Modeling Lifetime Dynamics of Gold Hyperdoped Silicon Solar Cells

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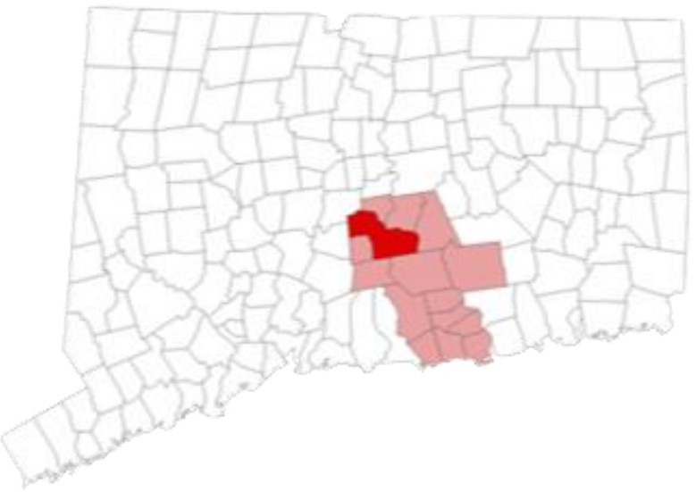
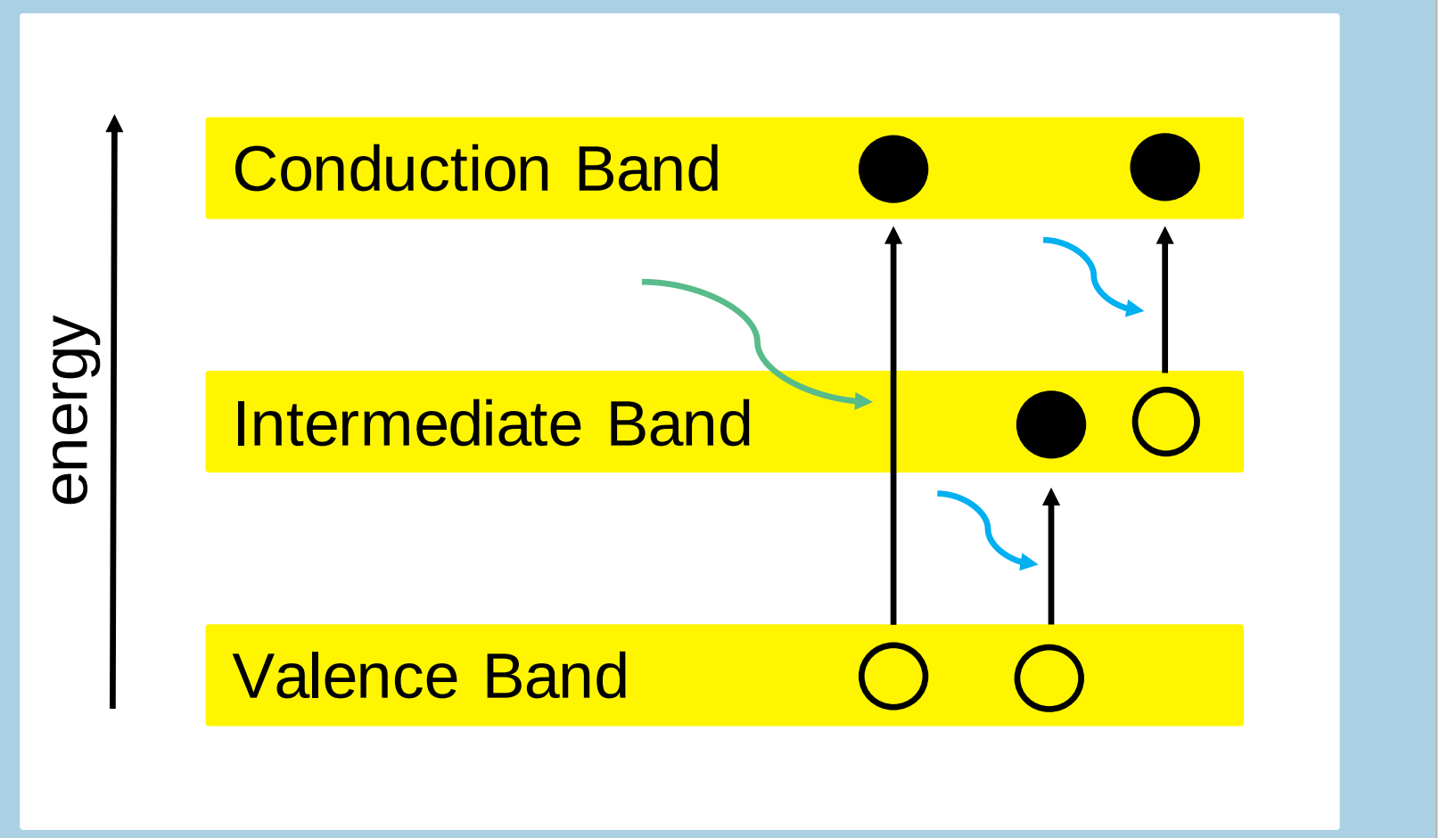


