ECE 695 Numerical Simulations Lecture 32: Finite-Difference Time Domain Band Structures

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April 5, 2017

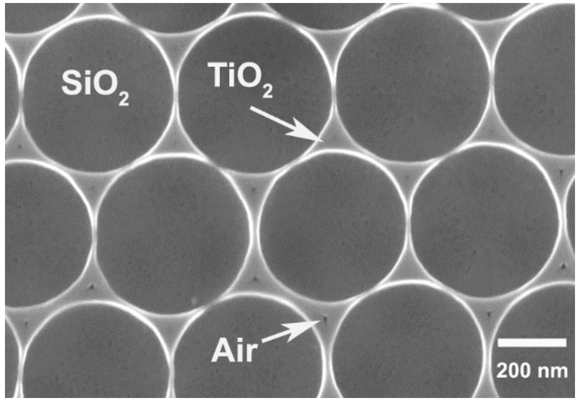
Outline

- Inverse Opal Photonic Crystals:
  - Photonic Band structures
  - Photonic Crystal Phosphors
- Photon recycling in PV
  - GaAs thin films
  - Nanowire solar cells
- Characterization of PV materials
  - Time-resolved photoluminescence
  - Plasmonic structures

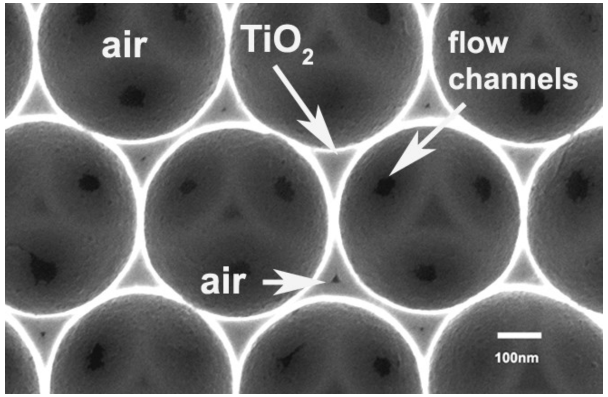
ALD of TiO_2 at 100ºC

(111)

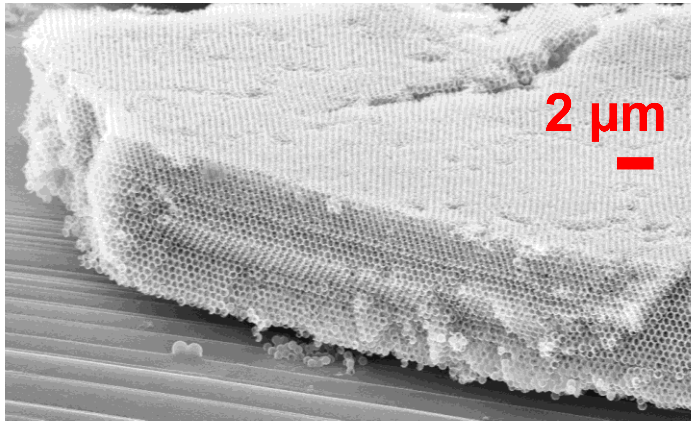
Cross-sections



433 nm opal infiltrated with TiO_2



433 nm TiO_2 inverse opal



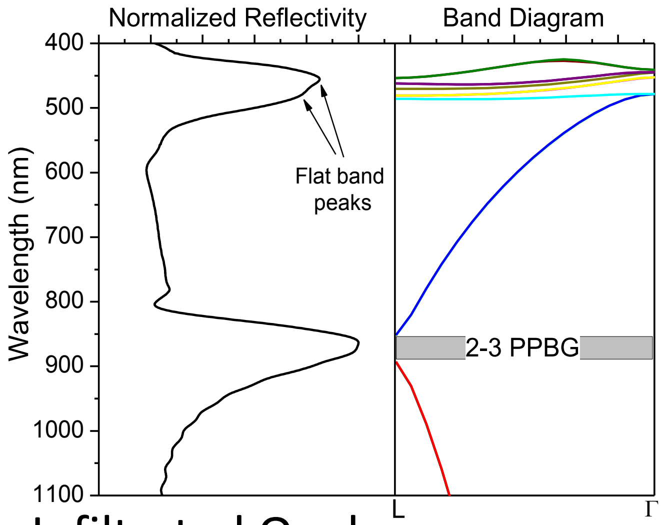
433 nm TiO_2 inverse opal

- TiO_2 infiltration at 100ºC produces very smooth and conformal surface coatings with rms roughness ~2Å.
- Heat treatment (400C, 2 hrs.) of infiltrated opal converts it to anatase TiO_2, increasing the refractive index from 2.35 to 2.65, with only a 2Å increase in the rms surface roughness.

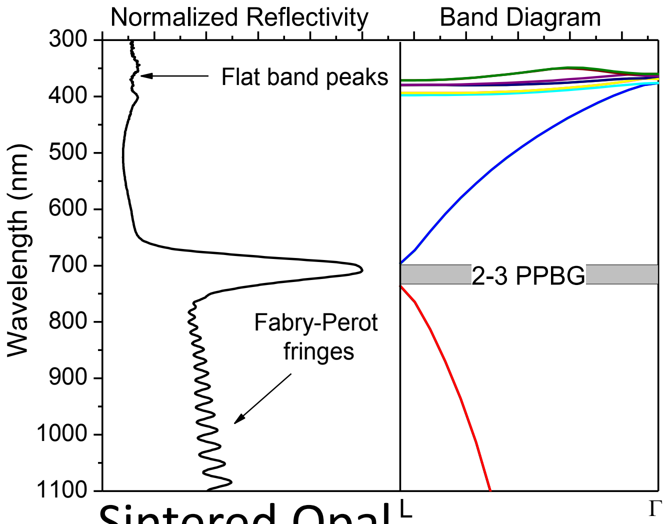
E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

Inverse Opal Reflectivity

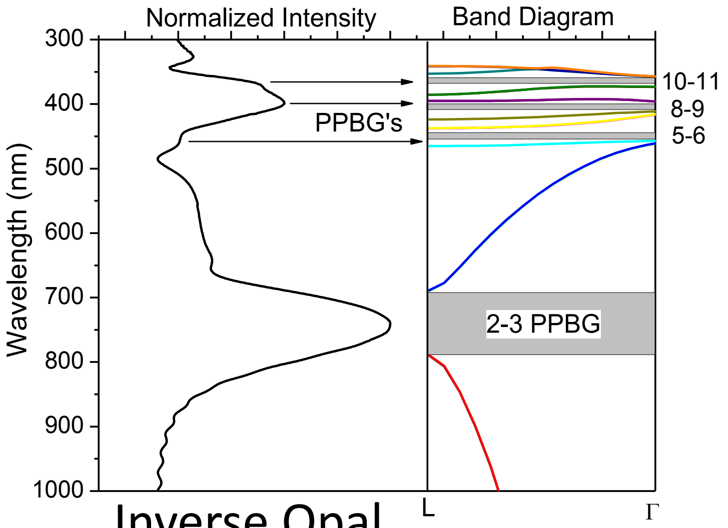
- TiO_2 infiltration of 330 nm opal.
- ~88% filling fraction
- 2.65 Refractive Index
- Agreement: full index attained!



Infiltrated Opal



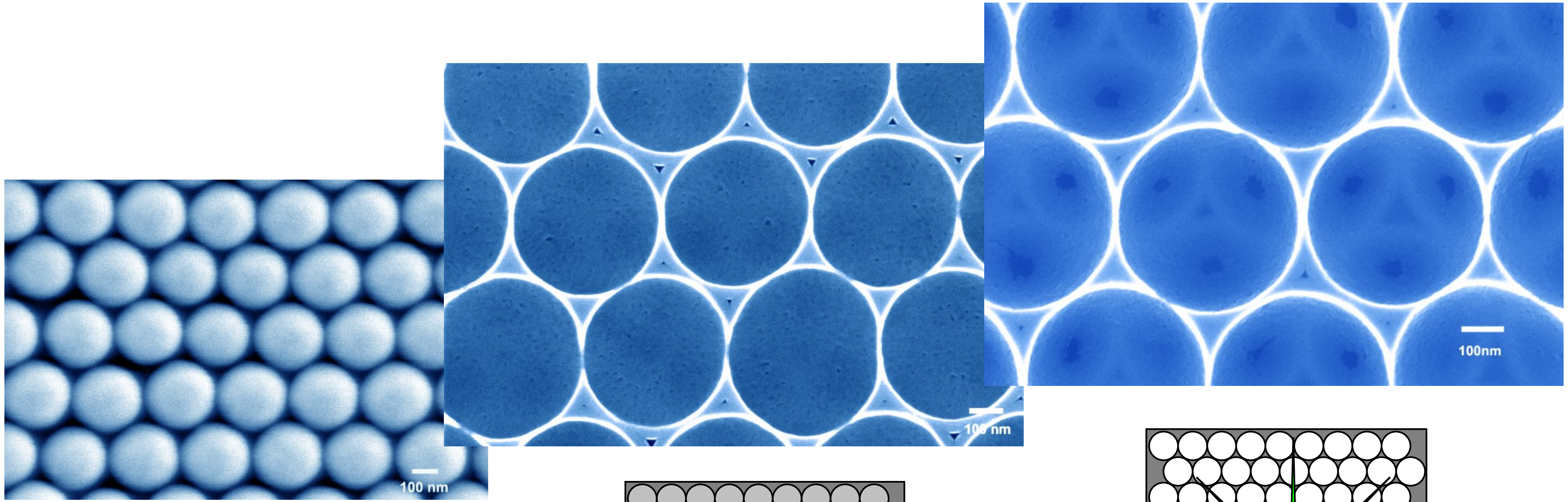
Sintered Opal

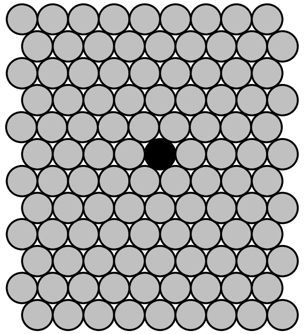


Inverse Opal

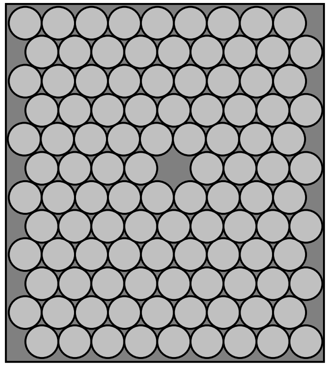
E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

Opal Defect Engineering

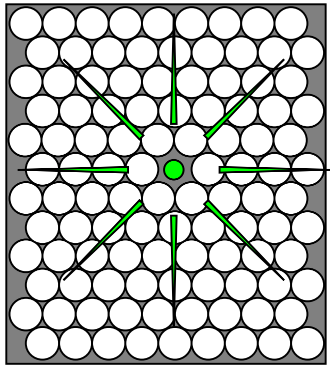




Silica Opal with Defect



Infiltrated Opal

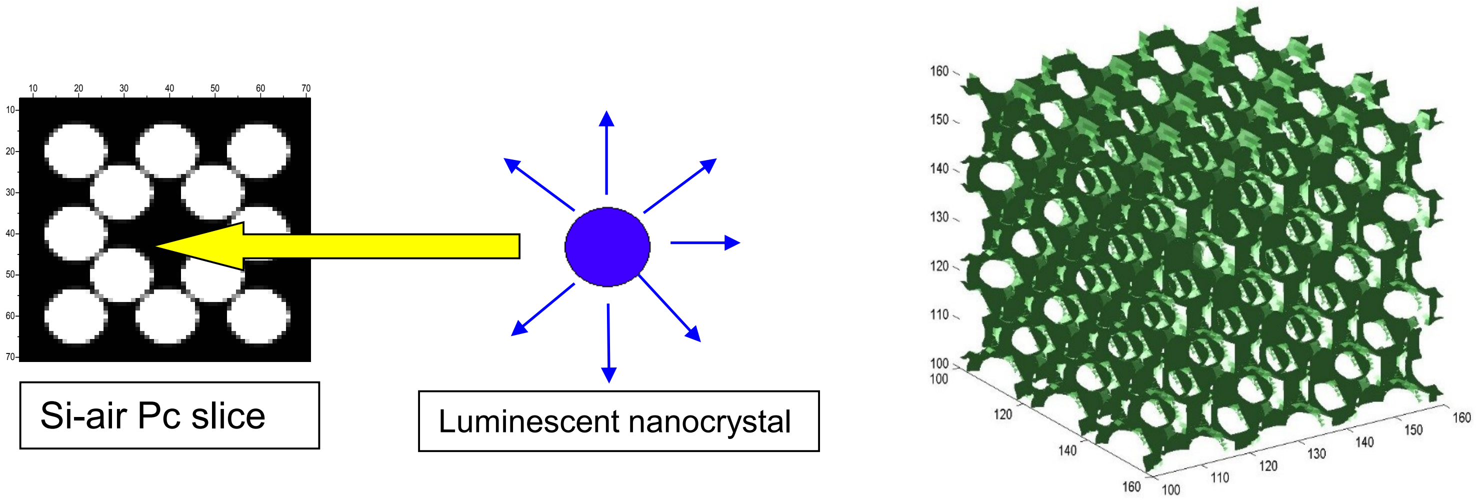


Inverted Opal Structure

(With Defect – soon!)

