Faculty of Engineering
School of Photovoltaic and Renewable Energy Engineering

UNSW SYDNEY | Australia's Global University

Solcore Workshop – Silicon Tandem Cell Computer Modelling

Sungkyunkwan University, 1 – 3 August 2023

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www.qpvgroup.org

EkinsNed

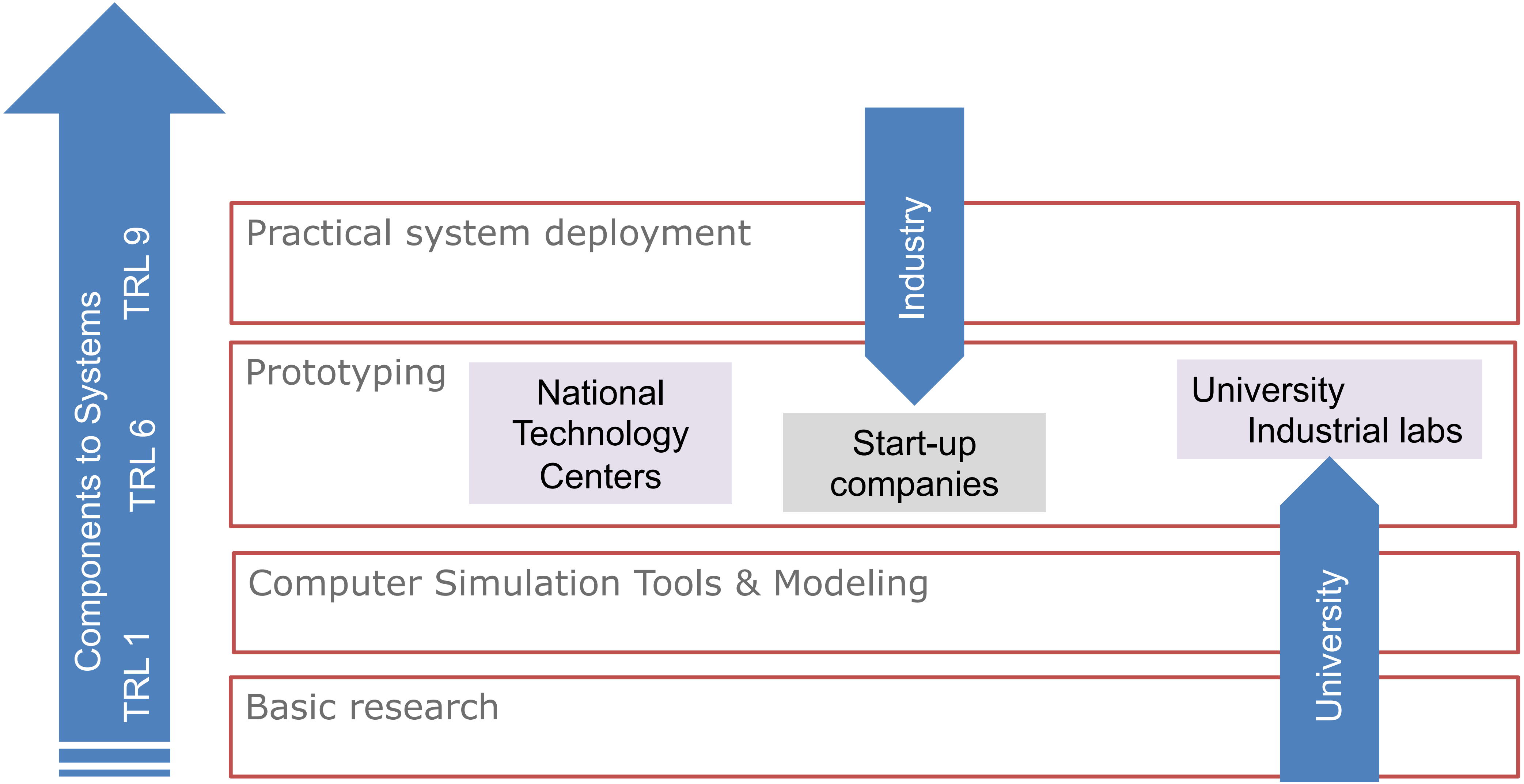
Faculty of Engineering
School of Photovoltaic and Renewable Energy Engineering

Session 1: Introduction

1 August 2023

Ned Ekins-Daukes, Phoebe Pearce

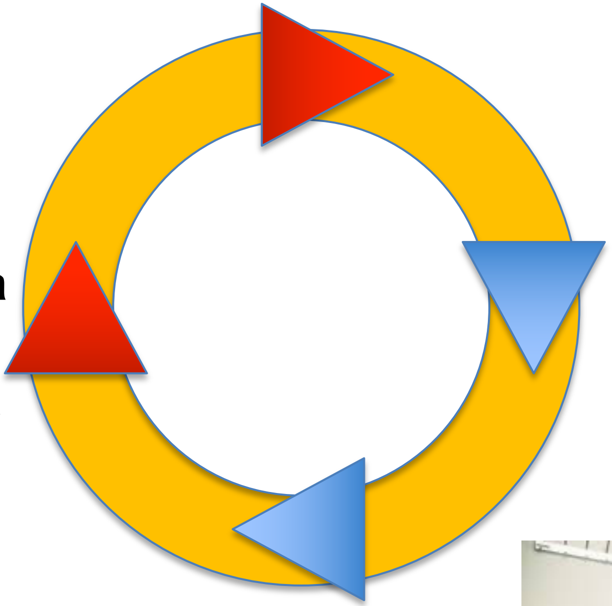
A Role for Computer Simulation in the Modern Technological Innovation Process



“Think Play Do: technology, innovation and organisation”, Mark Dodgson, David Gann and Ammon Salter, 2005, Oxford University Press, ISBN 9780199268092

The Present Value of Computer Modelling in Research & Development

Design aided by
a computer (TCAD):



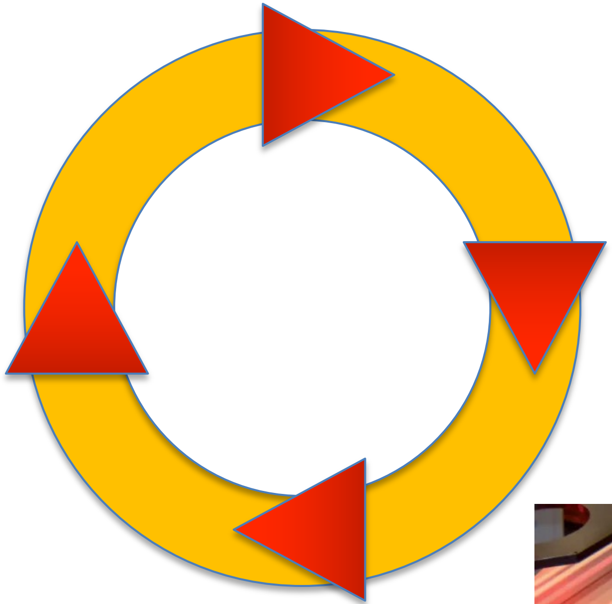
Evaluate data
through
fitting of data

Device
Fabrication

Device Test

The Future Value of Computer Modelling in Research & Development

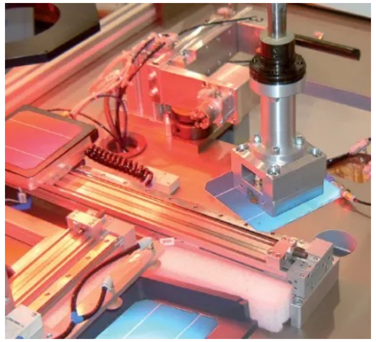
Design aided by a computer (TCAD):



Robot Device Fabrication

AI assisted fitting of test data

Automated Device Test

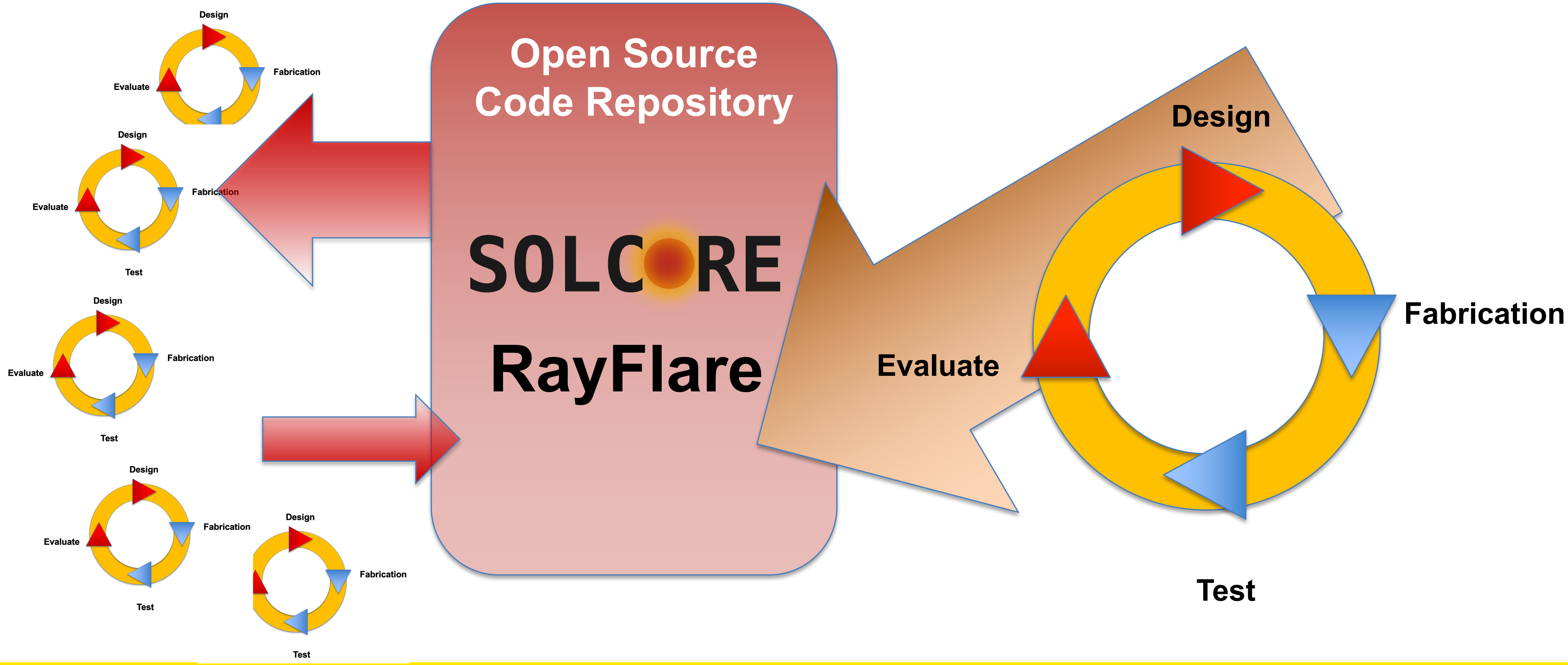


Rachel Kurchin, Giuseppe Romano, & Tonio Buonassisi,. 'Bayesim: A tool for adaptive grid model fitting with Bayesian inference'. Computer Physics Communications, (2019)