Motivation

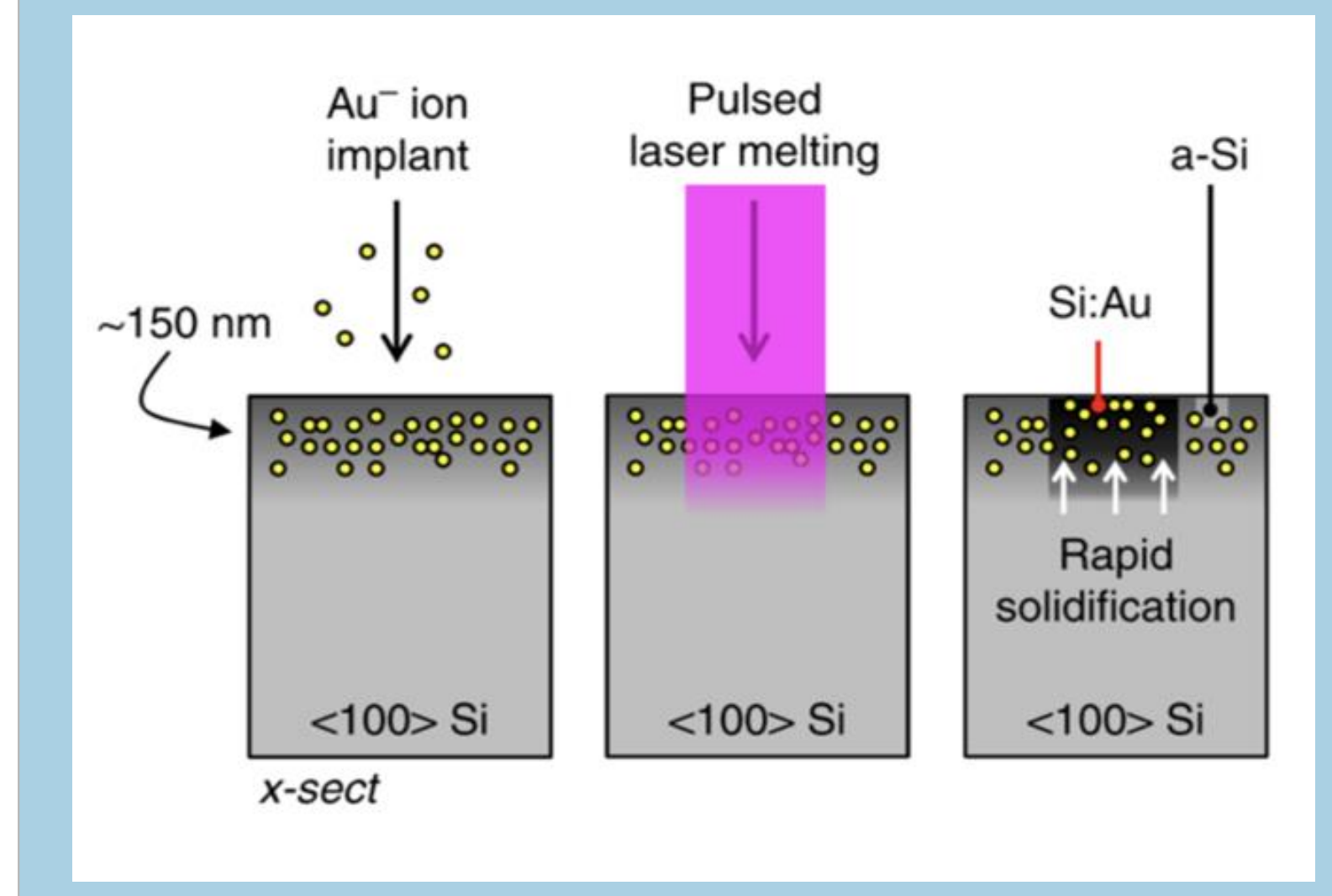
Using numerical simulation of charge carrier diffusion and electron recombination within gold-hyperdoped silicon solar cells, we studied how dopant concentration profile affects charge carrier lifetime. We found that lifetime increases with the dopant highly concentrated near the surface of the silicon.