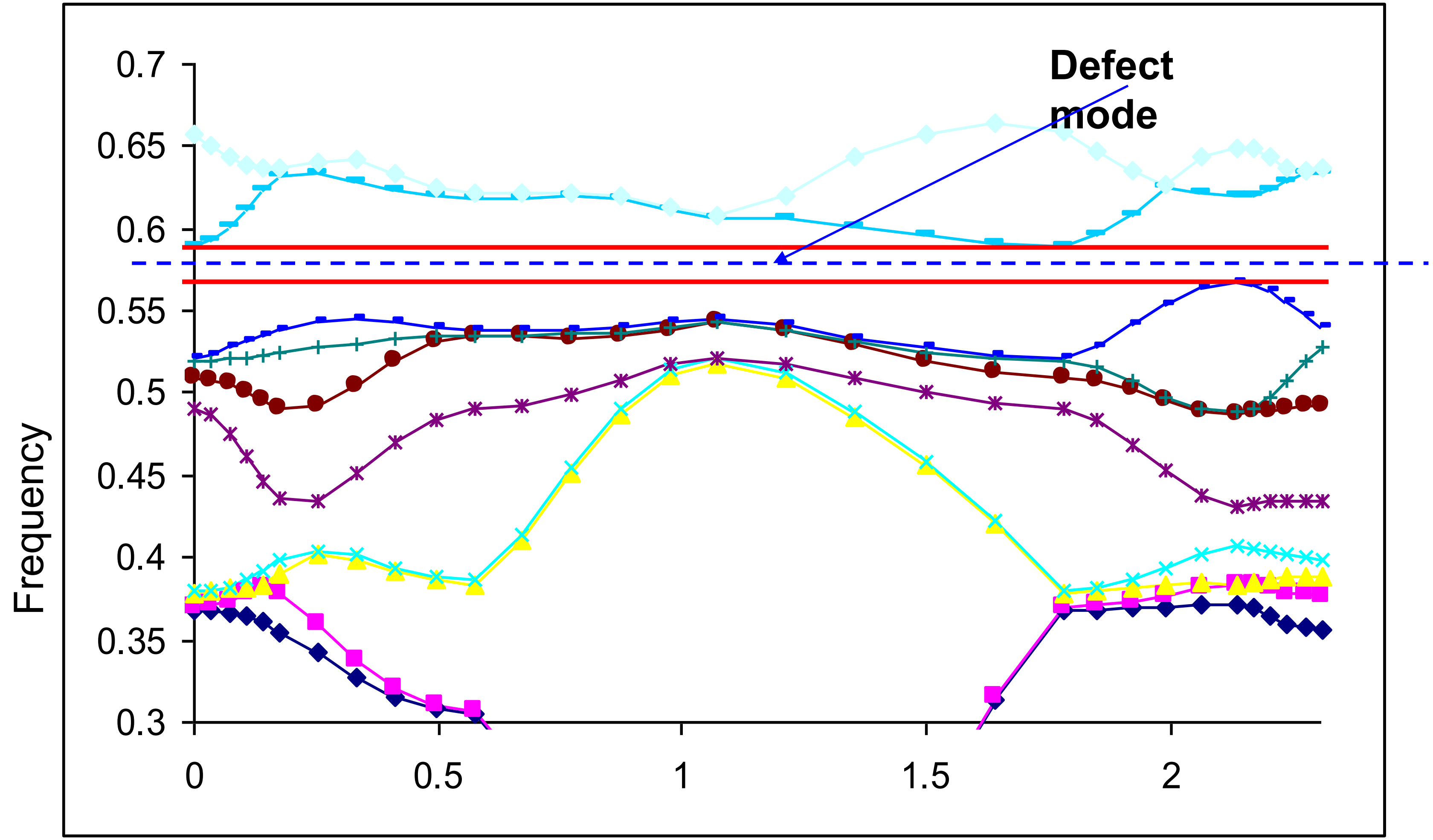
Inverse Opal Defect Mode Calculations for PhCPs

- What is the main idea behind Photonic Crystal Phosphor (PhCP)?
  - Combining a 3D inverse opal with nanophosphors as a local defect in the PhC lattice

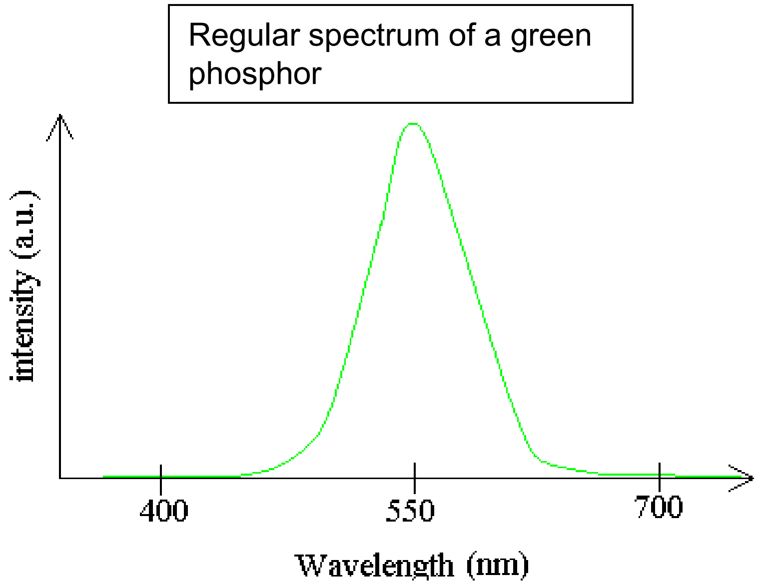


- Specific frequencies in the Photonic Band-Gap of the inverse structure are inhibited except for the defect modes
- A broad luminescent material spectrum within this band-gap would be filtered by the resonant frequency and therefore tuned up

Photonic Band-Gap Analysis



Spectrum analysis for PhCPs



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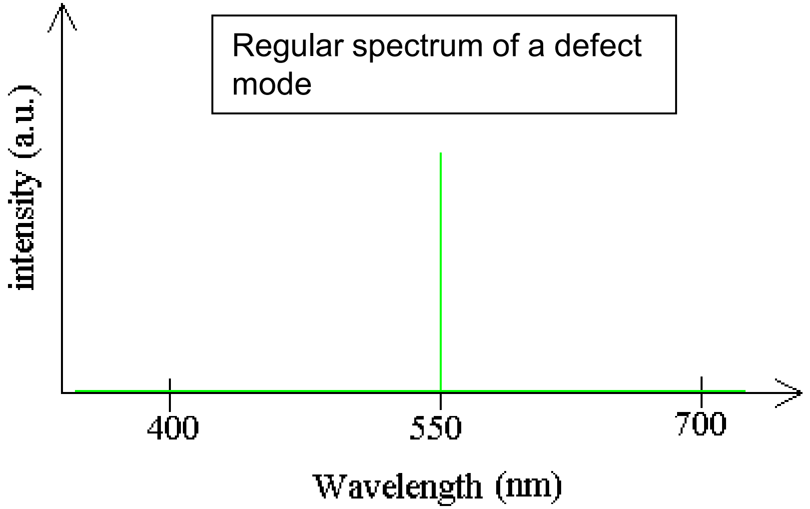

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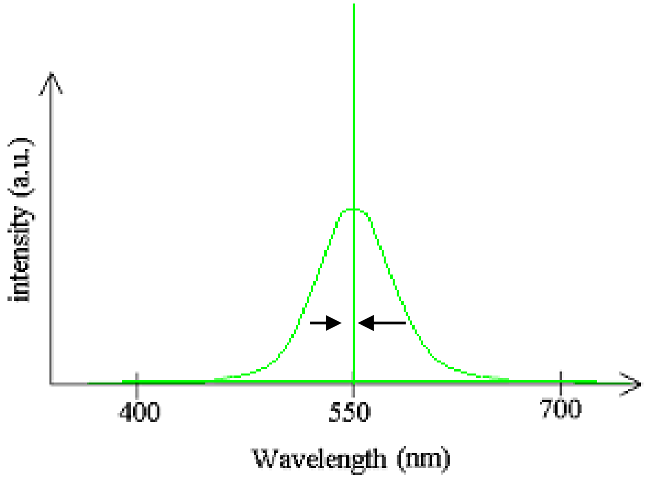


Both spectrum combine and

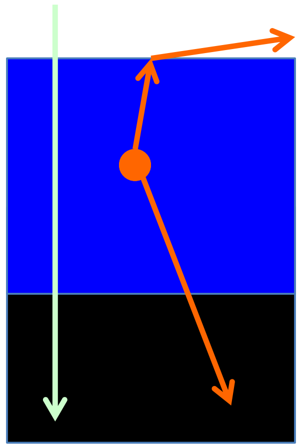
Emission Energy of phosphor is totally quenched into the defect mode

Main Characteristics of PhcPs

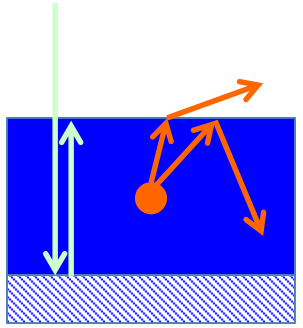
- The cavity mode emission spectrum lies within the phosphor emission spectrum
- The position and peak cavity spectrum from the host statically controls the color, luminous intensity and decay time
- Ultimate tunability would be achieved by tunable materials like liquid-crystal, PLZT, etc. to change both the position and peak of cavity mode