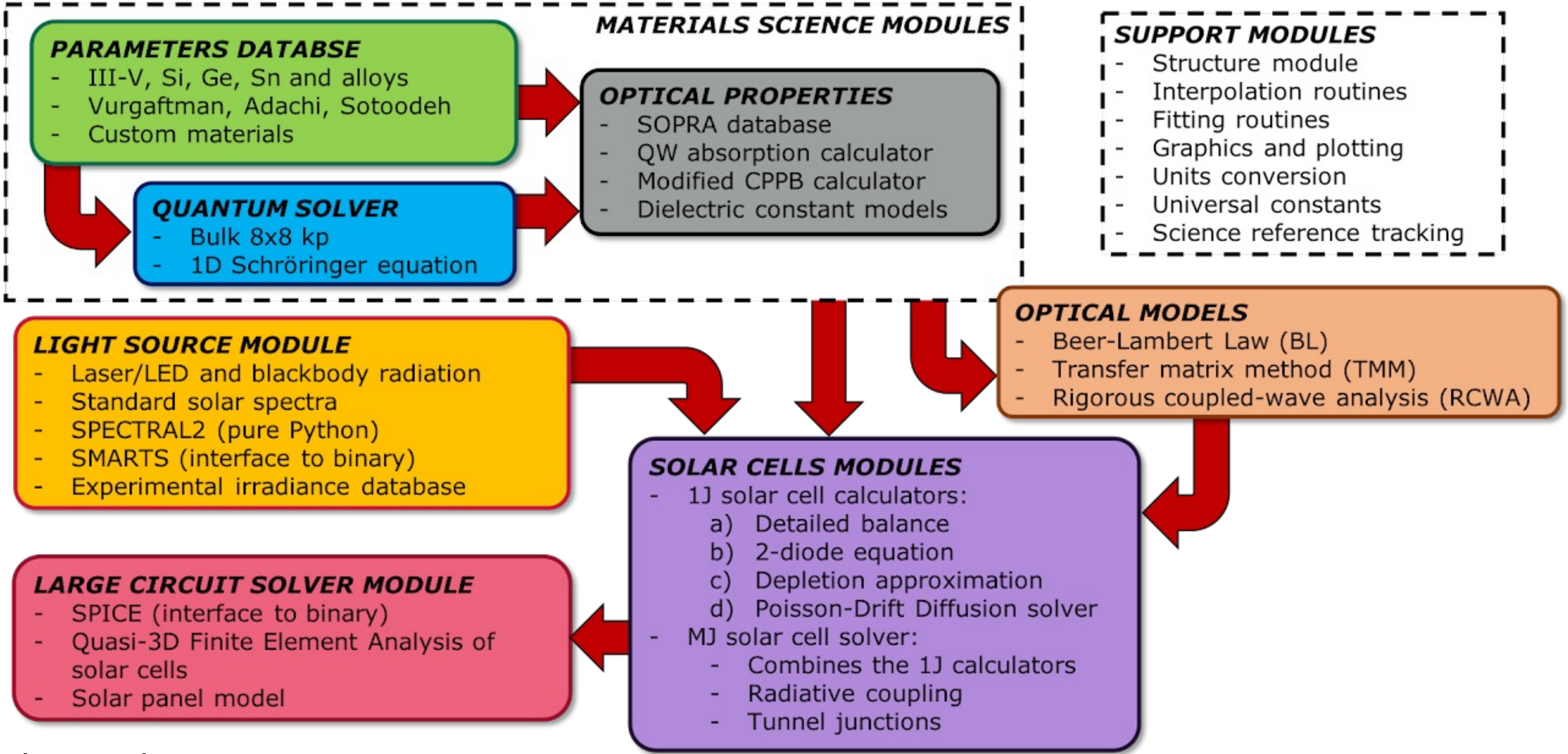
Development Process for our Computer Code:

Global PV R&D Community

QPV Research Group



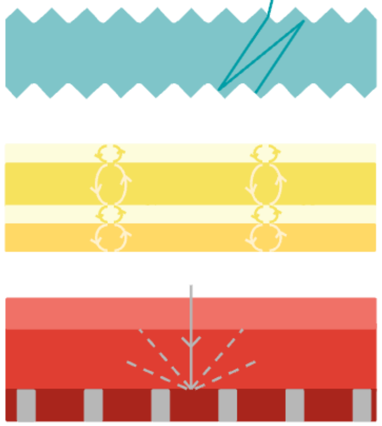
Solcore capabilities



www.solcore.solar

RayFlare capabilities

Simulations using a single method



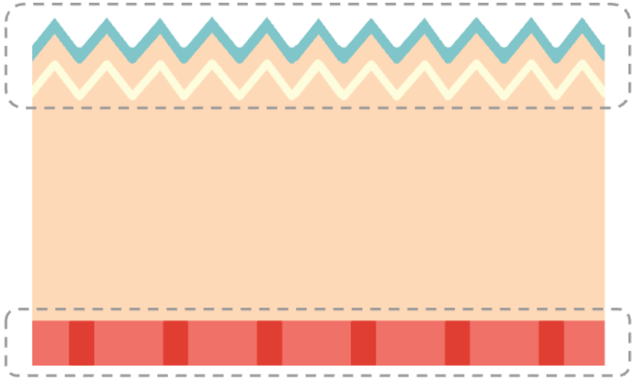
Ray-tracing: Geometric optics for large-scale textures without diffraction effects

Transfer-matrix method: Wave optics for planar layers (coherent and incoherent)

Rigorous coupled-wave analysis: Wave optics for planar or periodic structures e.g. gratings, photonic crystals

Ideal cases: E.g. perfect mirrors, Lambertian scattering

Simulations using angular redistribution matrices
Each surface is treated separately with an appropriate method



Calculate e.g. reflection, transmission, absorption per layer, depth-dependent absorption profiles

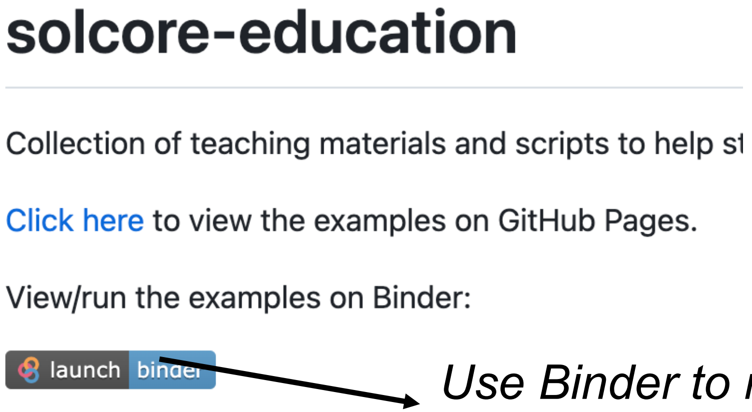
- Free, open source
- Anyone can contribute
- Modular
- Documented

https://rayflare.readthedocs.io

Course instructions

GitHub repository where the tutorials for this workshop are hosted:

https://tinyurl.com/2mn6rb64



Look at the tutorials + the expected outputs online

Use Binder to run Python in your browser & work through the examples

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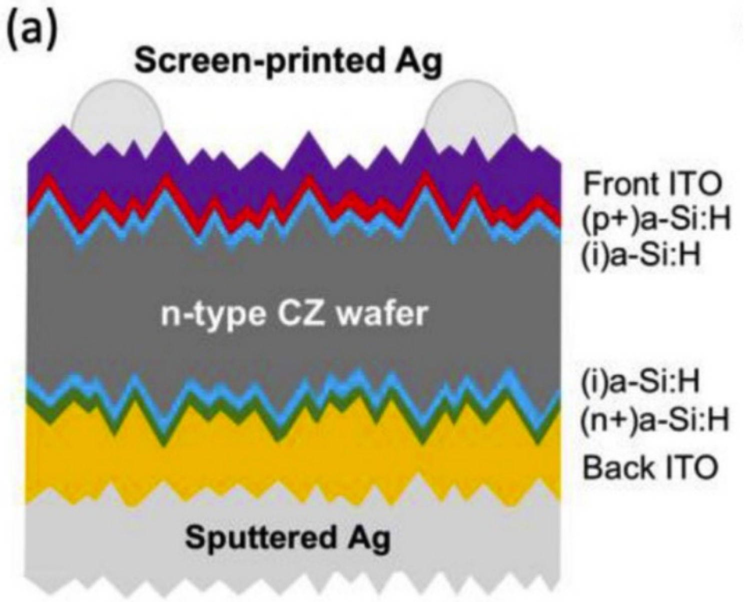
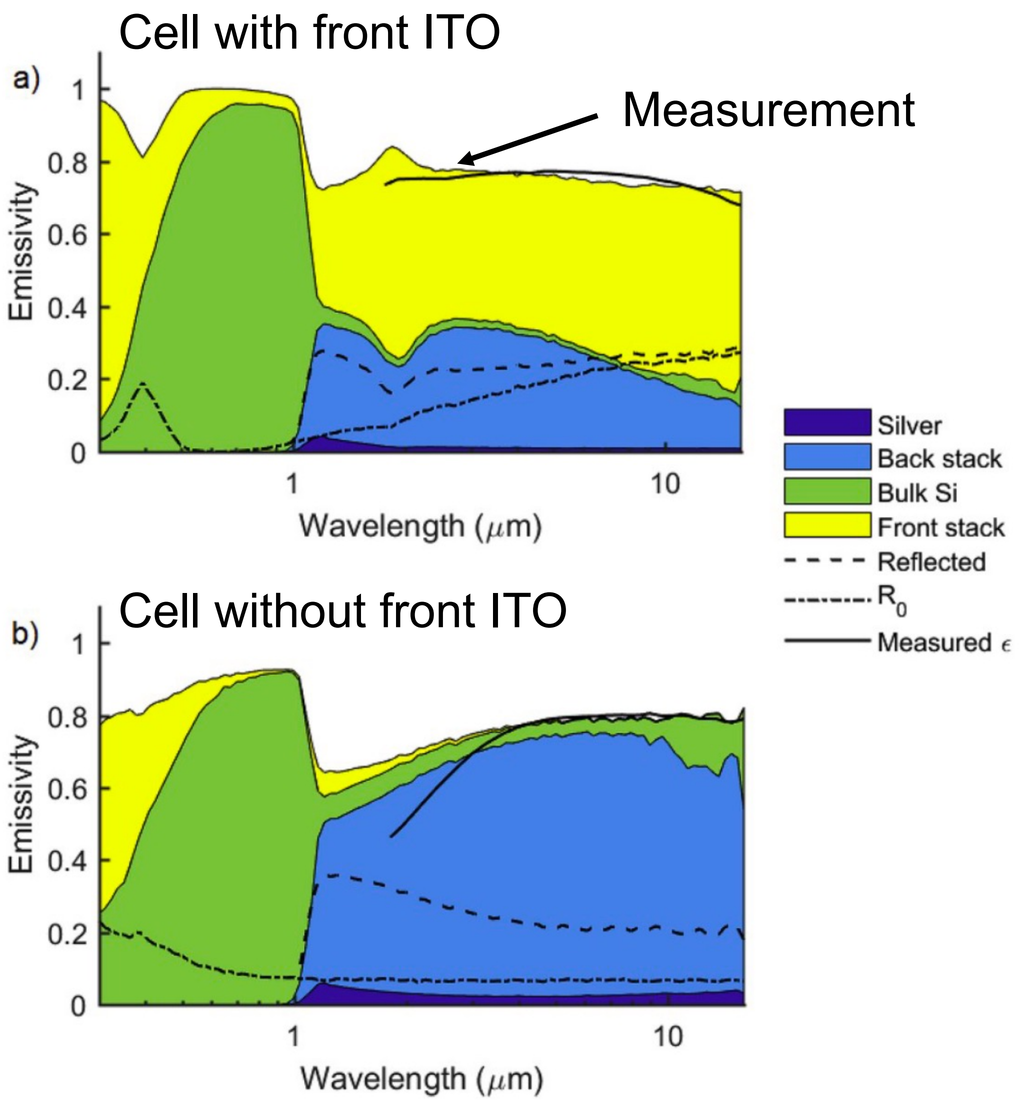
To run Solcore & RayFlare on your own computer, you will need to install Python (version 3.7 to 3.11):