Background

Hyperdoping is a process that incorporates other elements, such as gold, into a silicon lattice, which in theory can increase the efficiency of silicon solar cells. The gold creates an intermediate band between the valence and conduction band, so the solar cells can capture a broader range of light.



Energy band diagram of an intermediate band semiconductor. Figure adapted from Ref [1]



Hyperdoping process. Figure adapted from Ref [1]

One method of hyperdoping is pulse laser melting (PLM). In this method, gold is ion implanted into the silicon, then the material is pulse laser melted and rapidly solidified. PLM samples can be modified by etching, where a chemical reactant removes the top of the sample up to a certain depth.

Another variation of the PLM method is instead of ion implantation, a thin film of the dopant is deposited onto the surface of the silicon before the material is pulse laser melted.

Simulation

Conductivity as a function of time can be modeled by a bi-exponential decay curve with a fast and a slow decay. If the concentration profile of the dopant over the depth of the silicon were uniform, the lifetime would simply be modeled by a single exponential decay curve. However, most hyperdoping processes create a concentration profile with a pile up of the dopant near the surface, leading to more complicated decay dynamics.

Simulation (continued)

Our simulation helps us understand how the concentration profile affects the lifetime dynamics of hyperdoped silicon more accurately than the biexponential fit approximation.

$$\frac{\partial n_e(x,t)}{\partial t} = D\frac{\partial^2 n_e(x,t)}{\partial x^2} - \frac{n_e(x,t)}{\tau_b(x)}$$

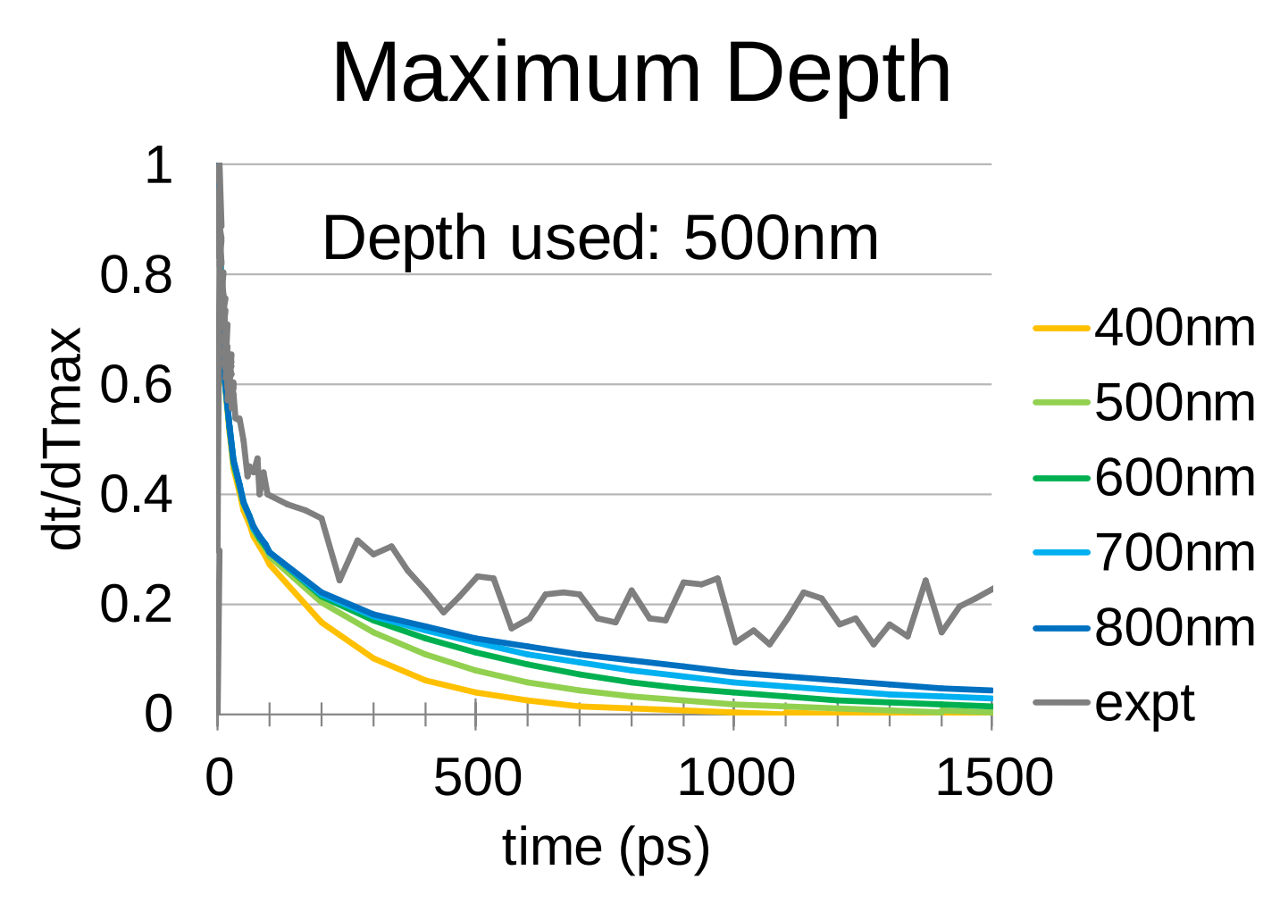
Equation 1: Density of charge carriers over time