PhCPs are candidates for High-Definition Display devices

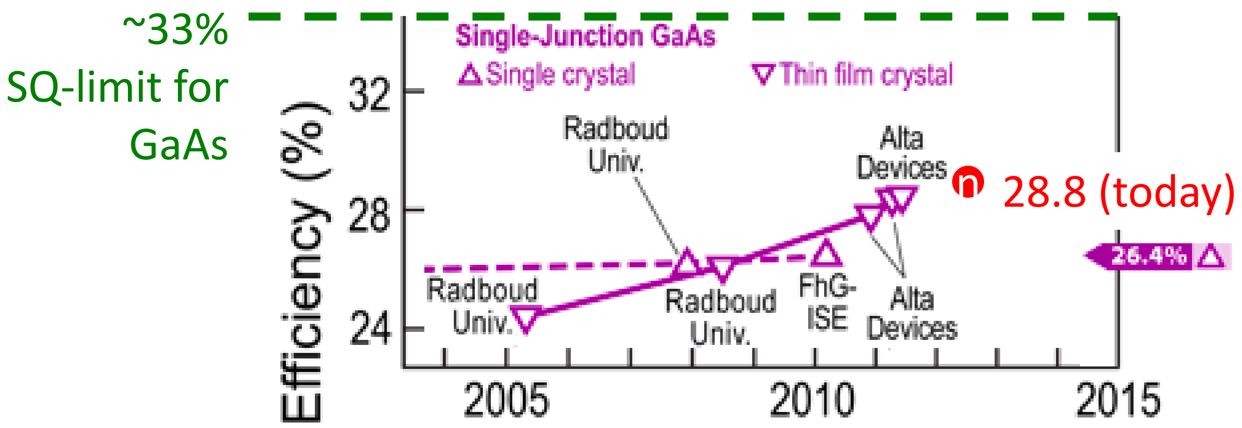
GaAs solar cell overview



Cell on substrate

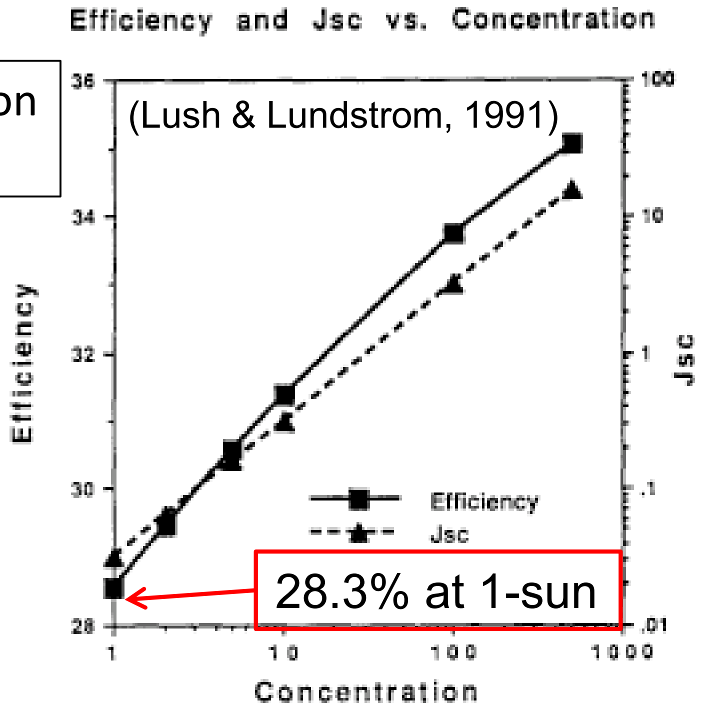


Thin film approach



Thin film approach increases photon recycling and thus the efficiency

(Alta Devices, 2012)

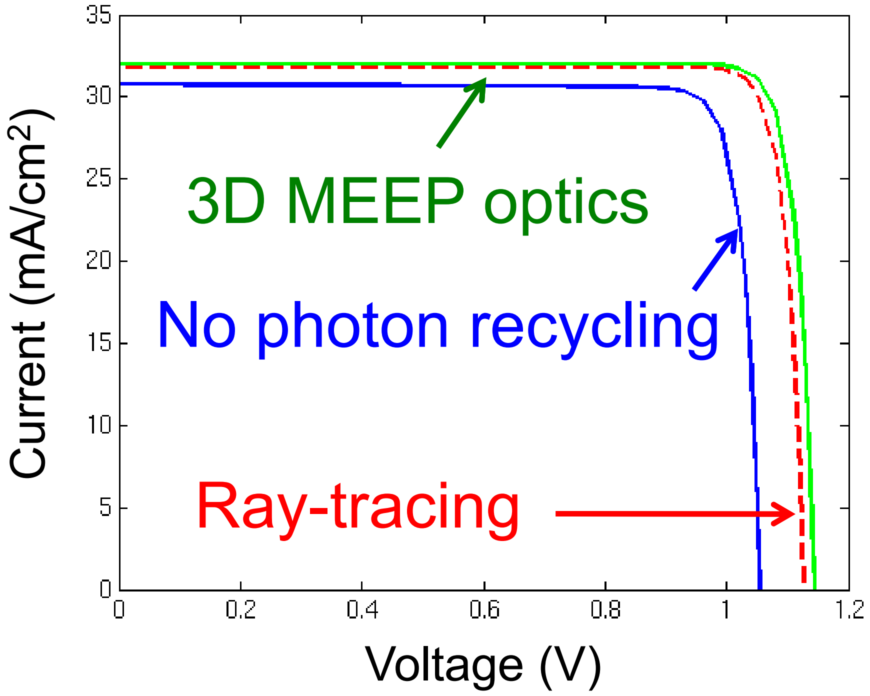


PV at SQ limits: coupling photons and electrons

Alta Devices 28.8%

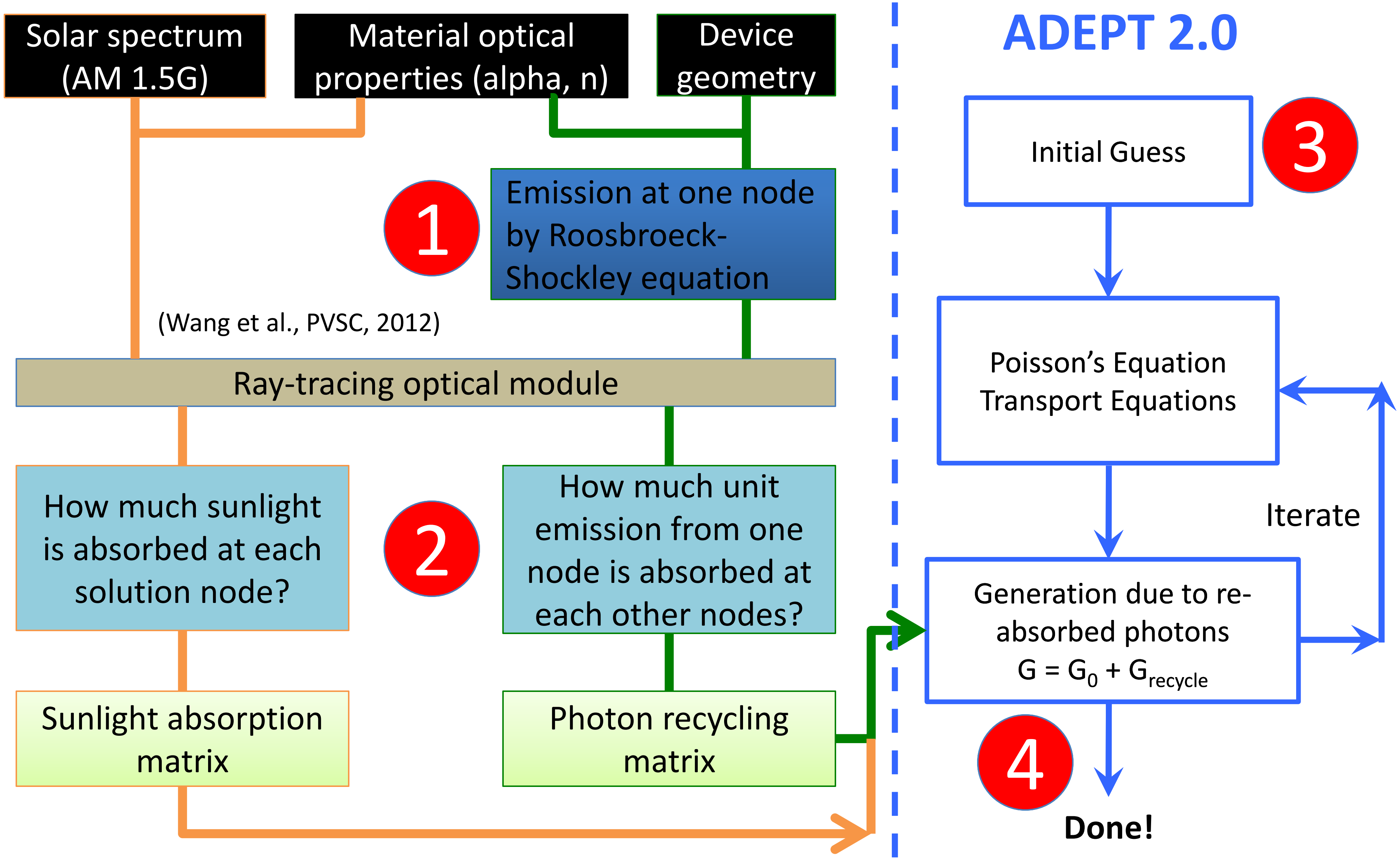
E. Yablonovitch et al., 38th PVSC (2012)

G. Lush and M. Lundstrom, *Solar Cells*, **30** 337 (1991).

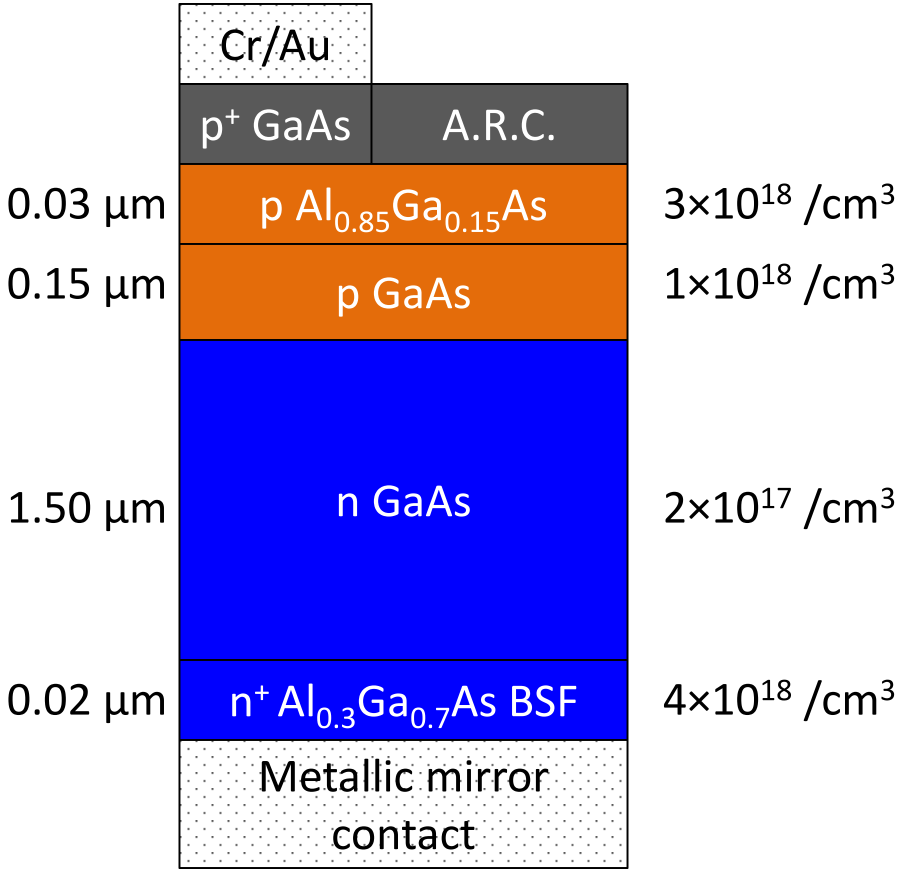


Xufeng Wang and PB (Purdue)