Recommendations:

- On **Windows**, use **miniconda** (https://conda.io/miniconda.html)
- On **MacOS**, use **Homebrew + venv (**see RayFlare's installation instructions for more detail)
- On **Ubuntu/Linux**, use **system Python + venv** (see RayFlare's installation instructions for more detail)

Example: Si cell emissivity

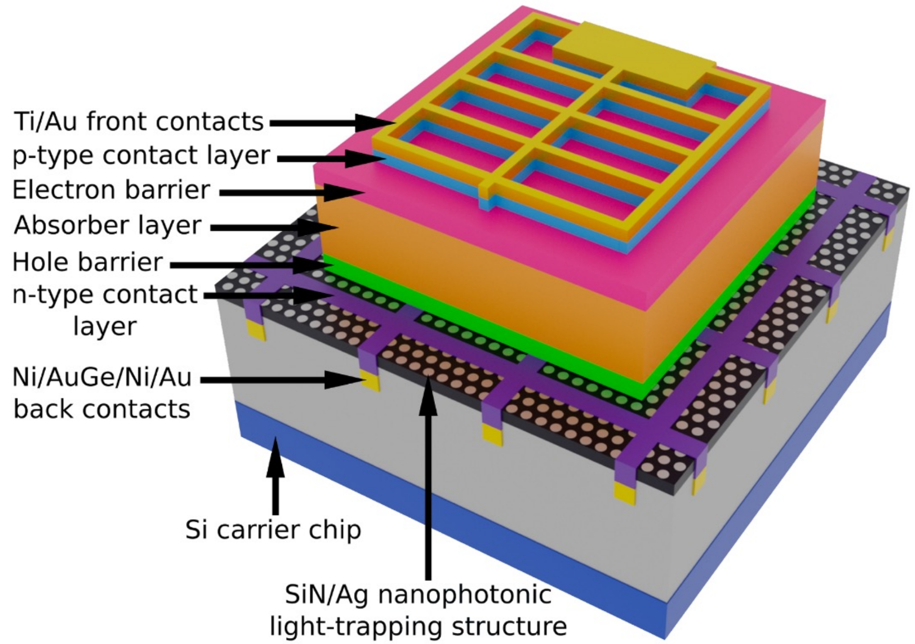


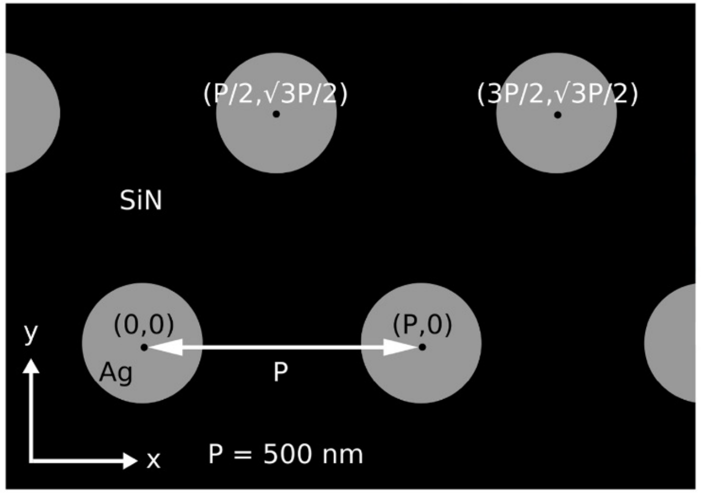


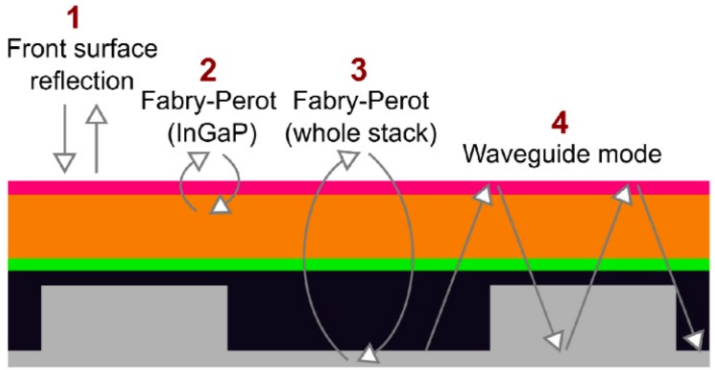
Simulations & measurement of cell absorptivity (emissivity) between 300 nm and 20 µm. This is relevant for the operating temperature of the cell. Due to free-carrier absorption in doped layers and very good light-trapping, the cell absorbs well even at wavelengths far beyond the bandgap.

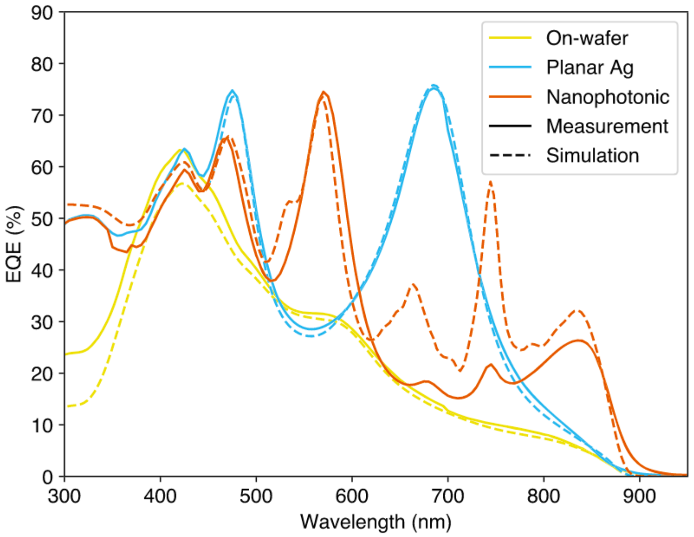
D. Alonso-Álvarez *et al.*, ‘Thermal emissivity of silicon heterojunction solar cells’, *Solar Energy Materials and Solar Cells*, vol. 201, no. May, p. 110051, 2019, doi: 10.1016/j.solmat.2019.110051.