Our simulation models the density of charge carriers over time (Eq. 1), which depends on two terms: carrier diffusion (1st term) and electron recombination (2nd term) within the material. Using this equation, we numerically simulated the decay in the number of charge carriers over time for different concentration profiles.

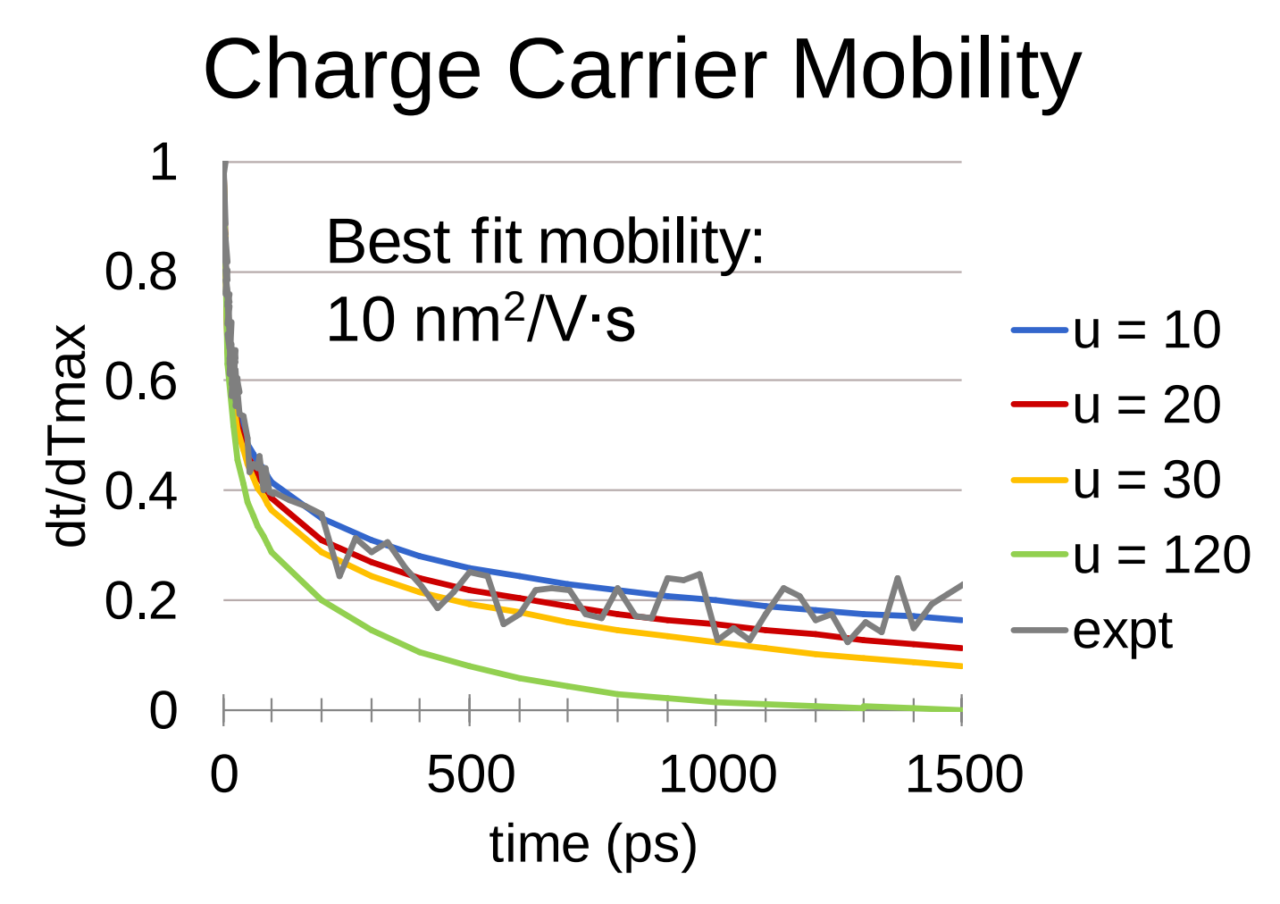
Fitting Parameters