Photon-recycling in device simulator



Baseline cell

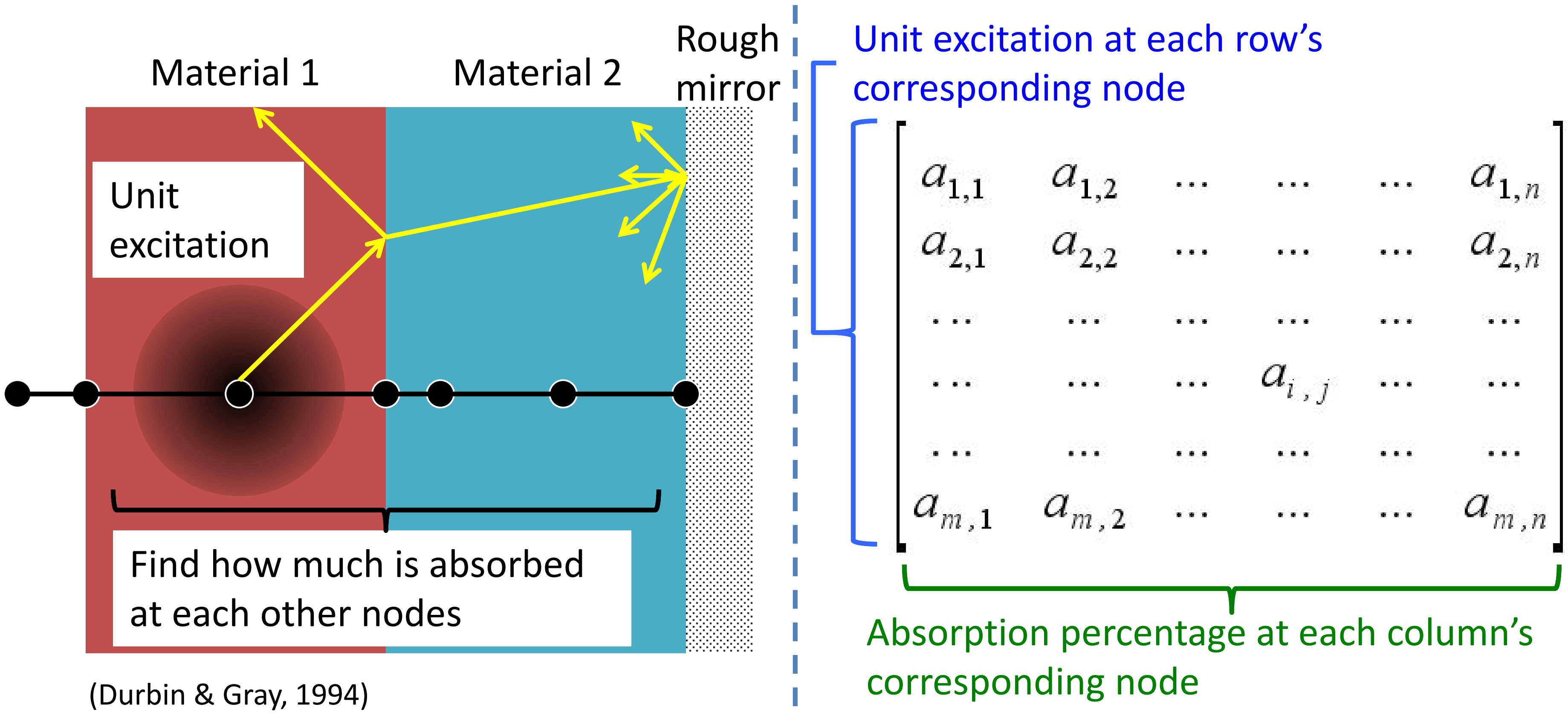


Parameter	Value
SRH lifetime	0.5 us
Auger Coeff.	7×10^{30} cm^6/s
Shadowing + Refl.	6.6 %
Rear mirror refl.	85 %
Ambient index	1.35
GaAs index	3.3
Series resistance	0.7 ohm

(Kayes et al., 2011)

Here we will evaluate the design of a planar, single-junction GaAs solar cell near the Shockley-Queisser limit.

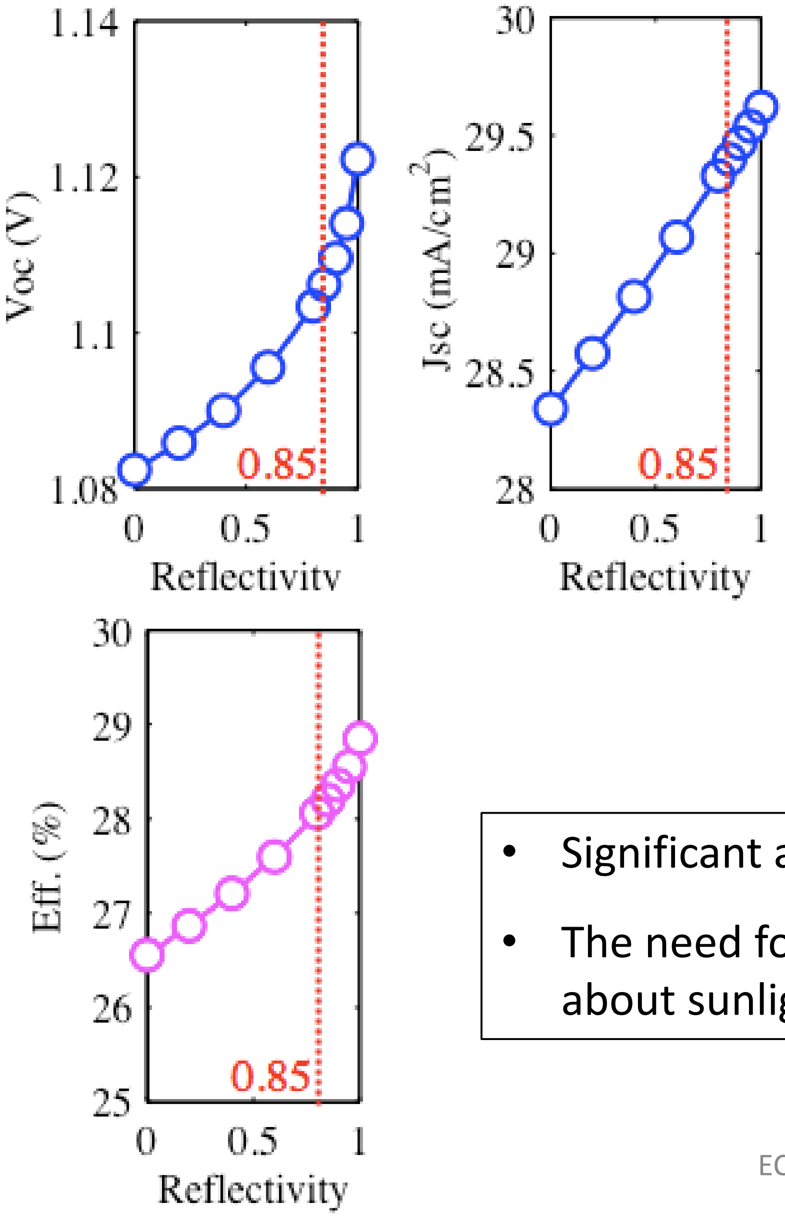
Ray tracing optics

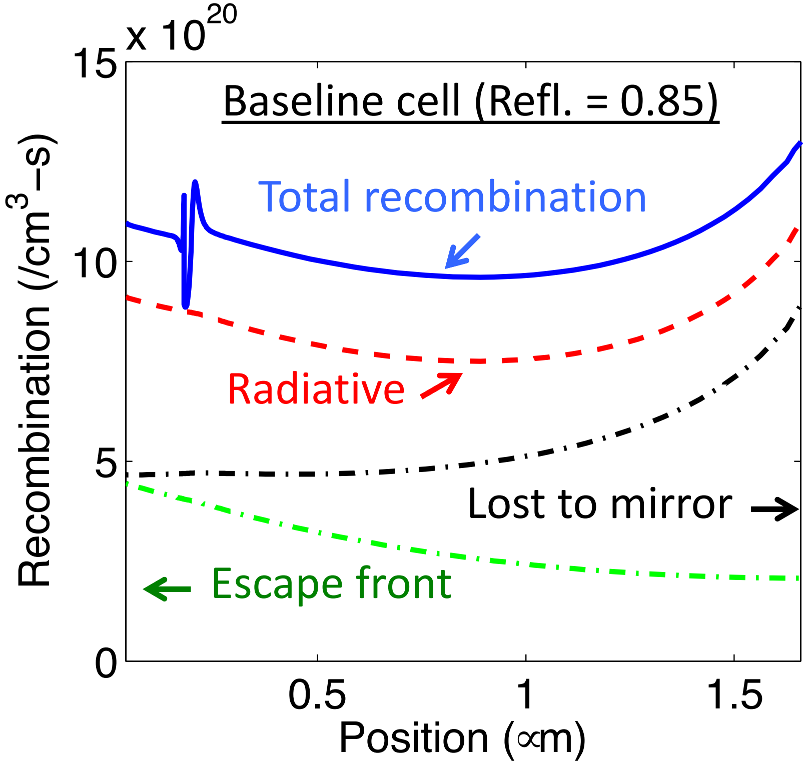


(Durbin & Gray, 1994)

- Treats planar and textured interfaces, and also mirrors with certain reflectivity.
- Treats photon recycling emission isotropically; each direction is traced independently

Impact of backside mirror quality

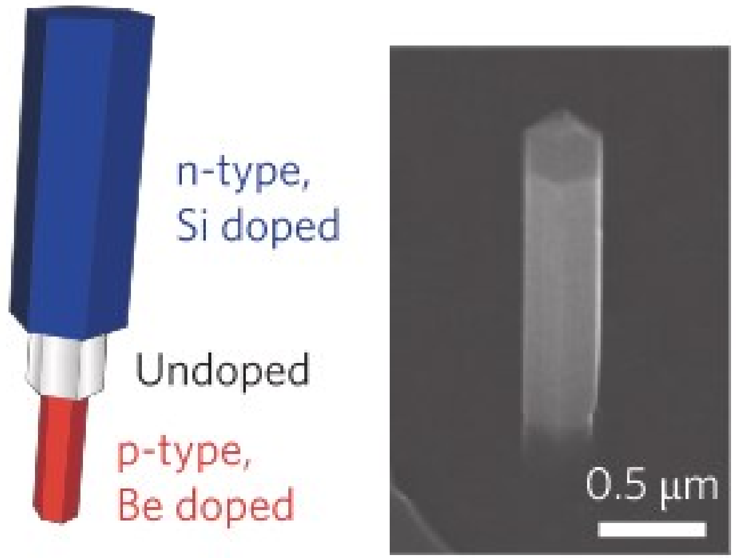




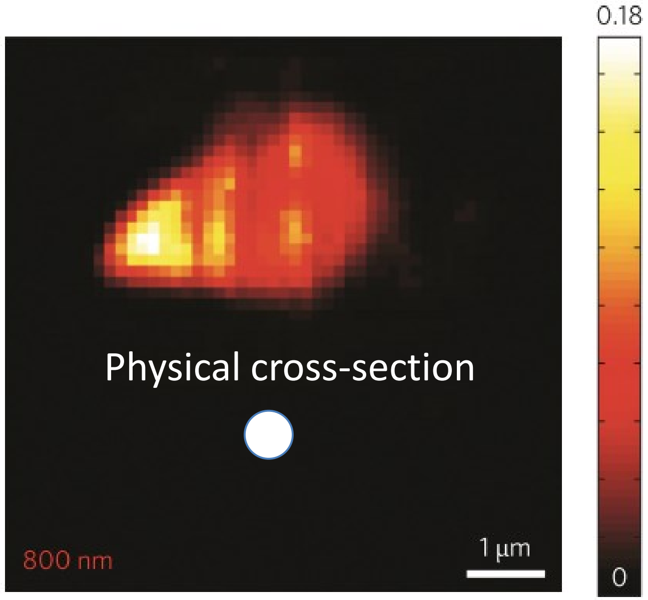
- Significant amount of radiative loss is due to rear mirror.
- The need for ultra-high mirror reflectivity is no longer about sunlight absorption—it is about photon recycling.