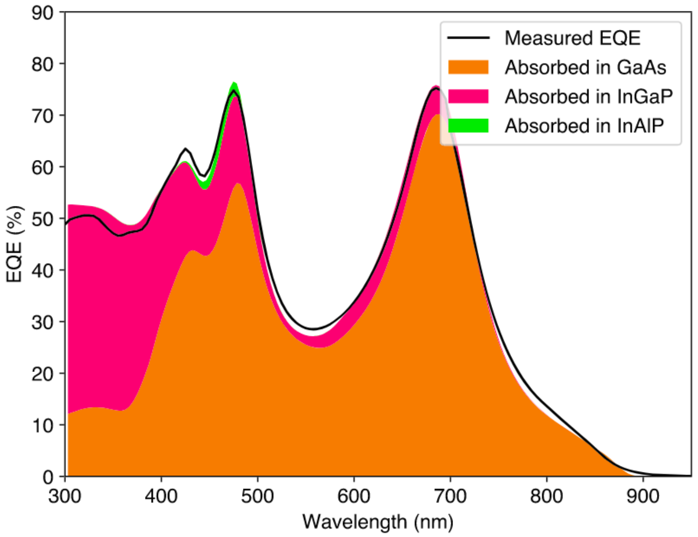
Example: ultra-thin GaAs cell





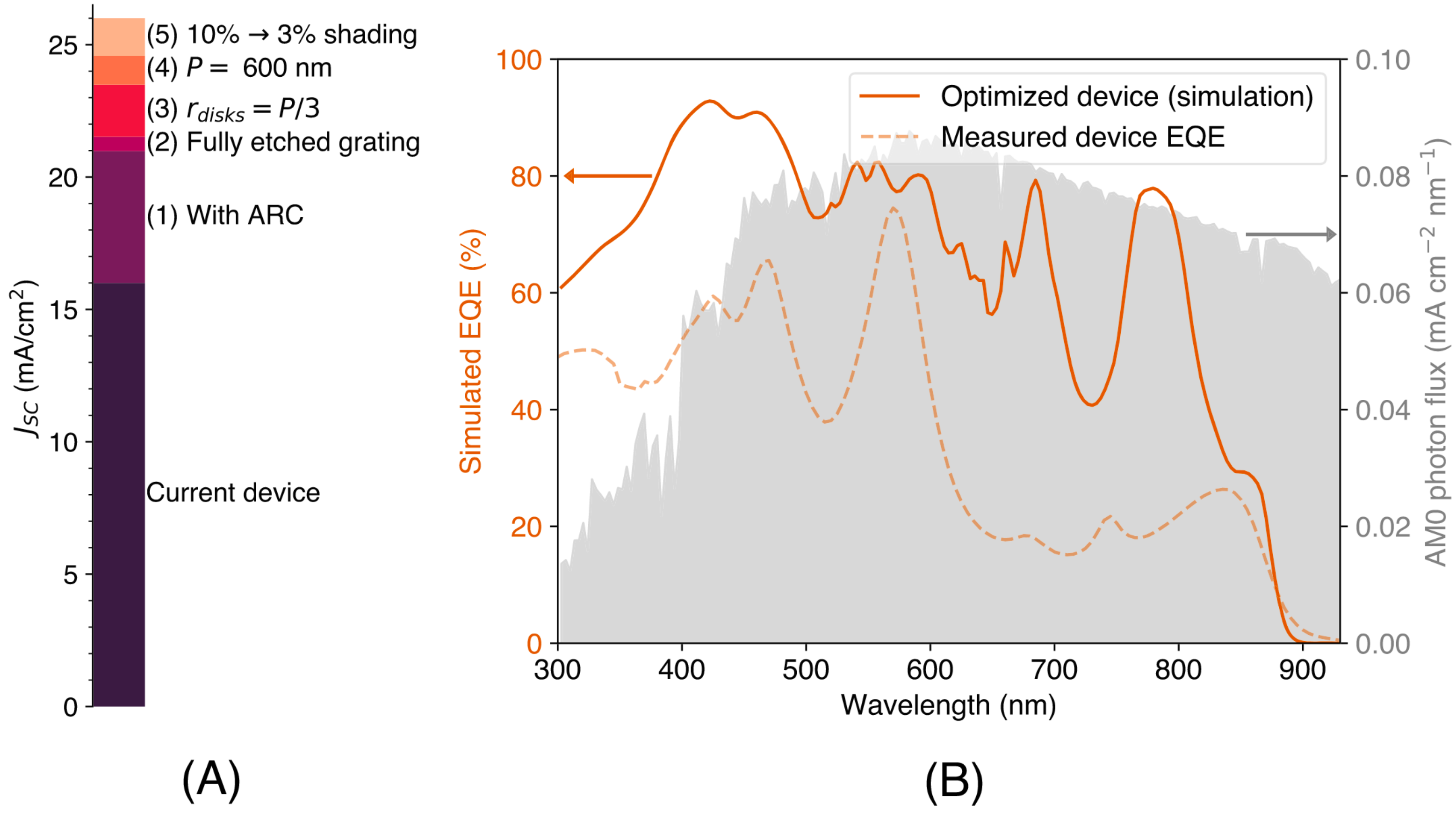




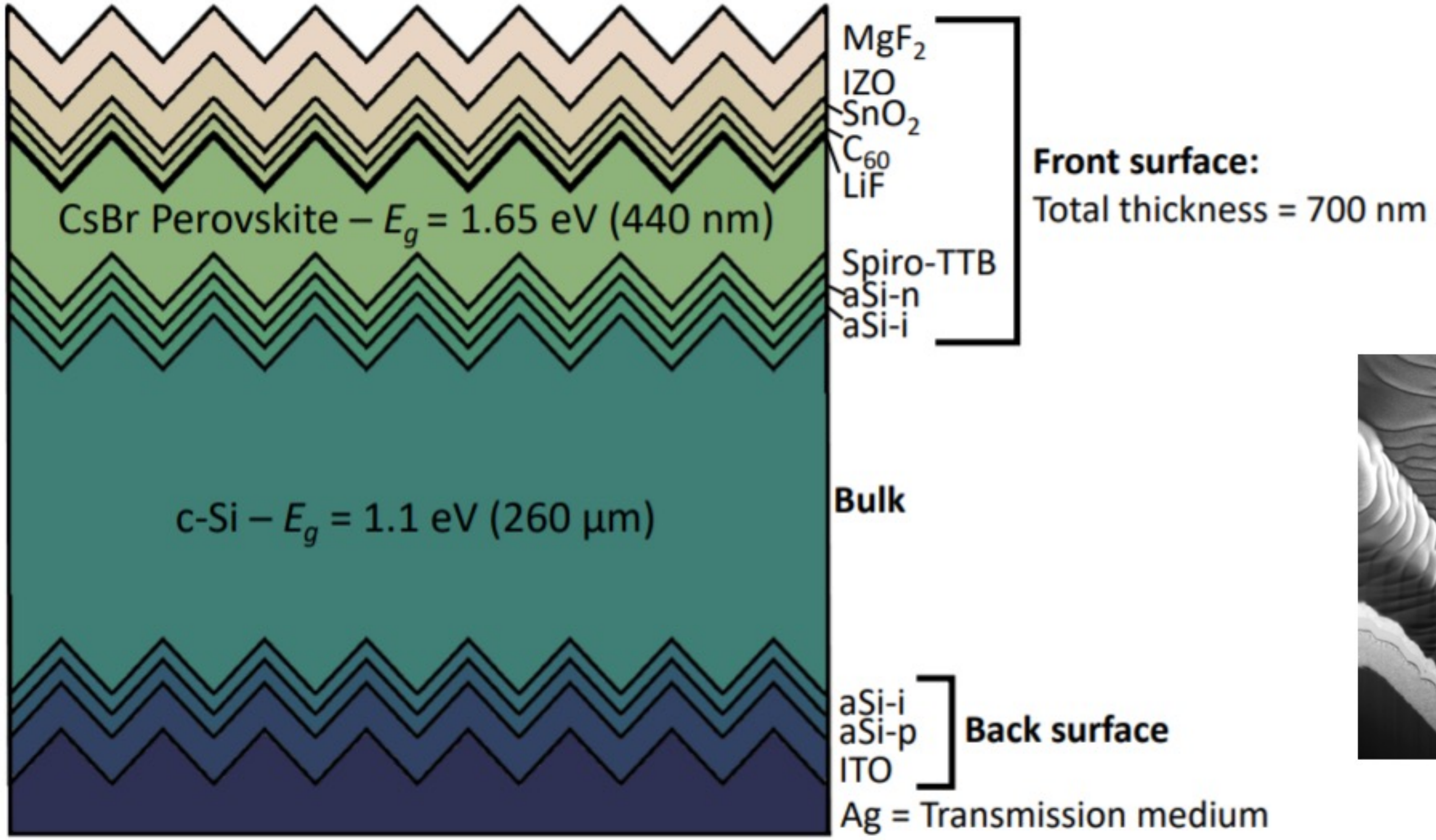


[1] L. Sayre *et al.*, 'Ultra-thin GaAs solar cells with nanophotonic metal-dielectric diffraction gratings fabricated with displacement Talbot lithography', *Progress in Photovoltaics*, vol. 30, no. 1, pp. 96–108, Jan. 2022, doi: 10.1002/pip.3463.

Example: ultra-thin GaAs cell (cont.)

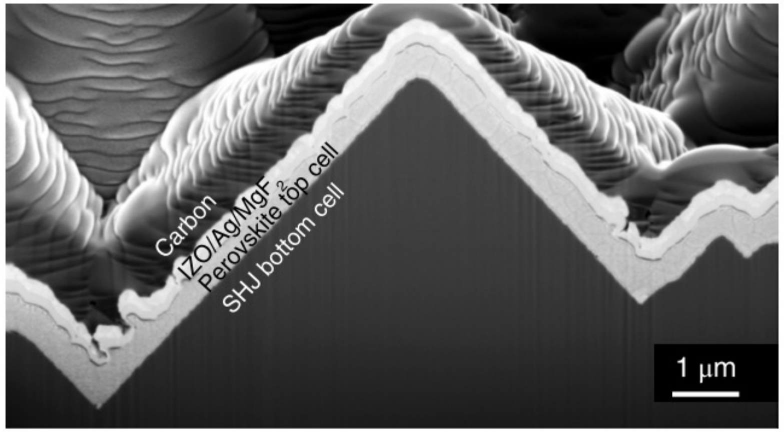


Example: Perovskite/Si tandem cell



Perovskite on silicon heterojunction (SHJ) tandem cell

Perovskite is deposited conformally on standard etched Si pyramid texture

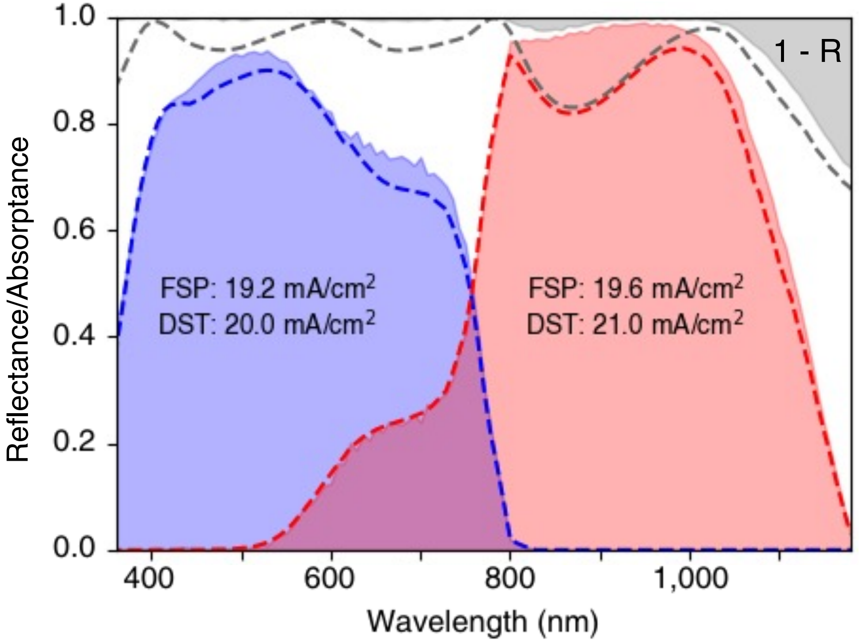


From [1]

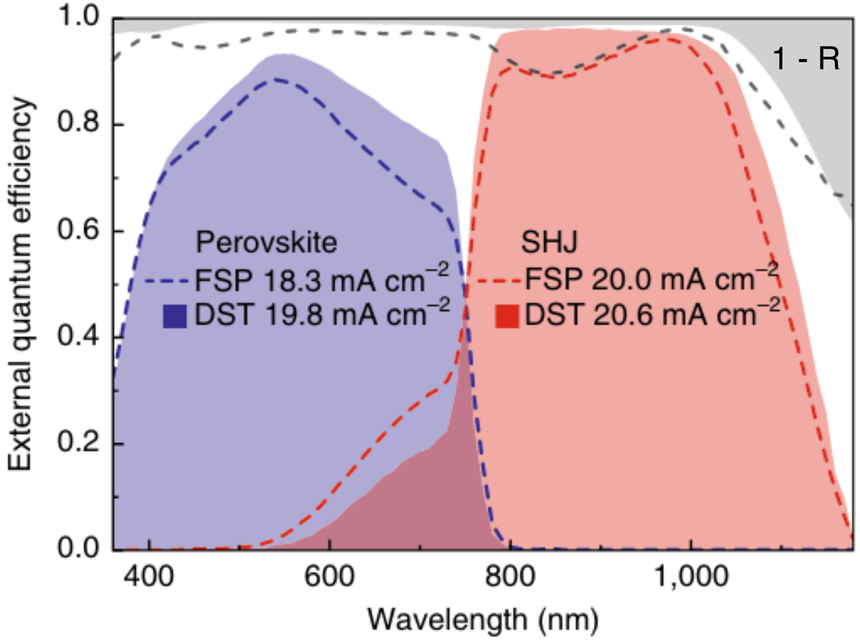
[1] Sahli, F., Werner, J., et al. (2018) 'Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency', *Nature Materials*. Springer US, 17(9), pp. 820–826.

