (2PE). Model considers a 10-micron diameter cylindrical grain with front (S_f), back (S_b), and grain boundary recombination (S_{gb}).

- Laser pulse time of 0.3 ps at 1.1 MHz frequency.
- Excitation wavelength for 1PE is 640nm and 2PE is 1120nm.
- Excitation power is 0.001-100mW for 1PE and 3-100mW for 2PE.
- Time-dependent Poisson and continuity equations solved using the finite element method in COMSOL Multiphysics®. 3D axi-symmetric model domains.
- Recombination mechanisms included radiative, nonradiative (Shockley Read Hall) in the bulk and at interfaces.
- Considered field screening and charge redistribution effects.
- PL intensity calculated by integrating the radiative recombination rate over the volume of the illuminated region:

Data Analysis

- PL decays curves were fit at the most linear state to determine τ.
- Obtained values plotted in Excel and OriginPro with other independent variables.
- Numerical results compared to analytical estimates (see Fig. 3).





1PE	Power (mW)	mu	Sfs	SRH	TH (mm)	slope	tau2
	1	1	1.00E+01	100	2.5	-0.00618	70.27508
	1	1	1.00E+01	100	3.5	-0.00618	70.27508
	1	1	1.00E+01	100	4.5	-0.00618	70.27508
	1	1	1.00E+01	100	5.5	-0.00618	70.27508
	1	1	1.00E+01	100	10.5	-0.00618	70.27508
	1	1	1.00E+02	100	2.5	-0.00636	68.28616
	1	1	1.00E+02	100	3.5	-0.00636	68.28616
	1	1	1.00E+02	100	4.5	-0.00637	68.17896
	1	1	1.00E+02	100	5.5	-0.00637	68.17896

Fig. 3. Process of determining lifetime (τ) by fitting TRPL simulations, collecting data, and comparing numerical (solid curves) to analytical calculations (dashed curves).

RESULTS

- Numerical and analytical calculations match reasonably well (Fig. 4).
- It appears that, at low mobility (μ), the analytical equation [Eq. (1)] is less reliable, but further analysis is required to quantify the discrepancies.
- TRPL lifetime becomes less dependent on thickness and surface recombination velocity (S_{fs}) as mobility decreases because most of the recombination occurs in the bulk.
- For any mobility, TRPL lifetime is less dependent on thickness as S_{fs} decreases.
- Bulk lifetime (τ_{SRH}) can be estimated by the y-intercept of the data.

$$\frac{1}{\tau} = \frac{1}{\tau_{SRH}} + \frac{1}{\tau_{rad}} + \frac{1}{d/S + d^2/D} \quad (1)$$

d – material thickness, D – diffusion coefficient
S – surface recombination velocity
τ_{rad} - radiative recombination lifetime

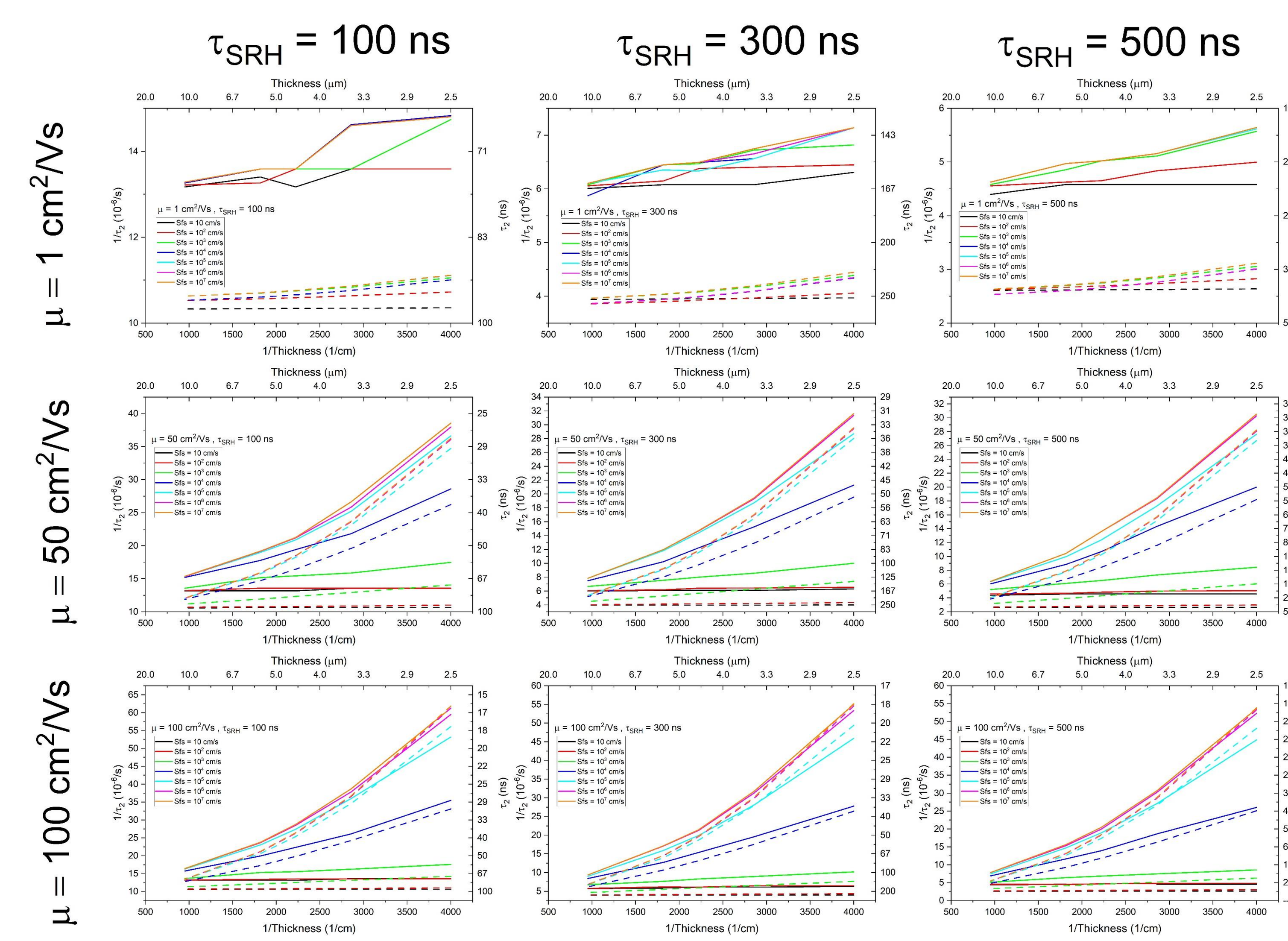


Fig. 4. Plots of $1/\tau$ vs. Cd(Se,Te) thickness for numerical (solid curves) and analytical (dashed curves) calculations at various bulk lifetimes (τ_{SRH}), mobilities (μ), and front surface recombination velocities (S_{fs}). TRPL simulations are for 2-photon excitation with a laser power of 3 μW.

CONCLUSIONS

- TRPL simulations can be used to better understand recombination in photovoltaic materials and devices.
- Analytical models can provide reasonable estimates, but additional work is required to quantify discrepancies and improve accuracy.

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