(Wang et al., JPV, 2013)

Nanowire solar cell



Nanowire geometry
(radial junction)



Spatially resolved light induced current

(Krogstrup et al., 2013)

Here, we can consider:

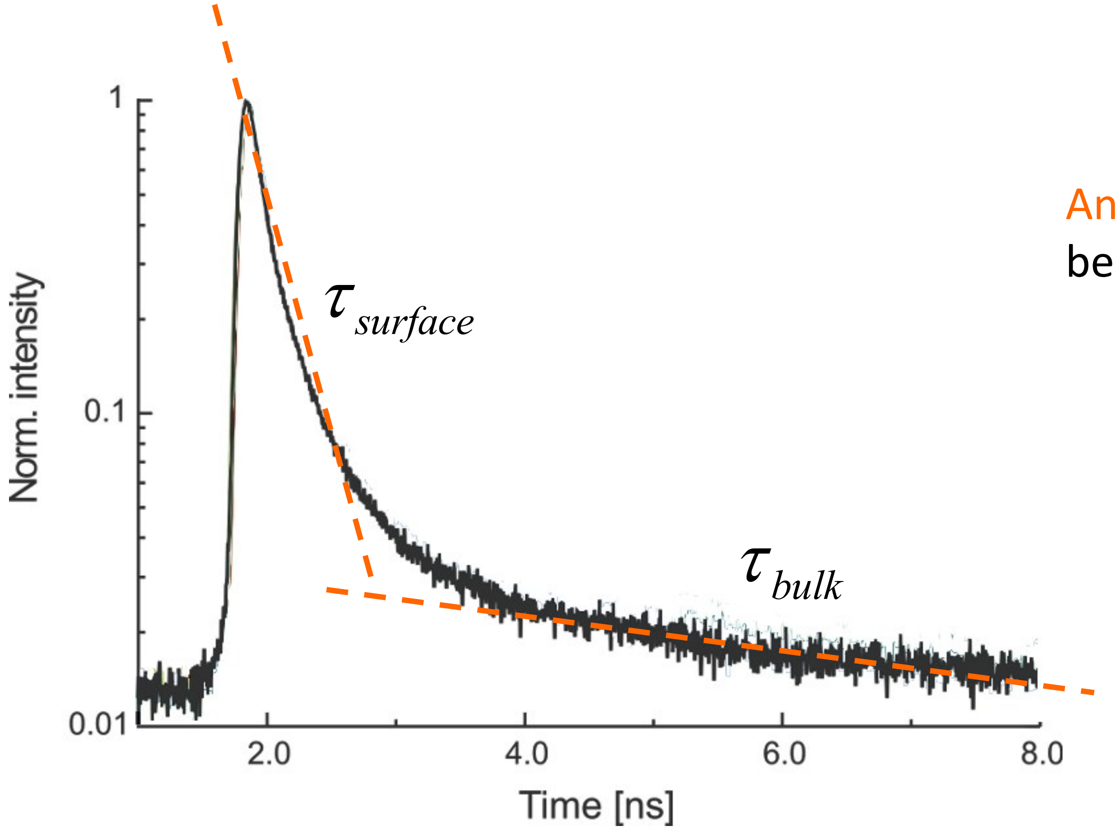
- How the design differs planar solar cells
- Major challenges to higher efficiency
- Maximum obtainable efficiency under realistic assumptions

Solar Material Characterization

Contactless, luminescence-based characterization

For deriving quantitative info. regarding surface and bulk recombination lifetime.

TRPL



Analytical, double-exponential fit can be difficult

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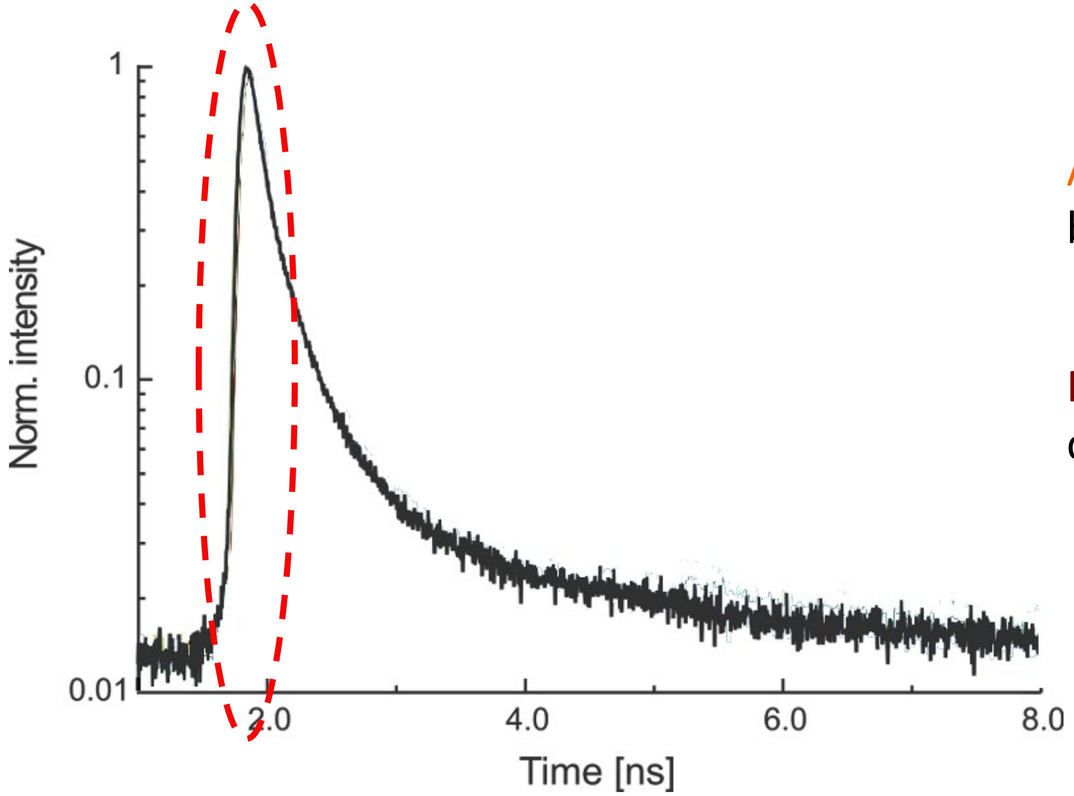
TRPL



Analytical, double-exponential fit can be difficult

Finite pulse width, instrument response decreases accuracy

Solar Material Characterization

Contactless, luminescence-based characterization

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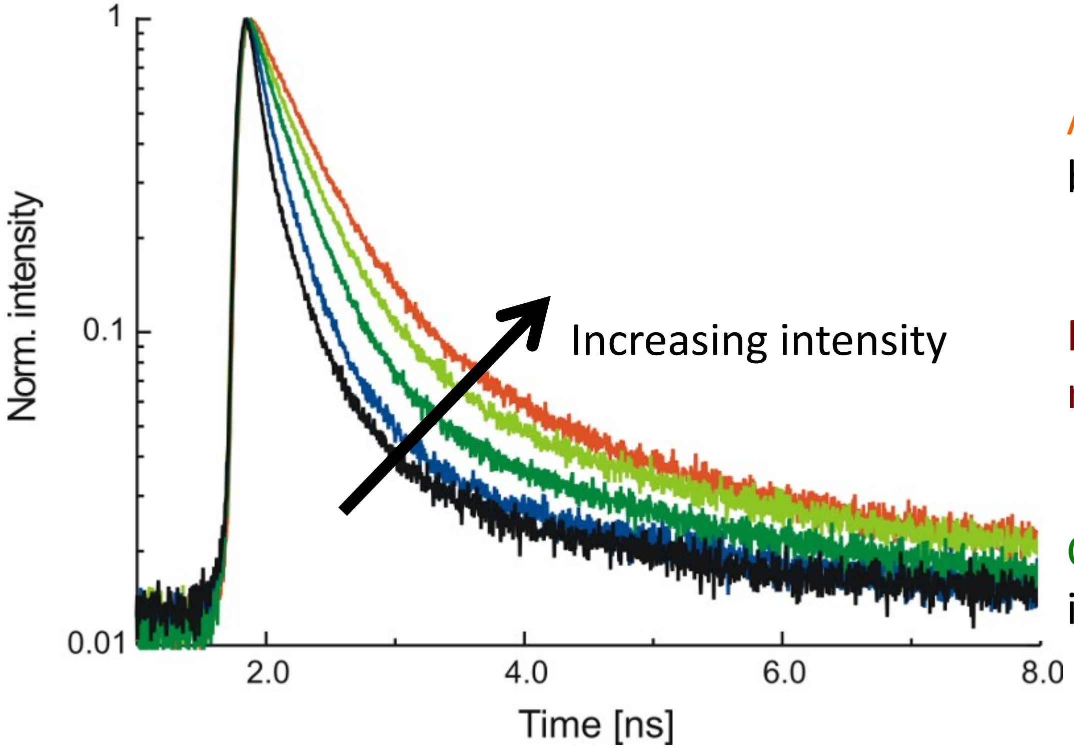
TRPL



Analytical, double-exponential fit can be difficult

Finite pulse width and instrument response decreases accuracy

Carrier dynamics complicate lifetime interpretation

Need for a new approach that can

- Complement the weakness of TRPL
- Go beyond simple analytical parameter fitting

Solar Material Characterization Method

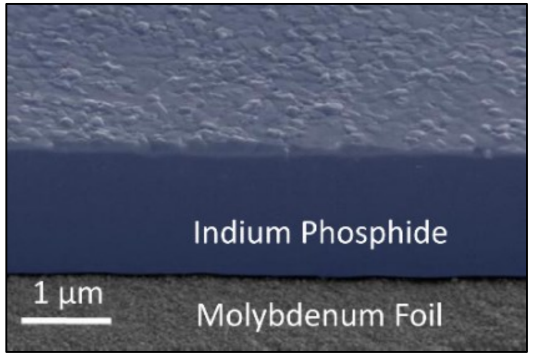
Dual characterization coupled with simulation

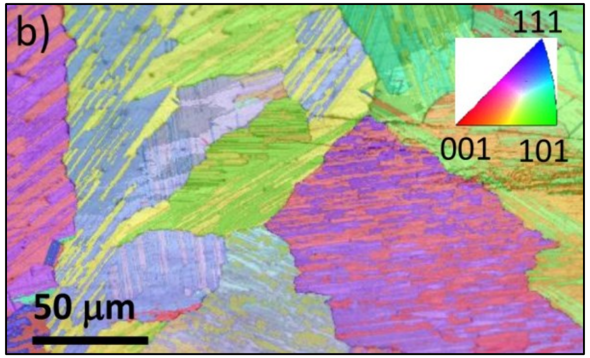
- Extract **surface** and **bulk SRH recombination** parameters.

Photoluminescence Excitation Spectroscopy (PLE) ⟷ **Time Resolved Photoluminescence (TRPL)**

E-O Coupled Simulator

Apply method on novel VLS-grown InP thin film





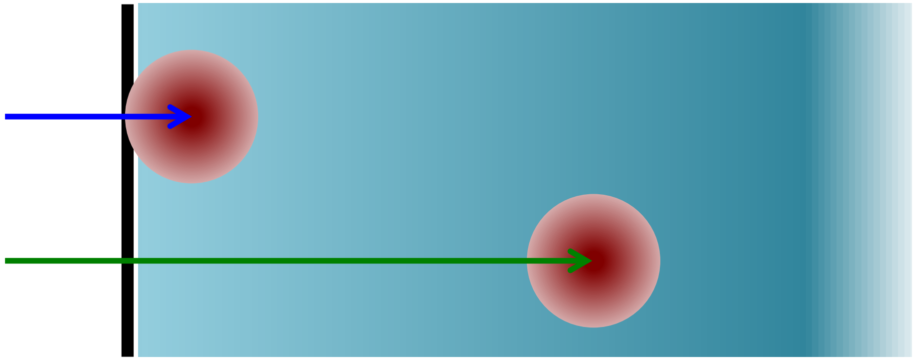
R. Kapadia et al., Scientific Reports 3, 2275 (2013)

Photoluminescence Excitation Spectroscopy (PLE)