Example: Perovskite/Si tandem cell (cont.)

RayFlare simulation

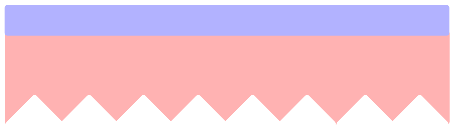


EQE measurement

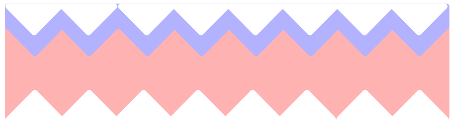


From [1]

FSP = Front-side polished



DST = Double-side textured



As a result of the front surface texture:

- Peak in R around 830 nm is reduced (lower front-surface reflectivity)
- Perovskite absorption slightly enhanced
- Boosts long-wavelength absorption (better light-trapping inside Si)

[1] Sahli, F., Werner, J., et al. (2018) ‘Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency’, *Nature Materials*. Springer US, 17(9), pp. 820–826.

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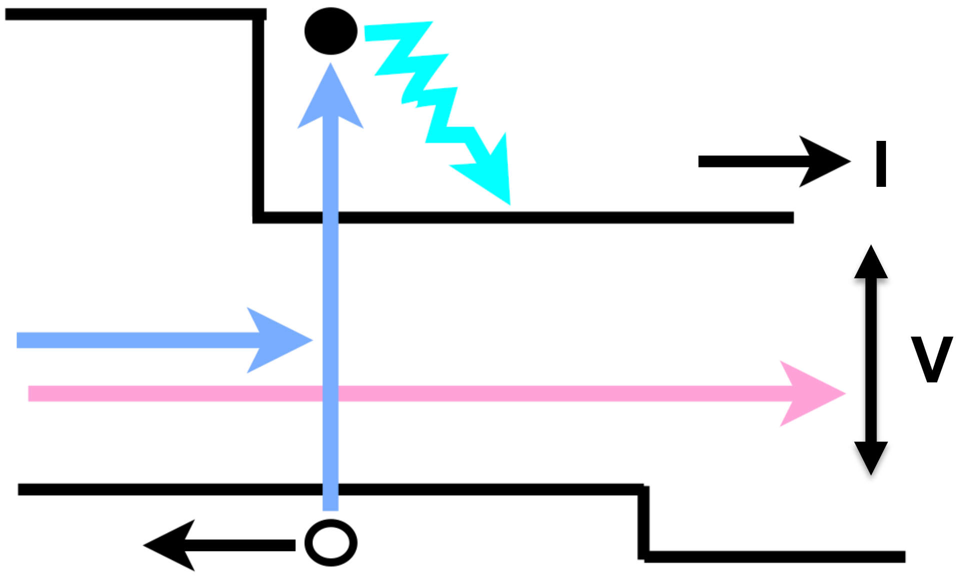
Session 2: Hands-on exercise
Using SolCore to calculate the Shockley-Queisser Efficiency limit

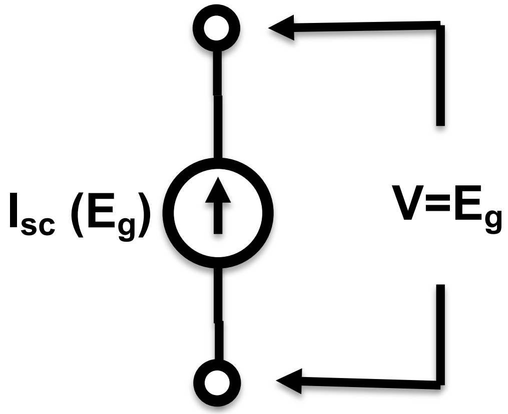
1 August 2023

Ned Ekins-Daukes, Phoebe Pearce

What is the Maximum Efficiency of a Solar Cell?

Trivich-Flynn Limit (1955)





Warning : Limit is invalid for T > 0K !

Trivich D, Flinn PA. Maximum efficiency of solar energy conversion by quantum processes. In Solar Energy Research, Daniels F, Duffie J (eds). Thames and Hudson: London, 1955.

Green, Martin A. 'Analytical treatment of Trivich-Flinn and Shockley-Queisser photovoltaic efficiency limits using polylogarithms'. Progress in Photovoltaics: Research and Applications, 20(2) (2012) 127

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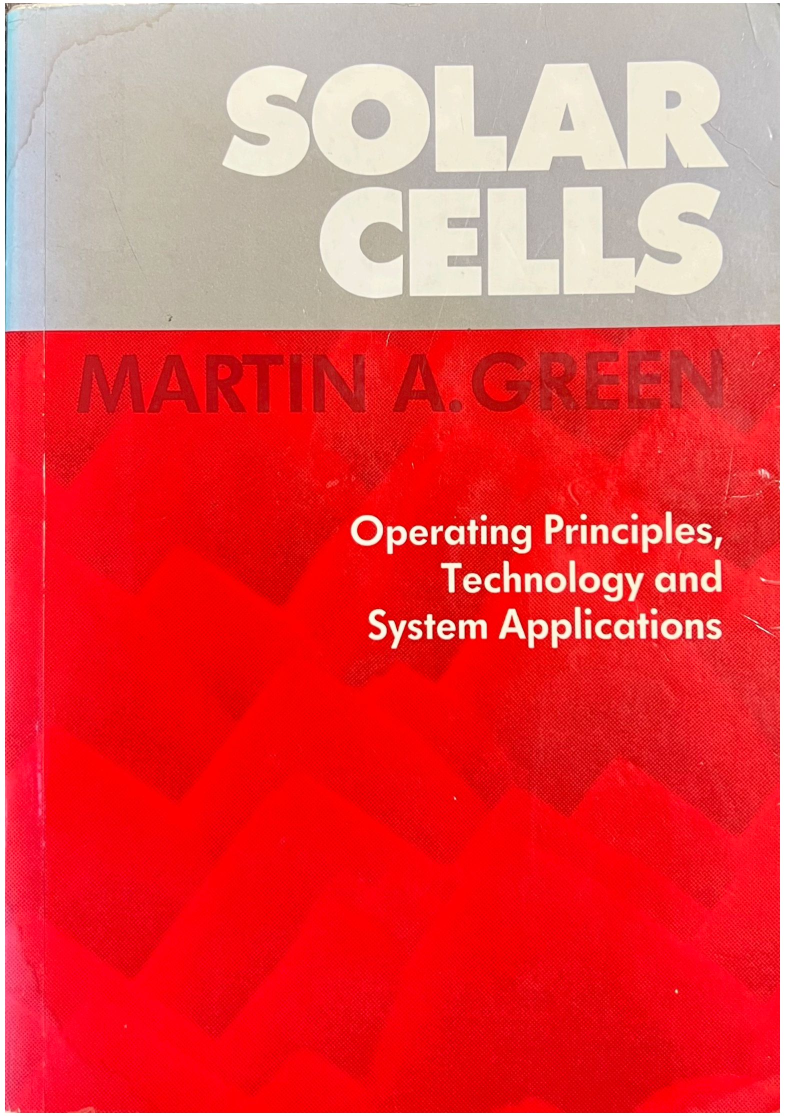
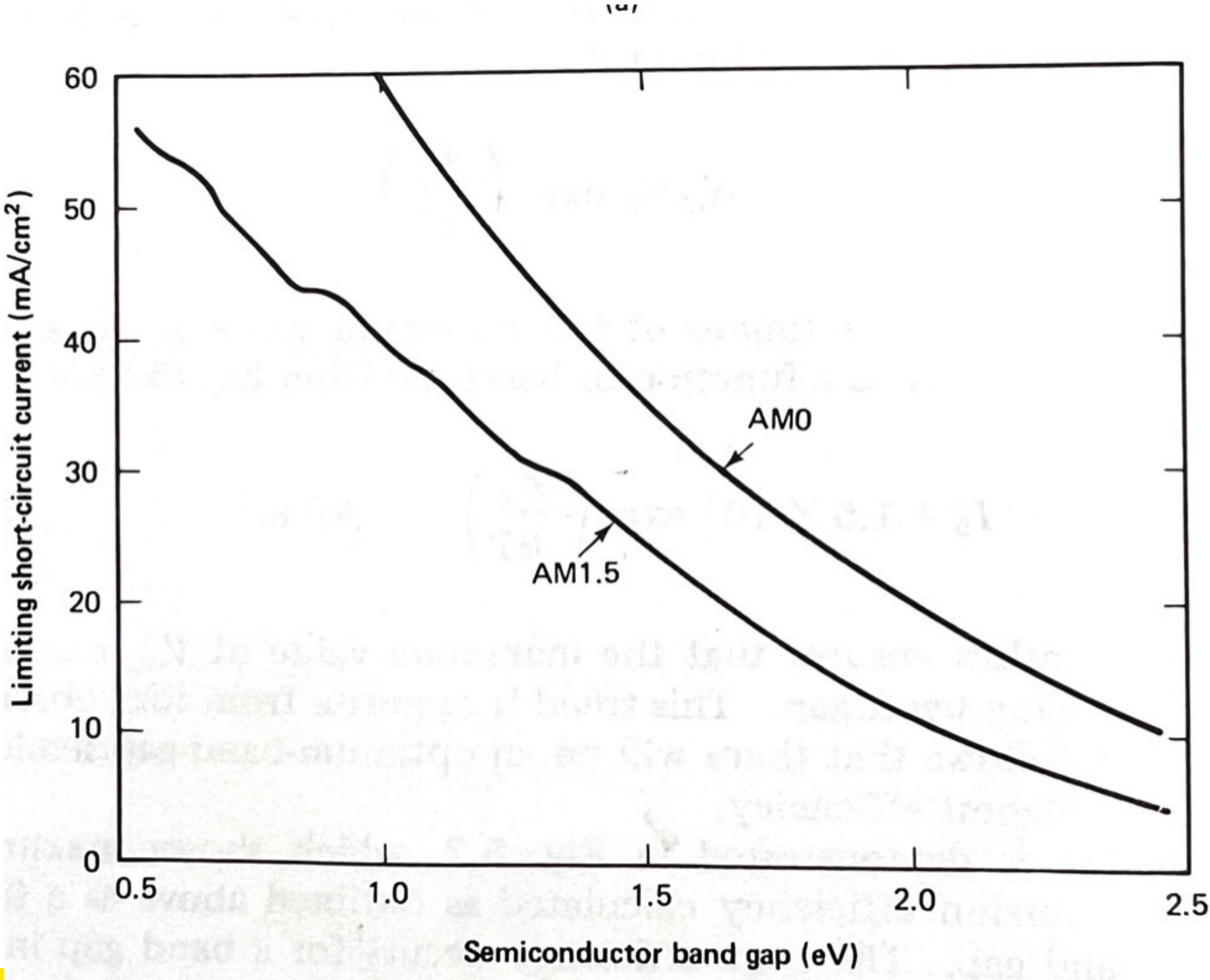
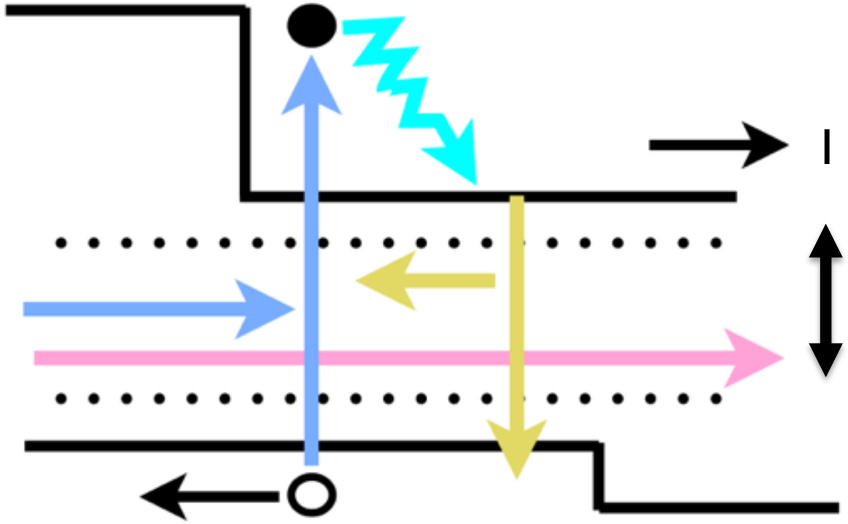
Limit to the Short-Circuit Current