We used three parameters to fit our simulation to experimental data of a film PLM unetched sample: maximum depth, charge carrier mobility, and capture cross section.

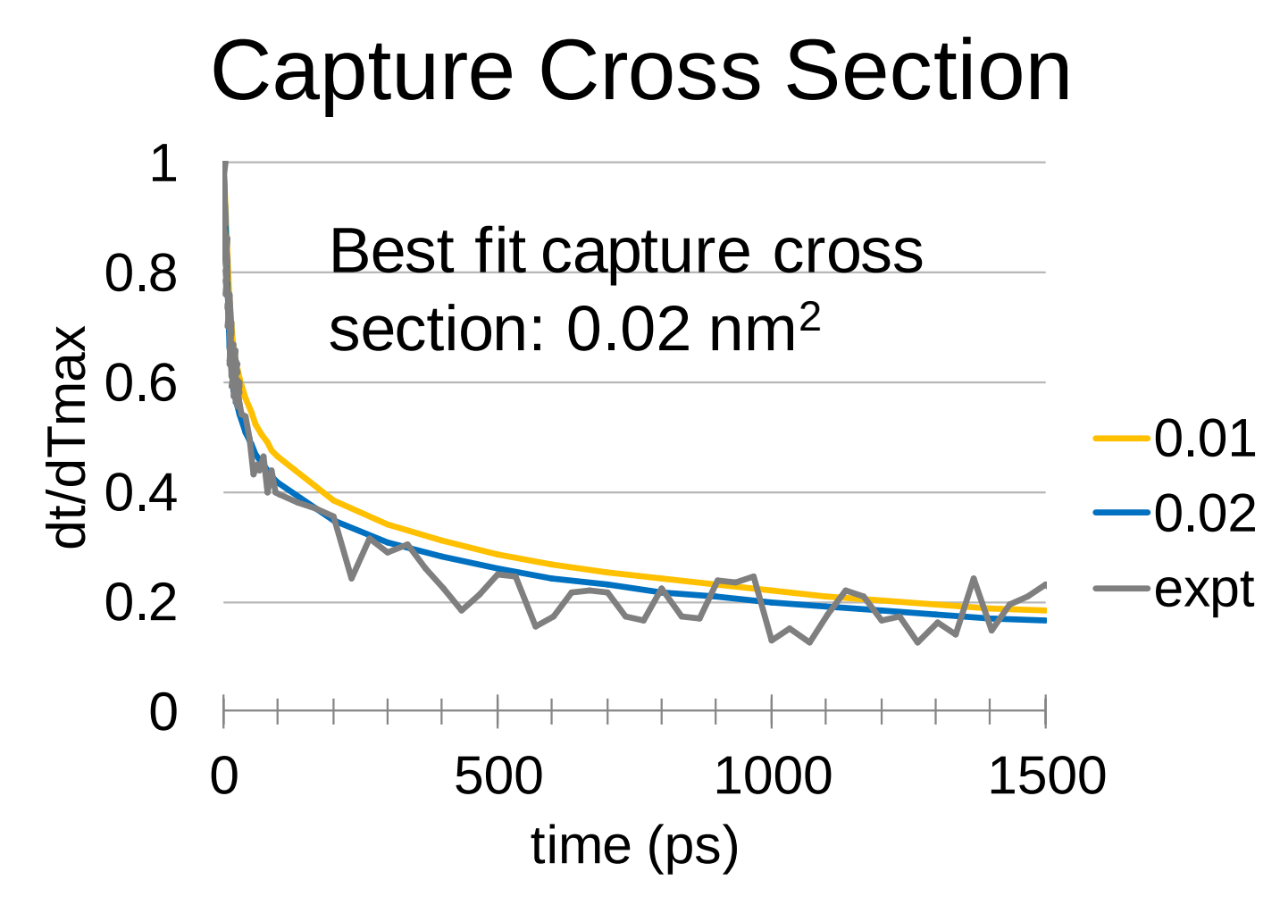
Maximum depth is the maximum diffusion depth of the simulated electrons. The simulation fits better with experimental data as the maximum depth increases, however the difference becomes negligible at large values.