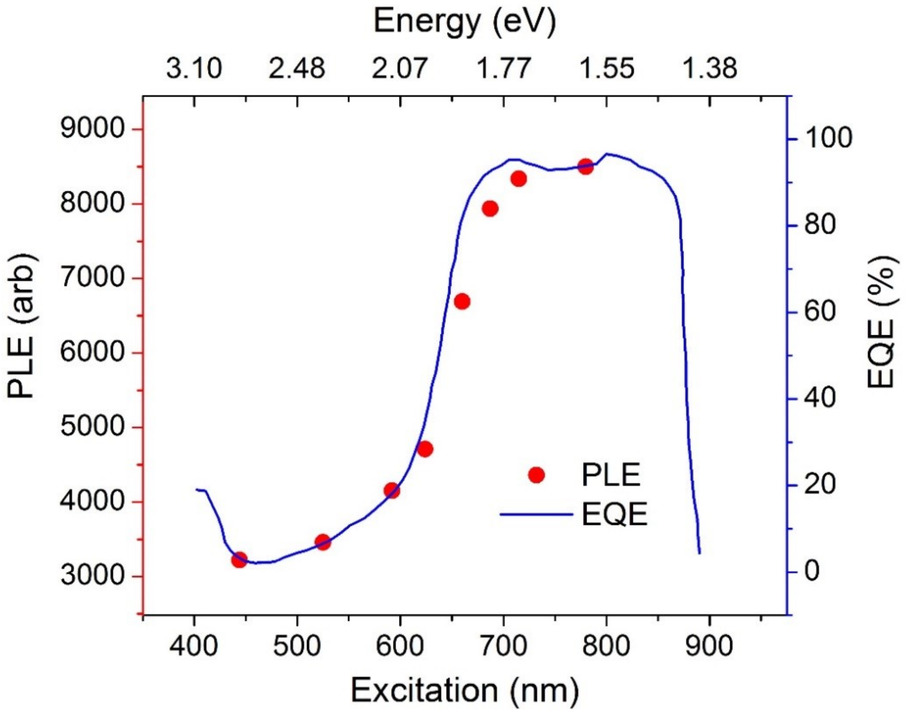
- Open-circuit version of EQE (emission instead of current)

$$PLE(\lambda) = \frac{emission}{input\ flux(\lambda)}$$

Thin film/cell



(wavelength -> position)

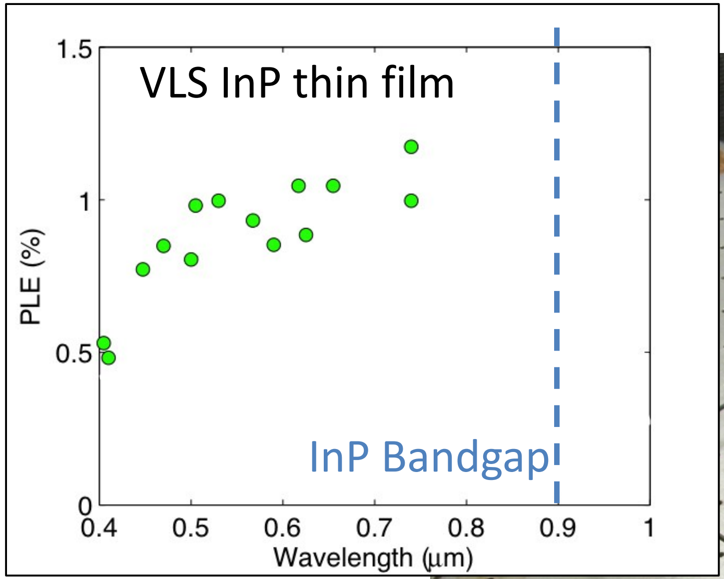


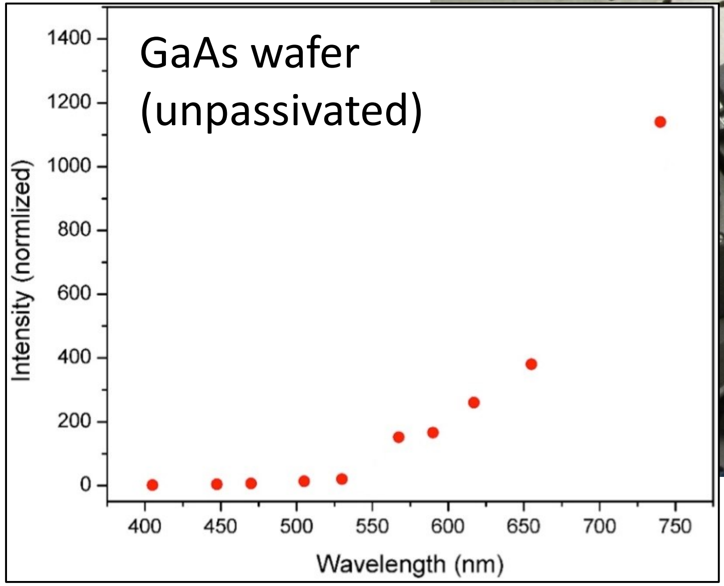
- **PLE** (open-circuit) is closely related to **EQE** (short-circuit) in high quality GaAs Solar cells.

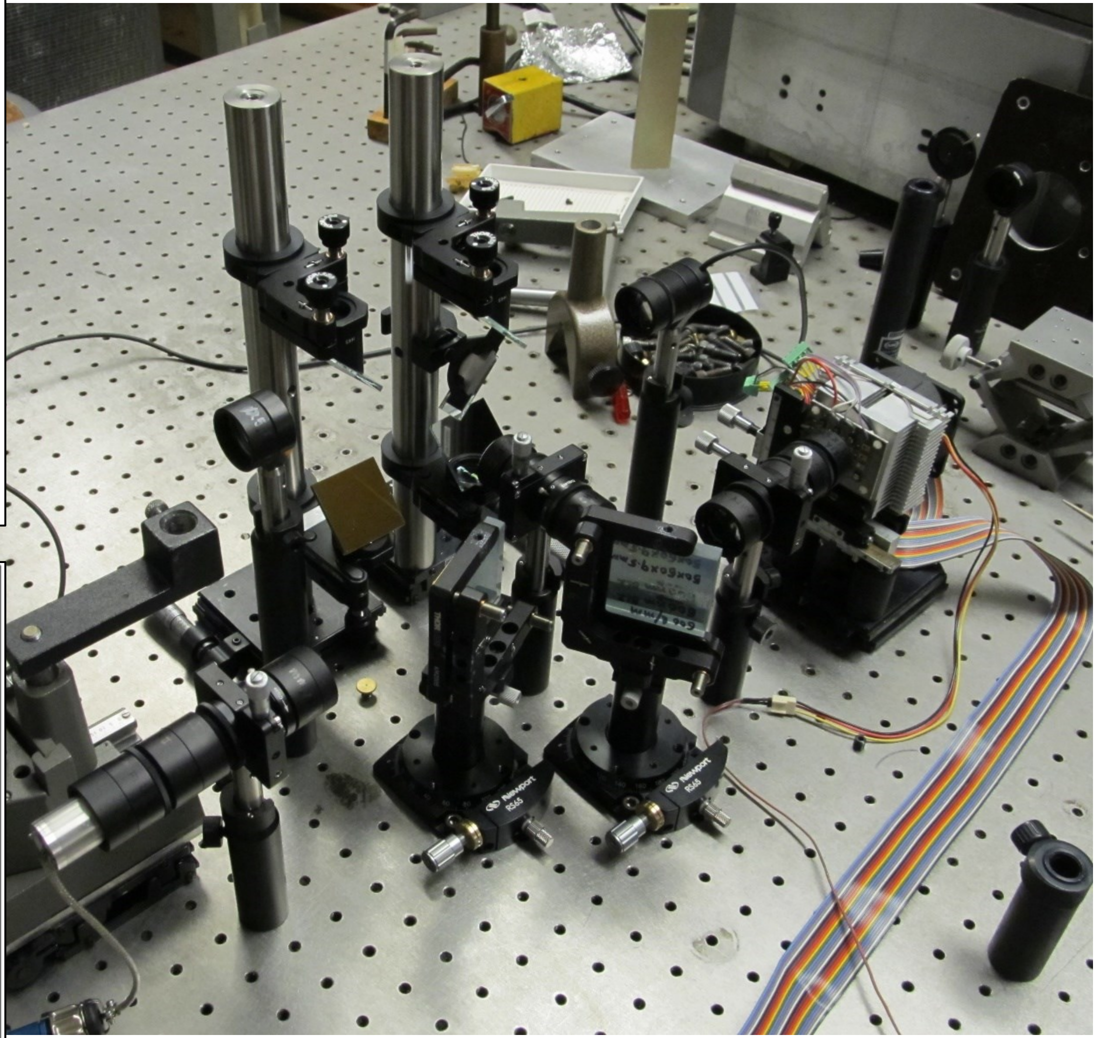
D. Berdebes et al., IEEE Journal of Photovoltaics 3, 1342 (2013)

PLE Measurement Result

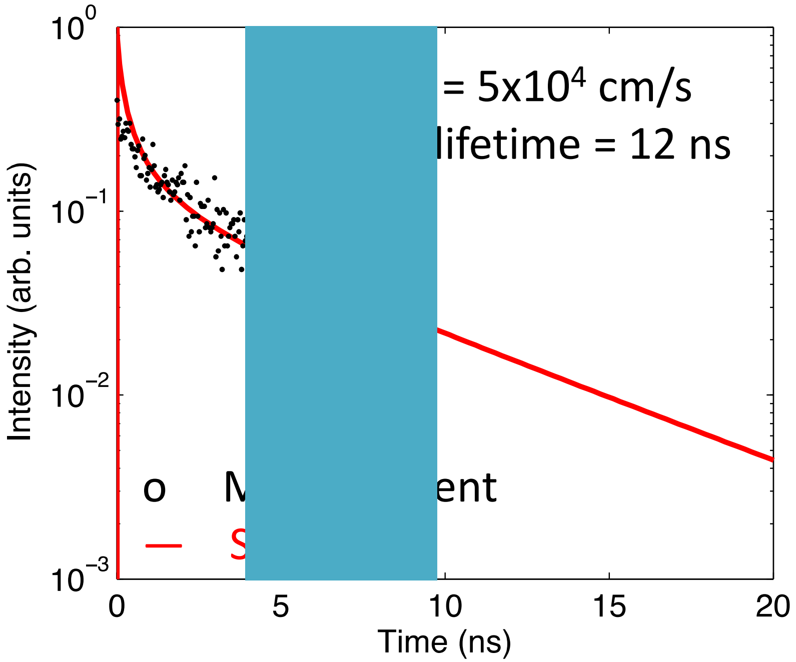
(See more results in X. Wang et al., JPV 2015)