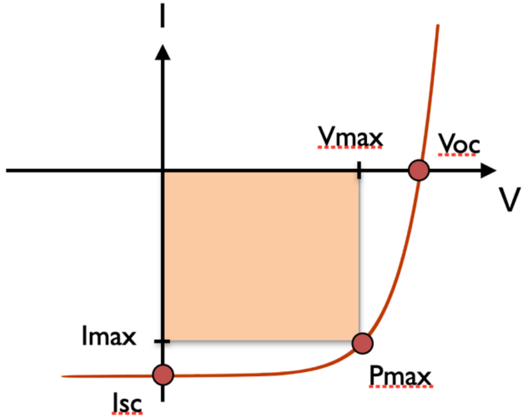


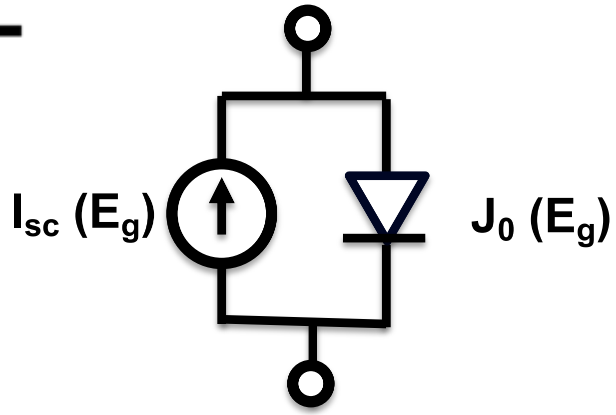


What is the Maximum Efficiency of a Solar Cell?

Shockley Queisser limit (1961)







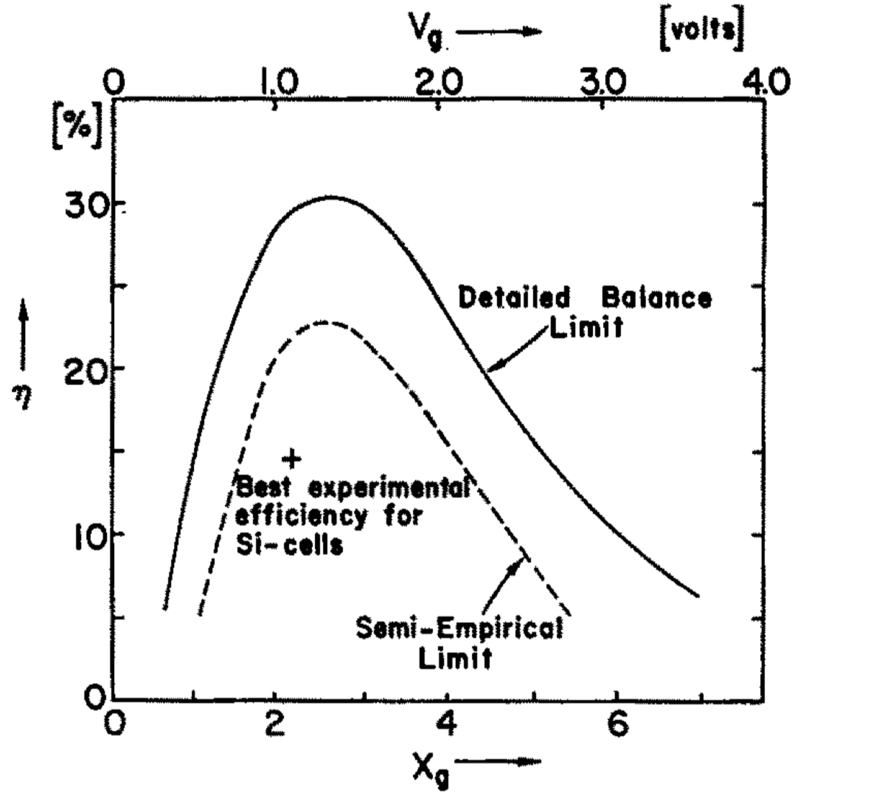


FIG. 1. Comparison of the "semiempirical limit" of efficiency of solar cells with the "detailed balance limit," derived in this paper. + represents the "best experiment efficiency to date" for silicon cells. (See footnote 6.)

Shockley, William, & Queisser, Hans J. 'Detailed Balance Limit of Efficiency of p-n Junction Solar Cells'. Journal of Applied Physics, 32(3) (1961) 510 https://doi.org/10.1063/1.1736034

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Session 3: Shockley-Queisser efficiency limit & detailed balance junction model

1st August 2023

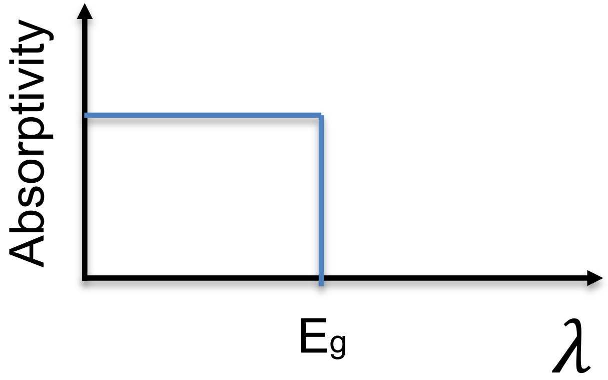
Ned Ekins-Daukes, Phoebe Pearce

Optical Models for PV Devices

Fundamental

Shockley-Queisser (Detail Balance)

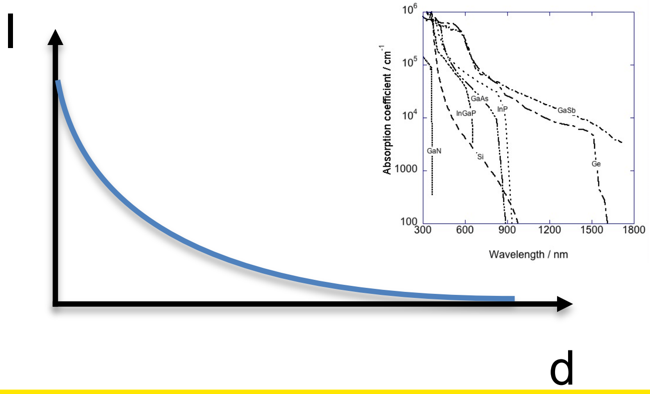
Complete absorption to band-gap energy Eg



Beer Lambert Law

$$I = I_0 e^{-\alpha d}$$

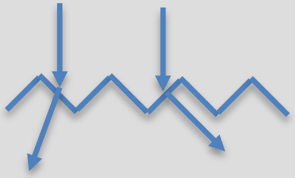
Intensity of light is attenuated exponentially with increasing thickness of absorber d [m] .
Absorption defined by a wavelength dependent absorption coefficient $\alpha(\lambda)[m^{-1}]$



Ray Optics

Non-uniform surfaces or PV structures $\gg \lambda$

Surface texture of a silicon solar cell

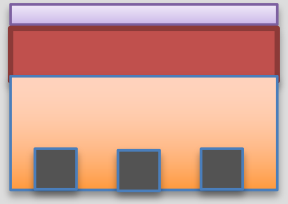


Wave Optics

Sub-wavelength structures $\ll \lambda$

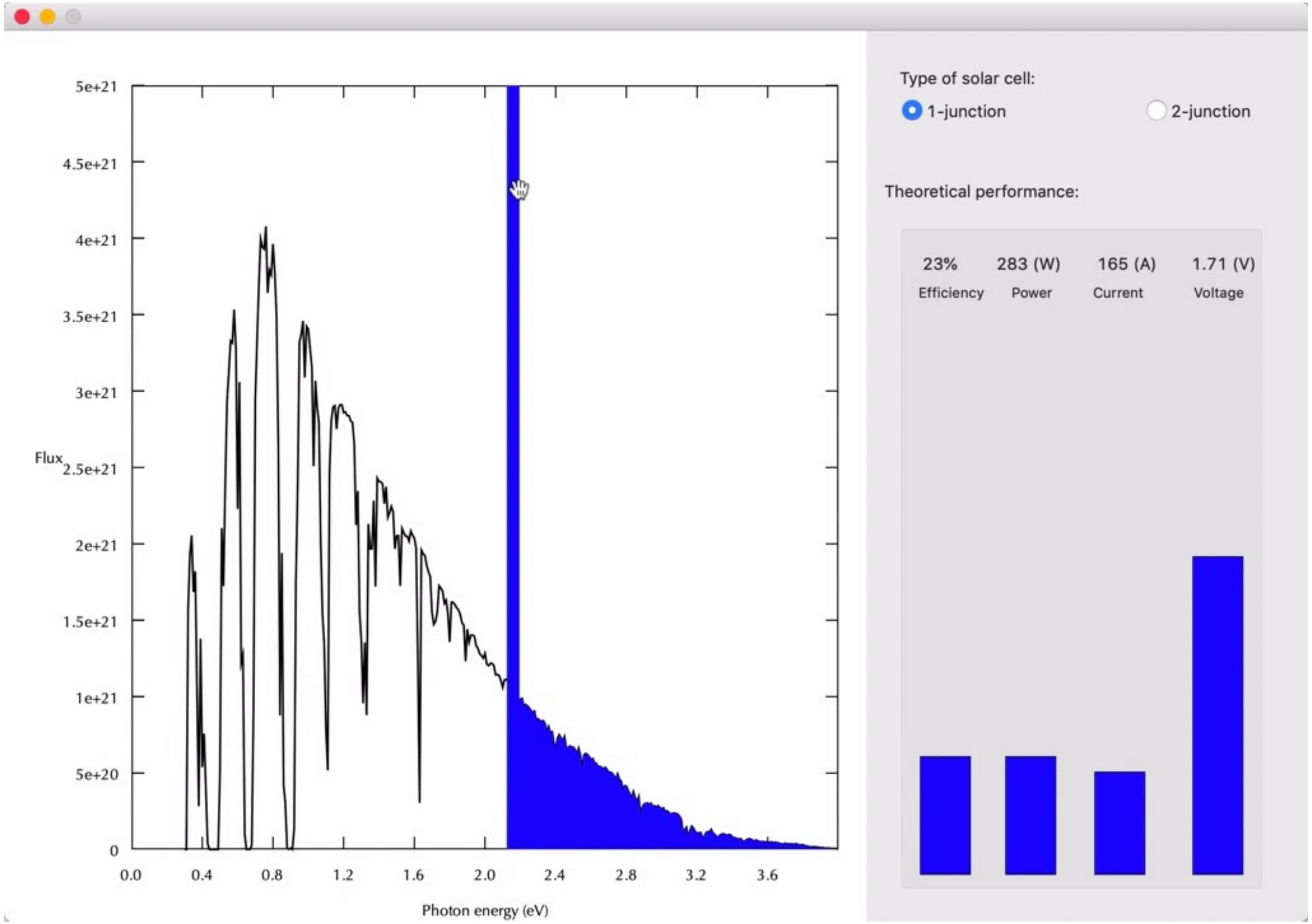
Anti-reflection coating
90nm p-doped layer