Charge carrier mobility measures how easily the electrons move throughout the material. At 400nm light, we found that a longer lifetime correlates with decreased mobility.

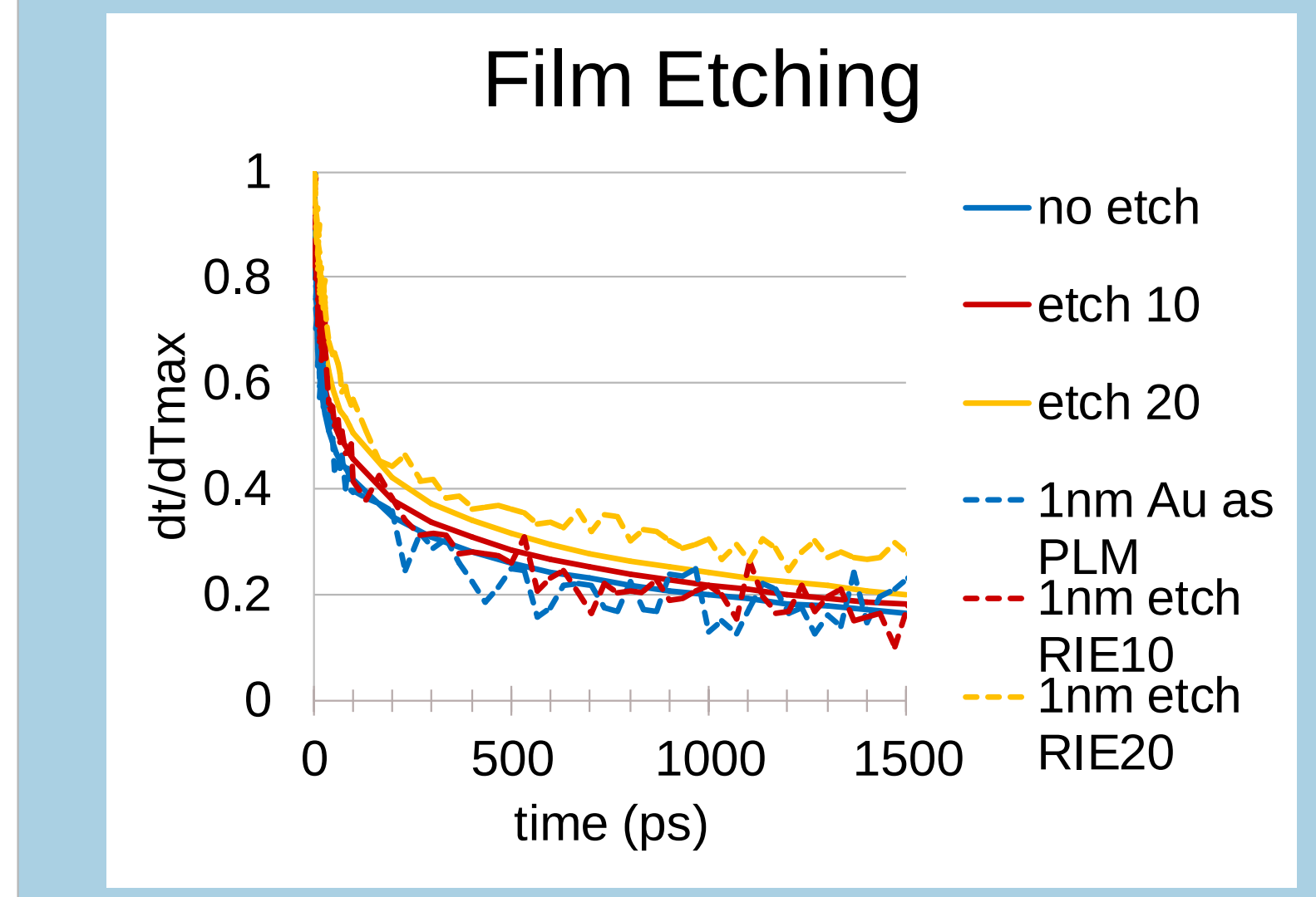