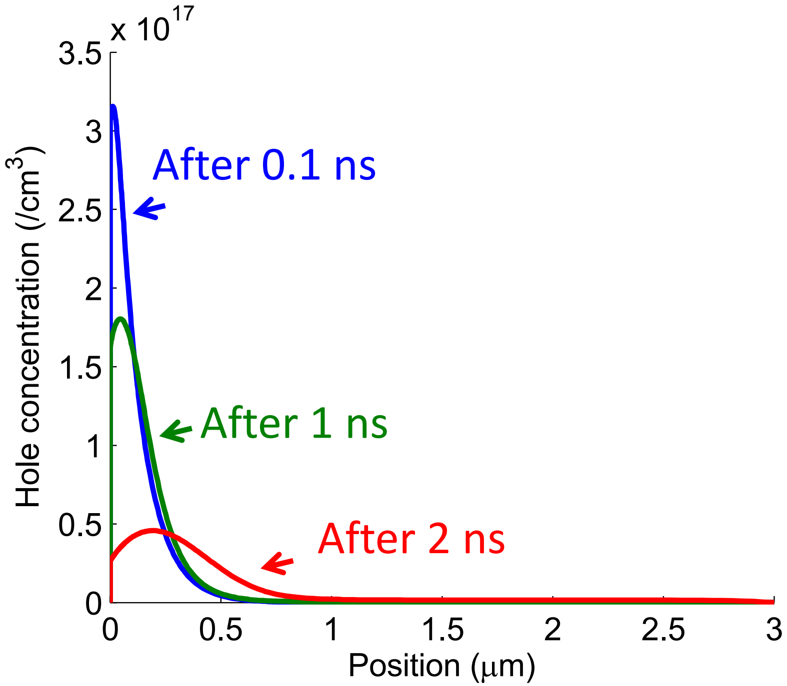


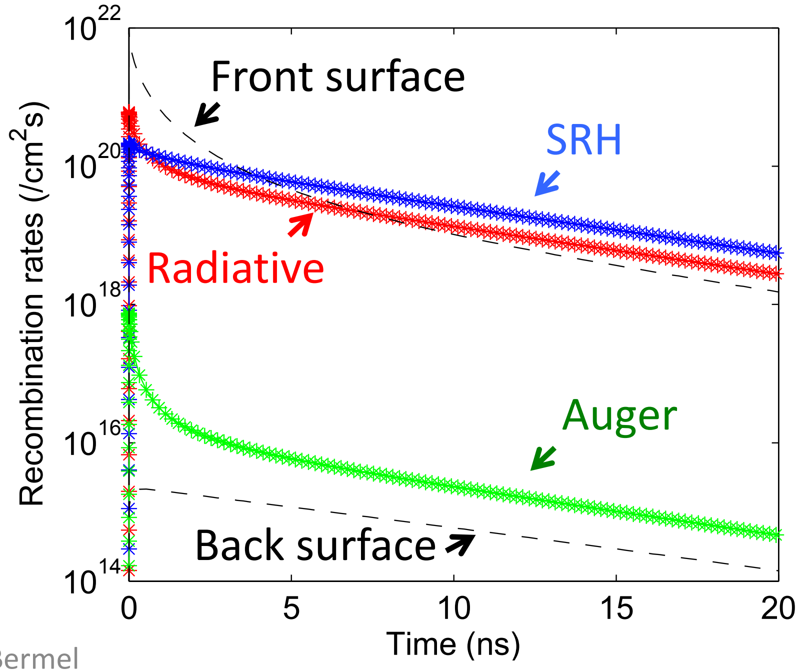




TRPL: VLS-grown InP thin film

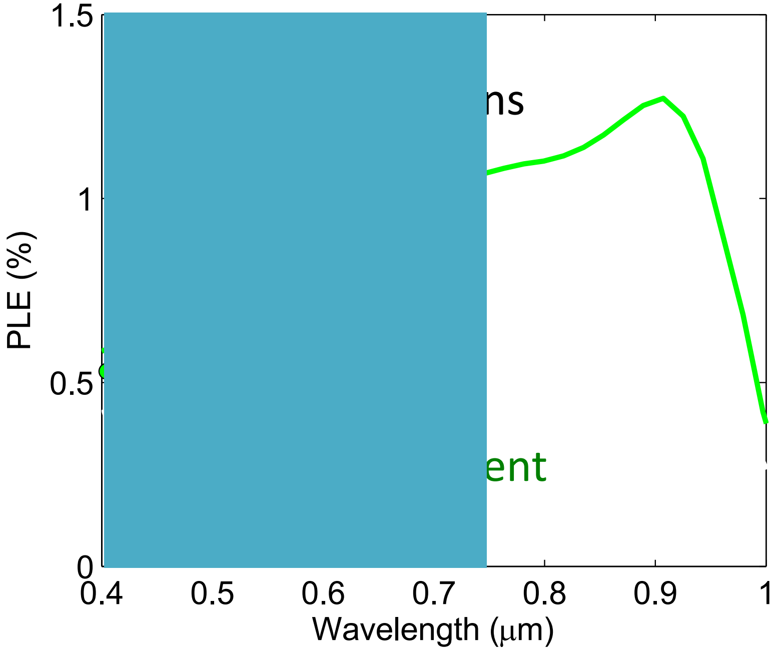


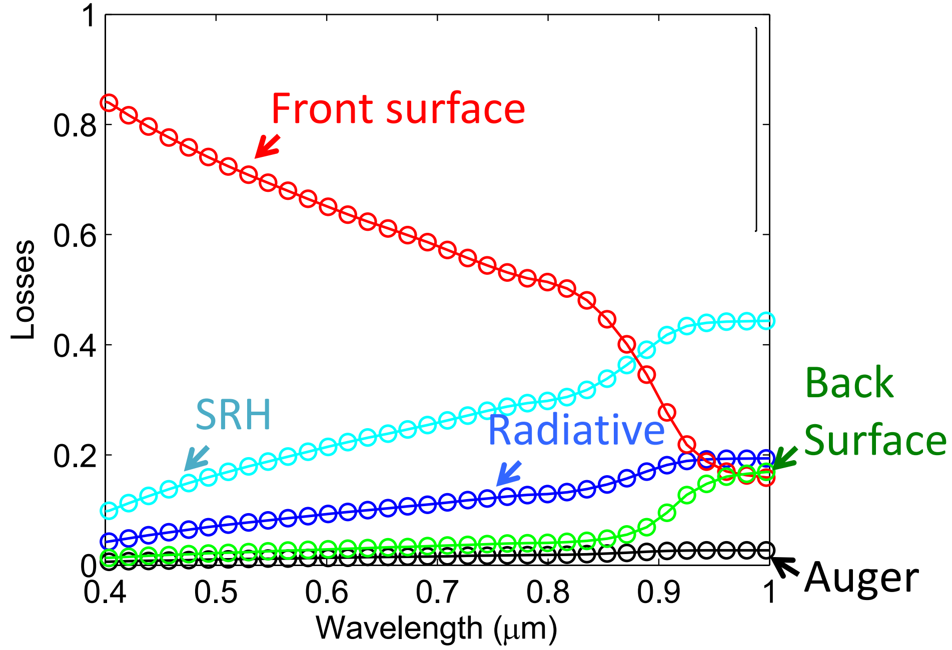




- **Initial (< 4 ns)**: Surface recombination dominates
- **Later (> 4 ns)**: Bulk recombination dominates.

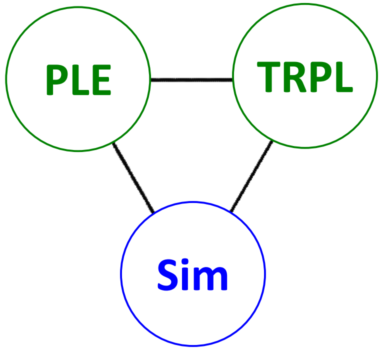
PLE: VLS-grown InP thin film

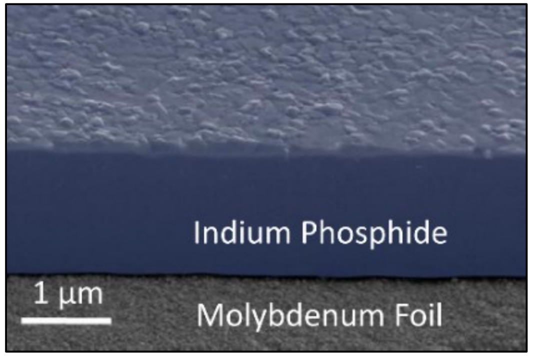




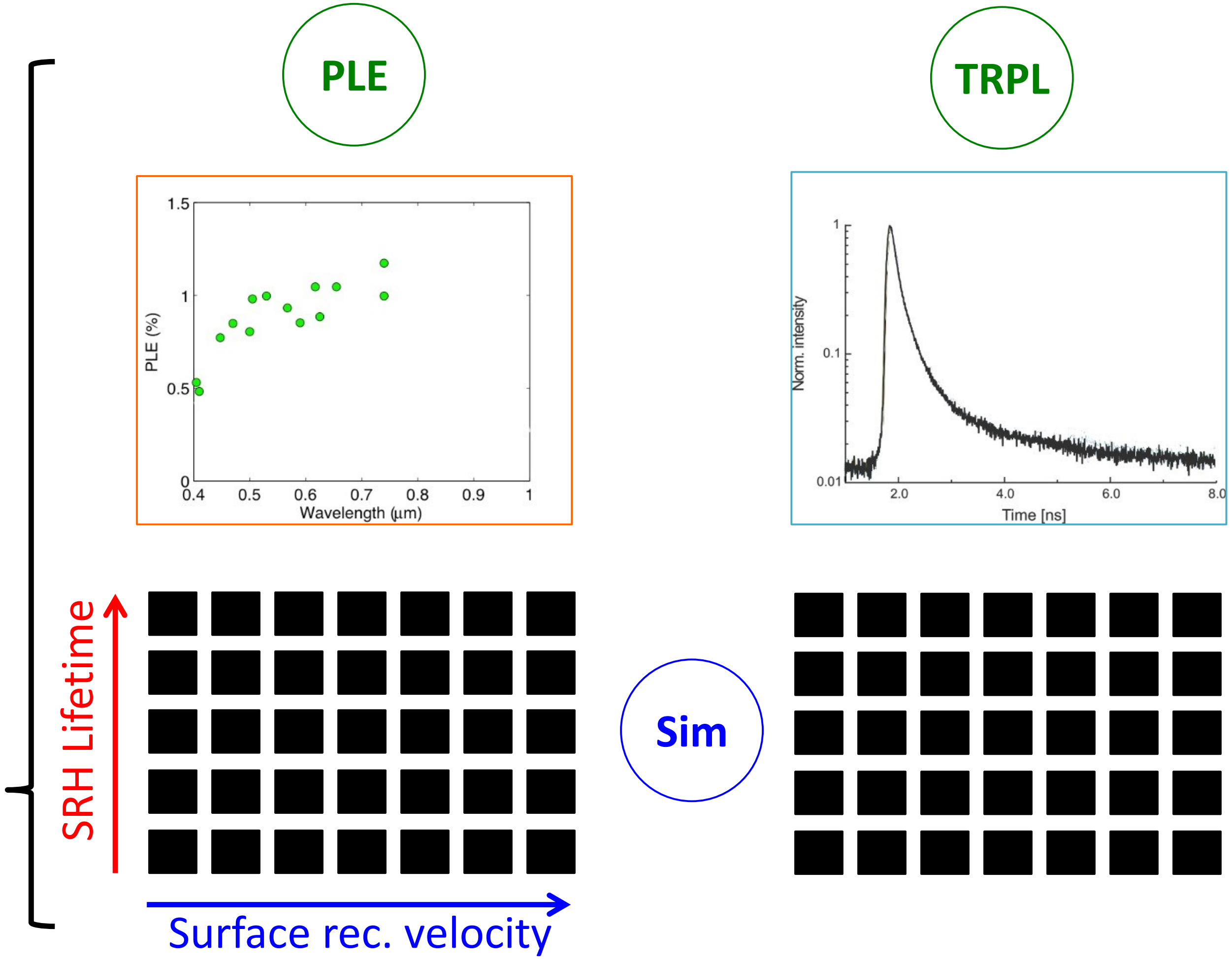
- **Short wavelength (< 870 nm)**: Surface recombination dominates
- **Long wavelength (> 870 nm)**: Bulk recombination dominates