800nm n-doped layer

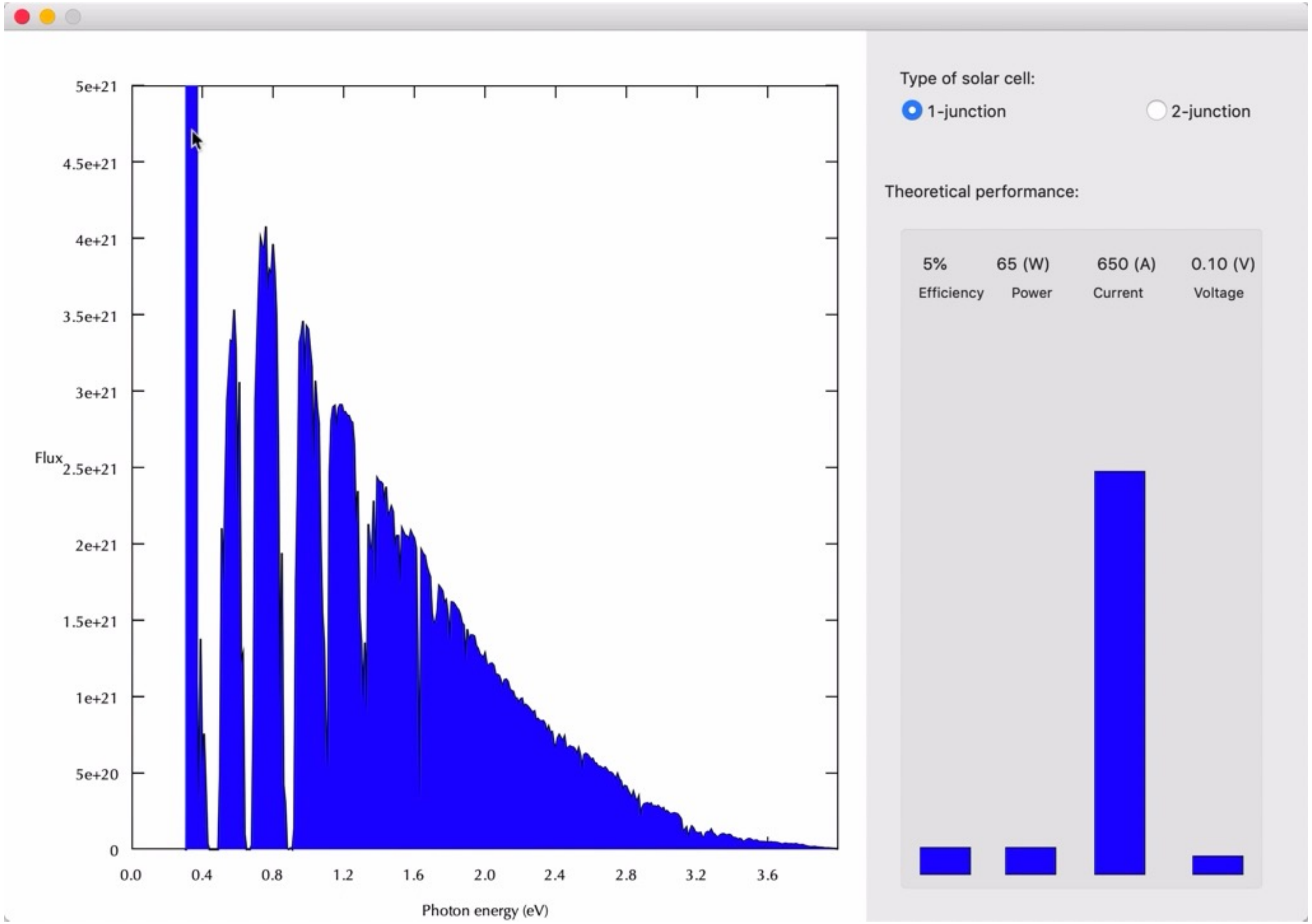


Diffractive grating on rear side.

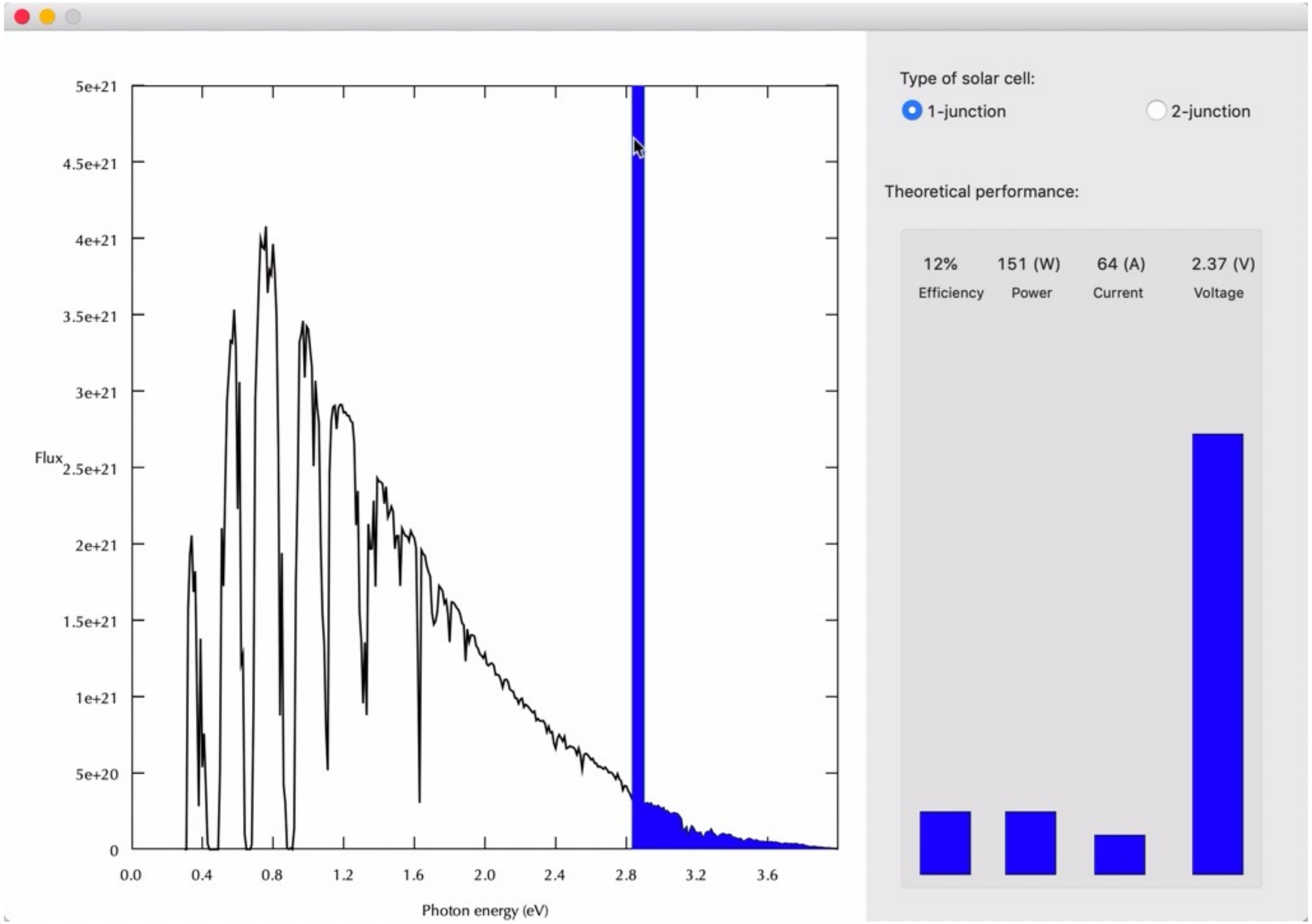
Current, Voltage, Power & Efficiency vs Eg