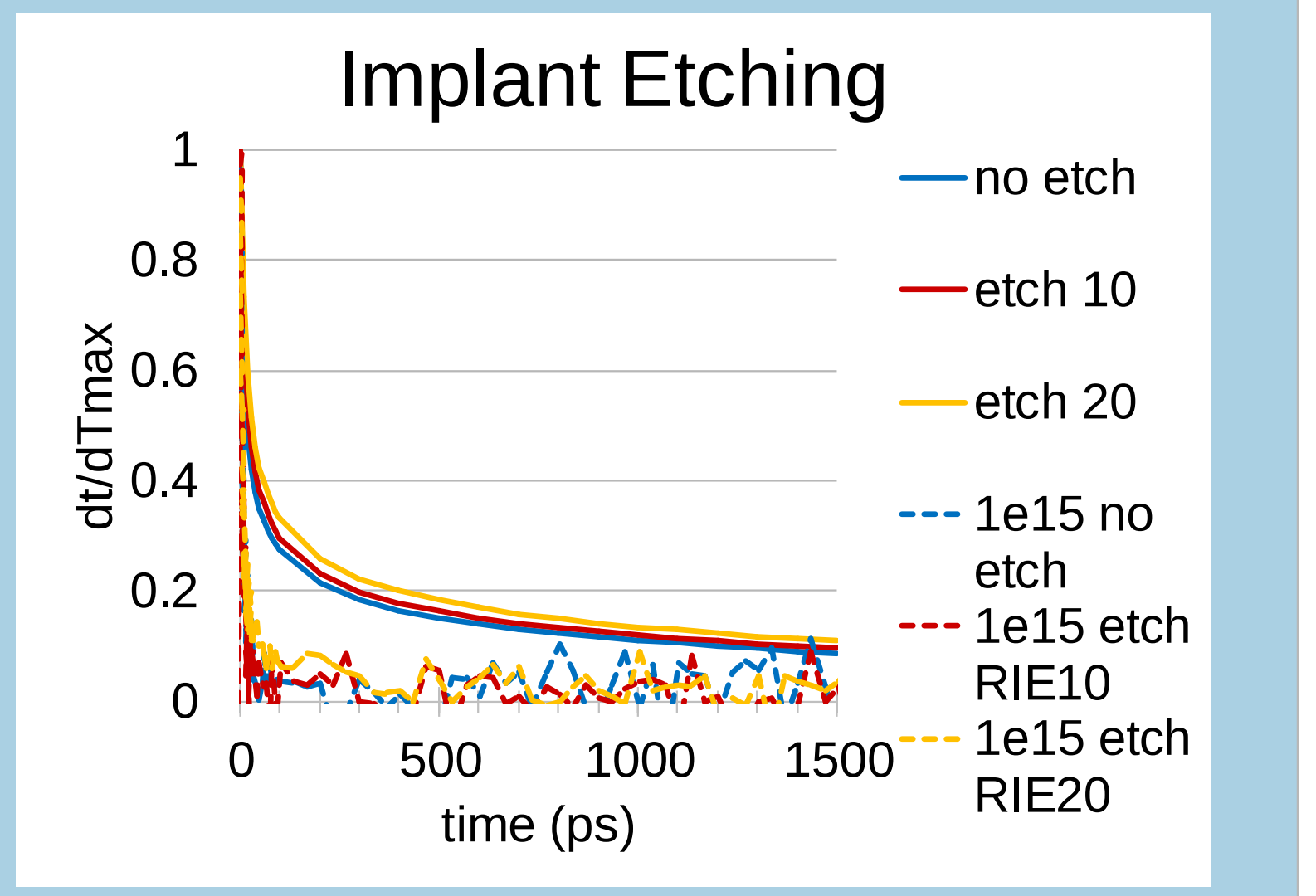
The capture cross section is the effective cross sectional area that traps electrons. With increased capture cross section, electron recombination is more effective, resulting in a shorter lifetime.