Overall scheme

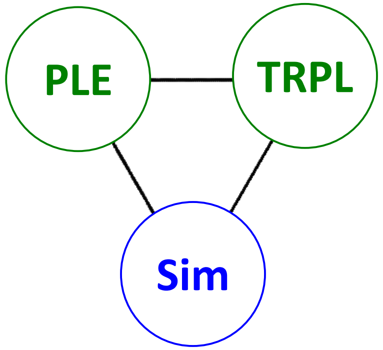


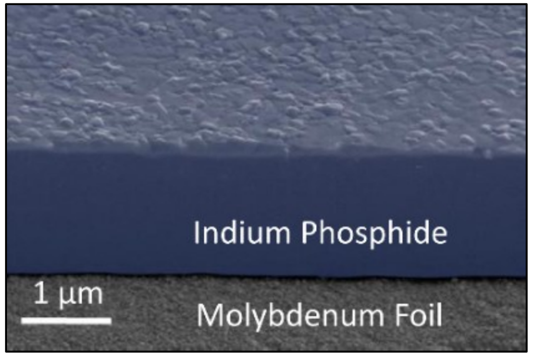


Sample under test



Overall scheme





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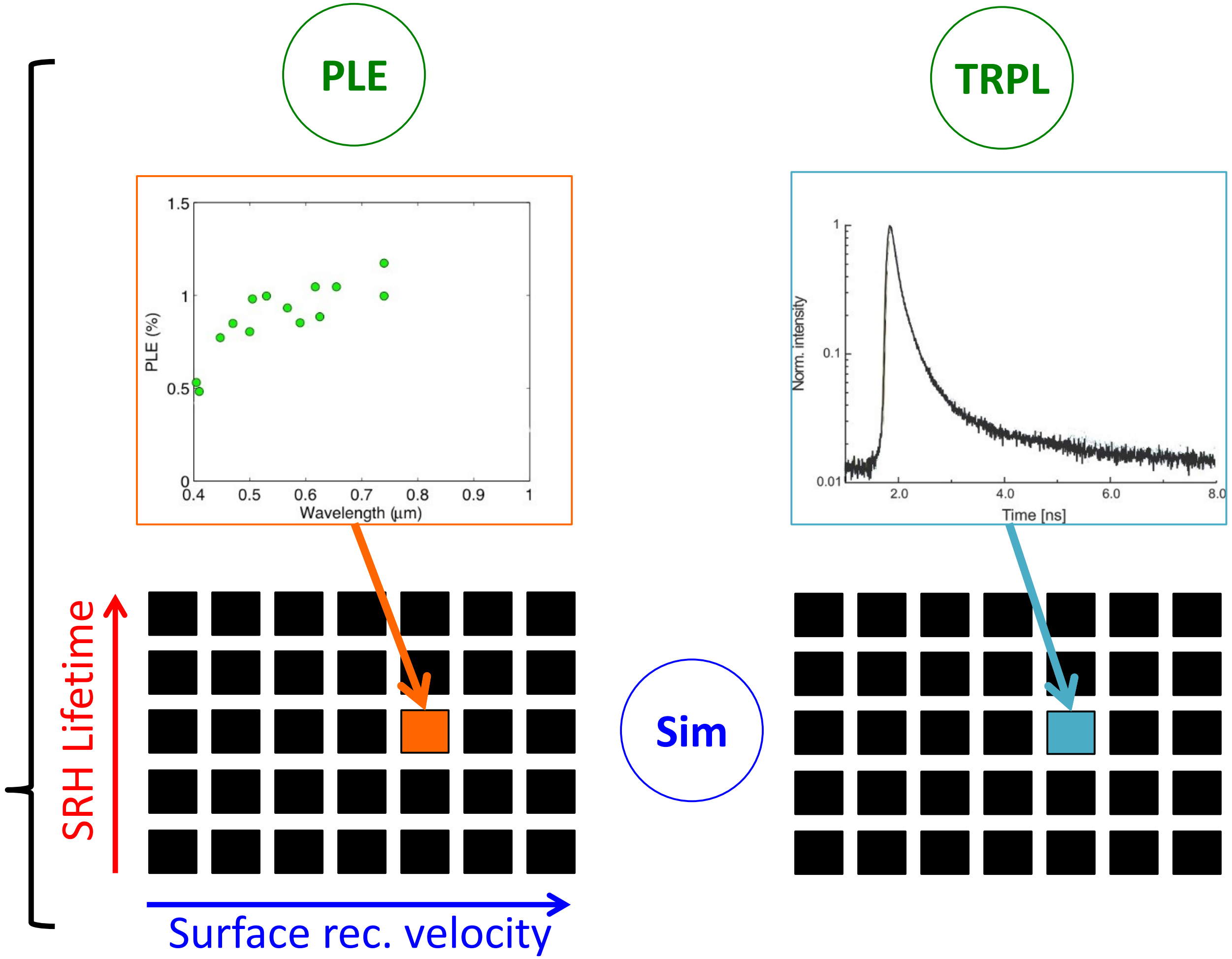

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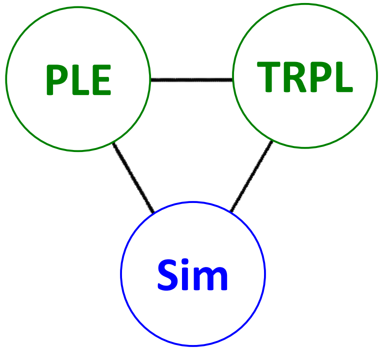

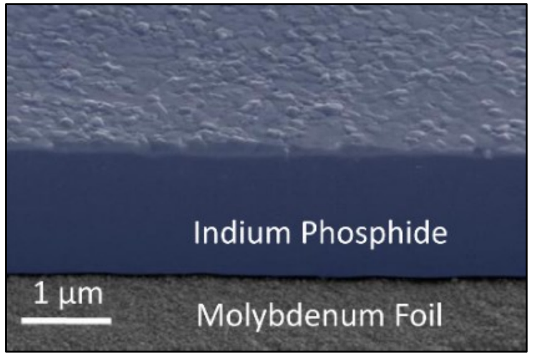

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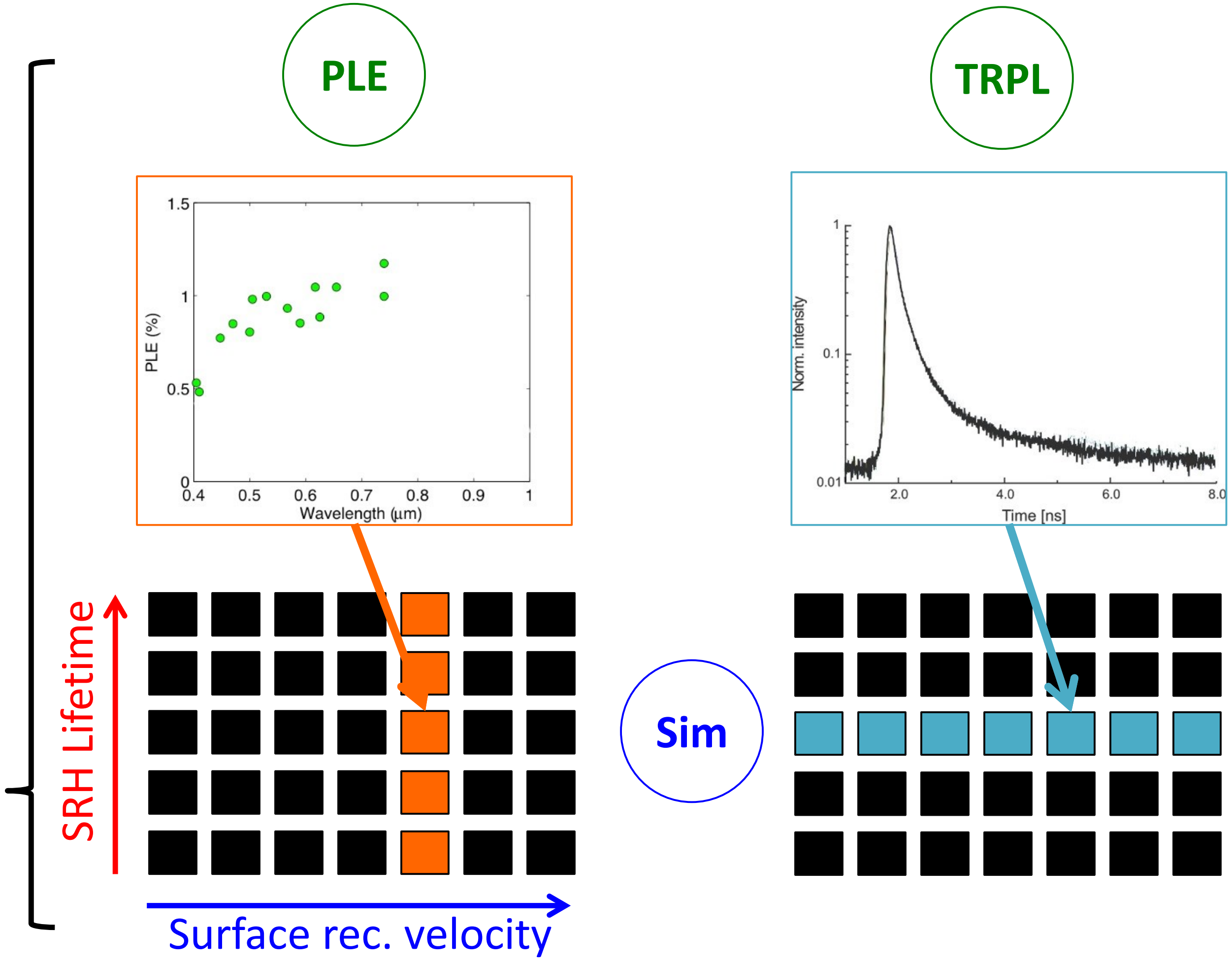
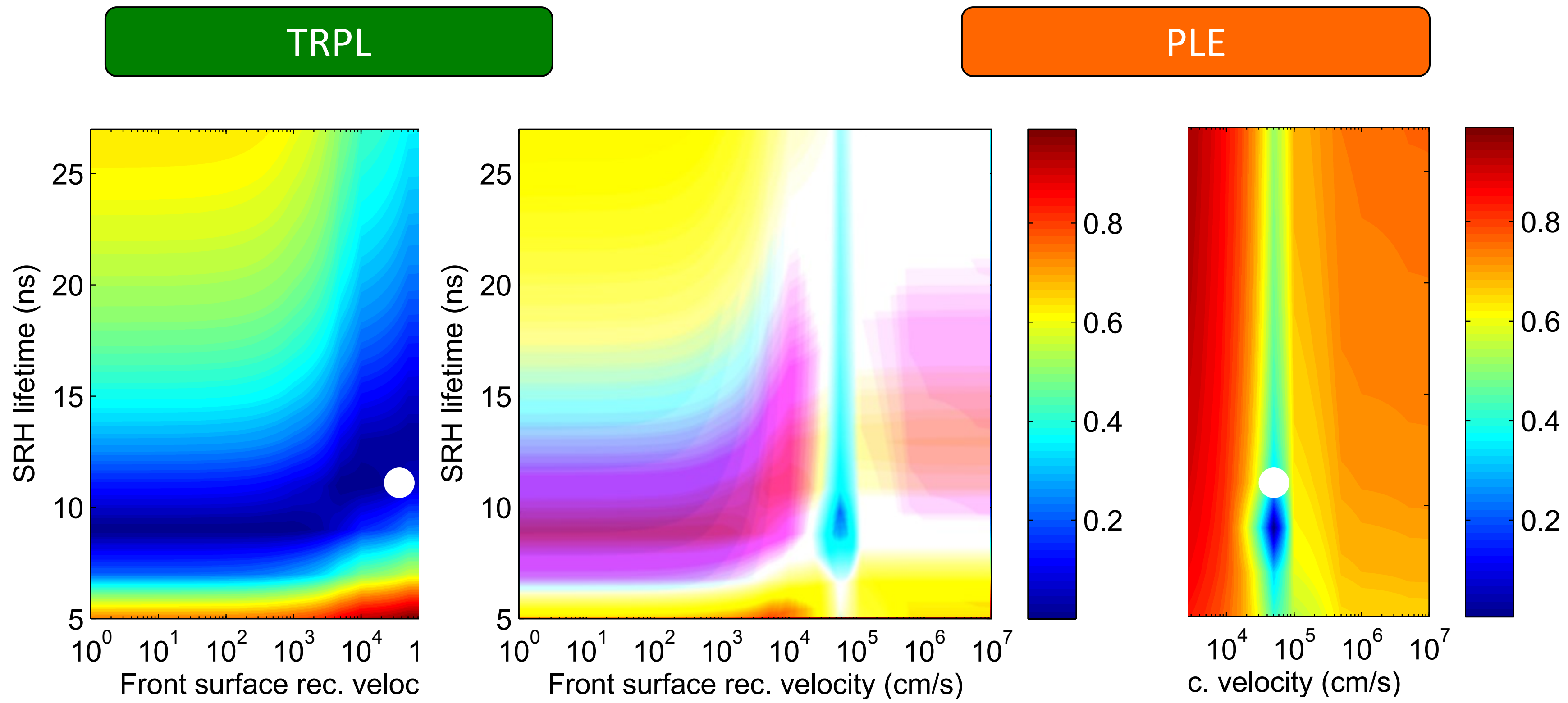


Least square error



- **TRPL is more sensitive to SRH lifetime, while PLE is more sensitive to front surface recombination.**
- For this particular sample displays a bulk SRH lifetime of **12 ns** and surface recombination velocity of **5×10^4 cm/s**

Next Class

- Next time: we will continue finite-difference time domain techniques, as applied to thermophotovoltaics
- Suggested reference: *Thermophotovoltaics: Basic Principles and Critical Aspects of System Design*, by Thomas Bauer