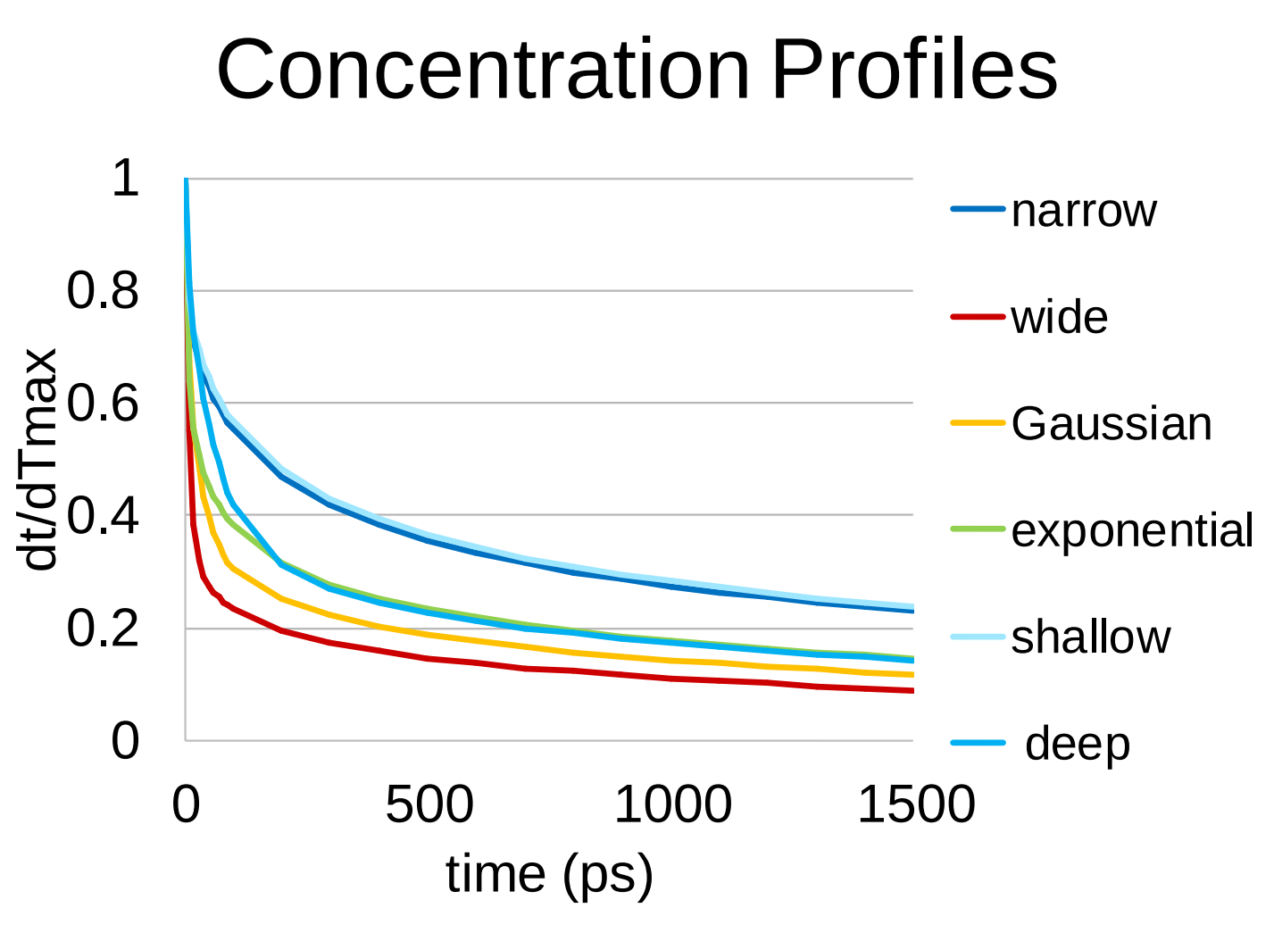
Results

The simulation fit well for the film PLM experimental data with various etching depths. However, the simulation predicted longer lifetimes for the implanted PLM samples, likely due to high damage concentration from implantation.





Using simulated concentration profiles, all containing the same amount of gold, we found that profiles with highly concentrated gold near the surface produced the longest lifetimes. Profiles with the same distribution at different depths (shallow and deep) produced different results.



An exponential profile closely represents a typical concentration profile of gold-hyperdoped silicon.

Conclusion

For gold hyperdoped silicon, we found that carrier lifetime increases when the gold is highly concentrated. This concentration profile is likely the ideal to maximize electron extraction and create more efficient solar cells. We also found that the implantation PLM process creates significant defects, resulting in a less efficient solar cell.

We can further use this simulation to determine which element hyperdoped with silicon would create the most efficient solar cells and which process of hyperdoping results in a concentration profile most similar to our ideal concentration profile.

Works Cited

[1] Fiutak, R. (2019). *Understanding Lifetime Dynamics in Gold Hyperdoped Silicon Solar Cells* (Undergraduate thesis). Wesleyan University, Middletown, CT, USA.