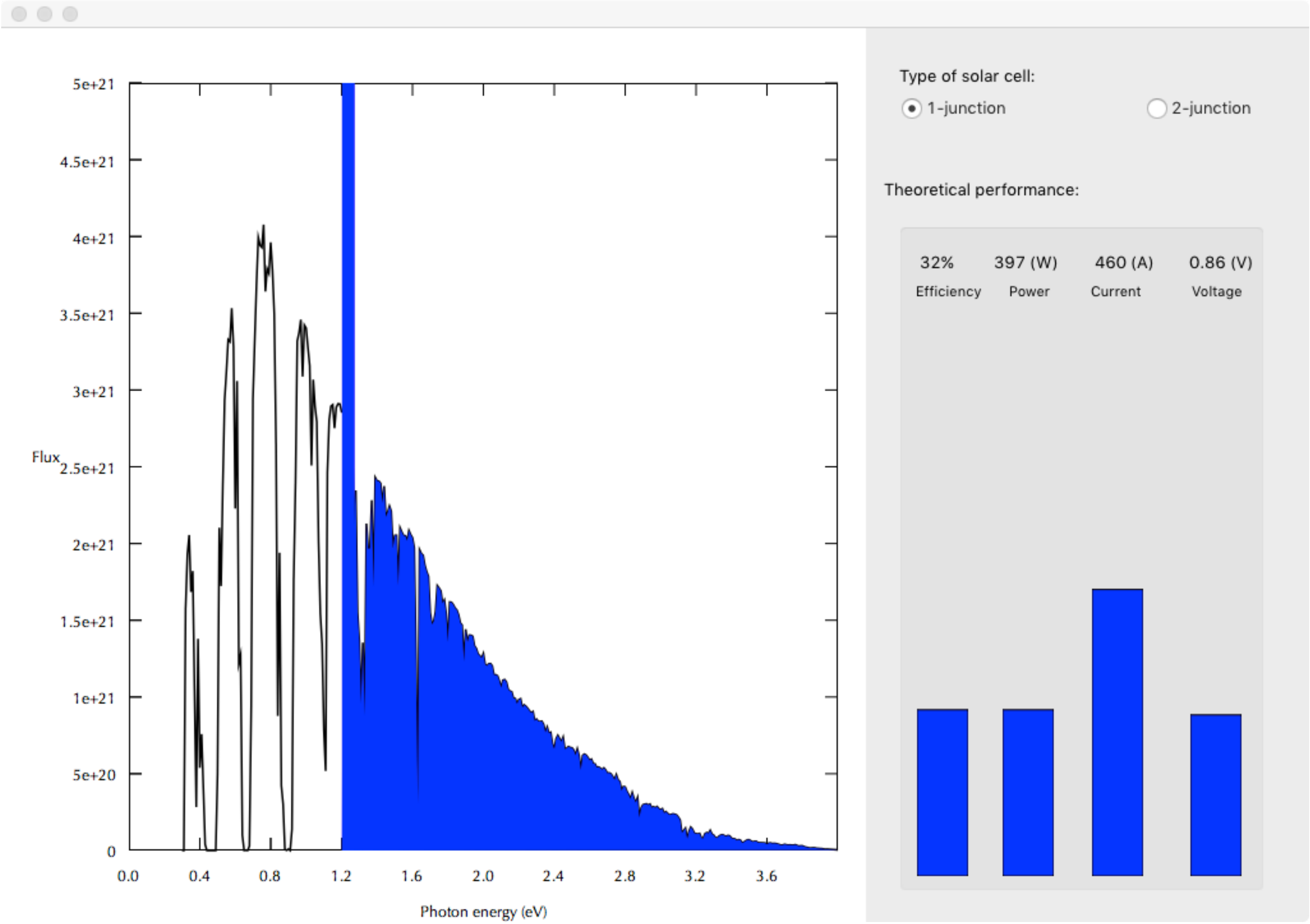
Current, Voltage, Power & Efficiency vs Eg



Current, Voltage, Power & Efficiency vs Eg



Current, Voltage, Power & Efficiency vs Eg

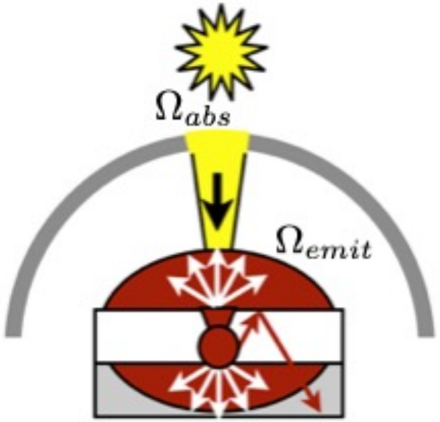


Electrical Models for PV Devices

Fundamental

Shockley-Queisser (Detail Balance)

Band-gap : Eg
Temperature : T

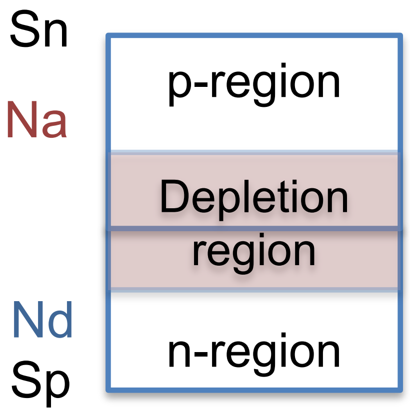


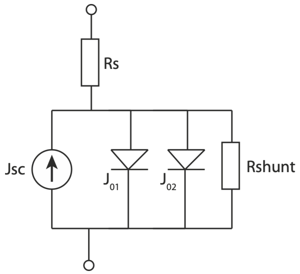
Depletion approximation

Analytical solutions to the drift-diffusion equations for homogeneous layers.
Shockley Diode Eqn

Band-gap : Eg
Temperature : T
Diode dimensions: x
Doping level: Na, Nd
Absorption coefficient α

Mobility μ
Surface recombination Sn,Sp
Diffusion length L,
Minority carrier lifetime τ



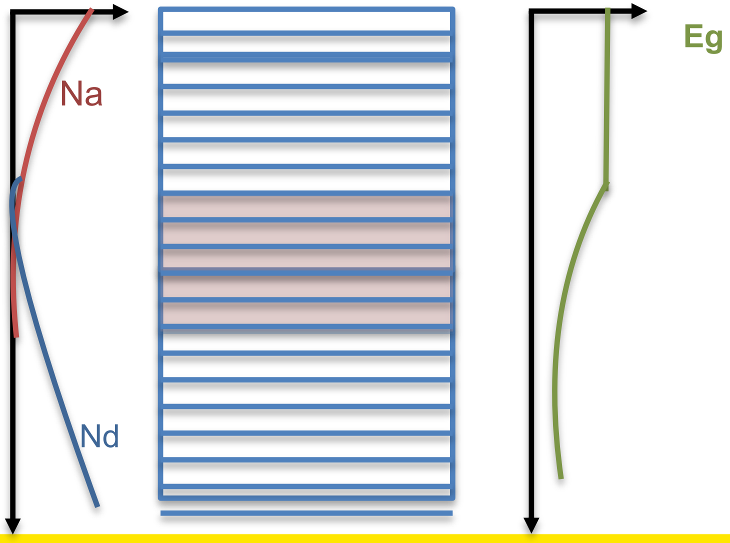


Drift-Diffusion

Numerical solution to the semiconductor drift-diffusion equations: 1D, 2D, 3D

Spatial variation of all parameters previously used in the depletion approximation.

- *Variable doping profile within a region (silicon PV)*
- *Variable band-gap within a region (CIGS PV)*
- *Mobile ions under dark and illuminated conditions (Perovskite PV)*



General Form of the Planck Equation

Stove

900K

Tungsten-Halogen light bulb

2800K

Sun

5800K

$$n(E) = \boxed{\epsilon(E)}\,\frac{\boxed{2\pi}}{\boxed{c^2 h^3}}\,\frac{\boxed{E^2}}{\boxed{e^{\frac{E-\mu}{kT}} - 1}}$$

Photon modes

Occupation probability

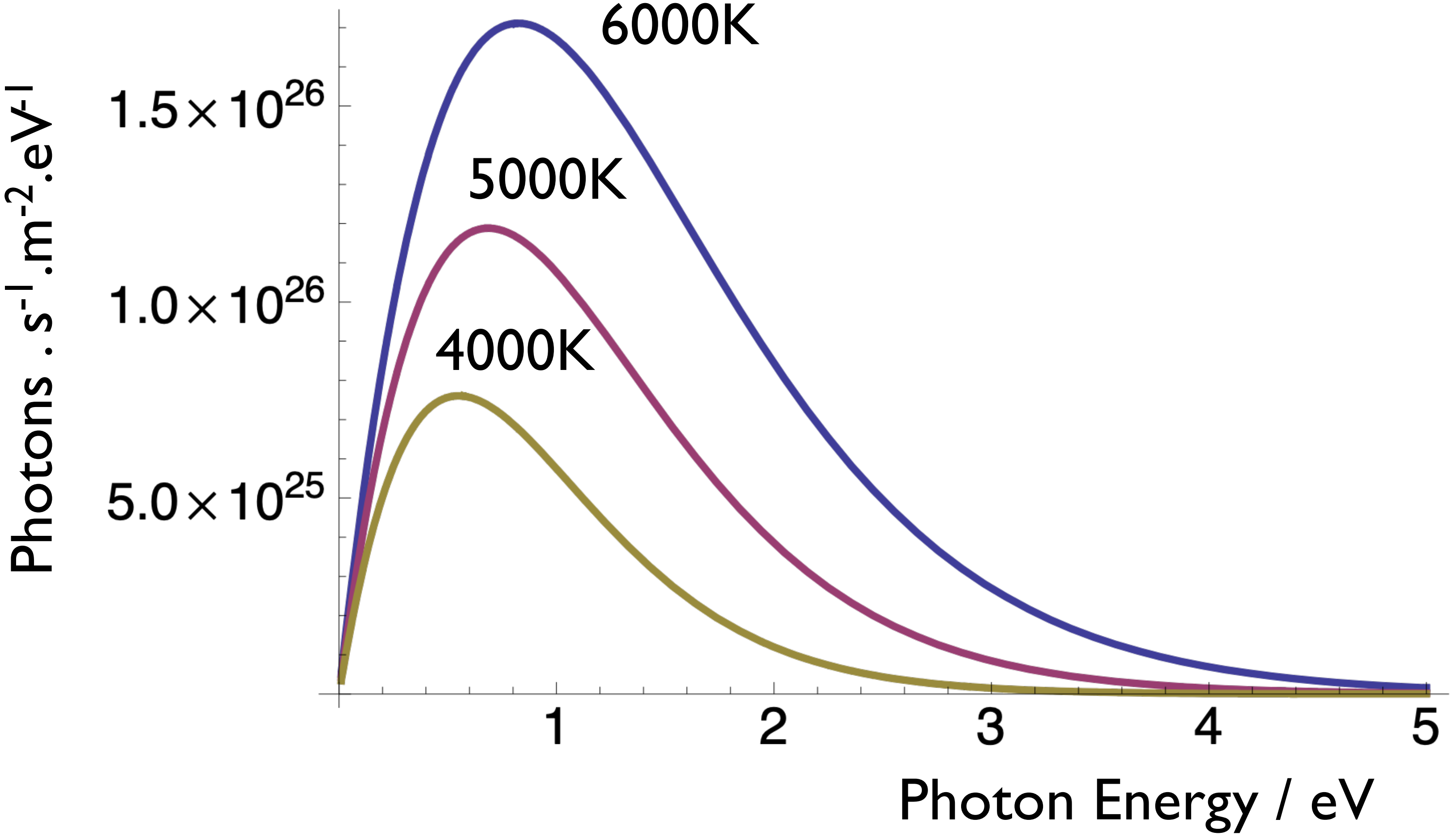
Encapsulates the electronic density of states.

Blackbody Emission

$$n(E) = \epsilon(E)\frac{2\pi}{c^2h^3}\frac{E^2}{e^{\frac{E-\mu}{kT}}-1}$$

$$\mu = 0$$

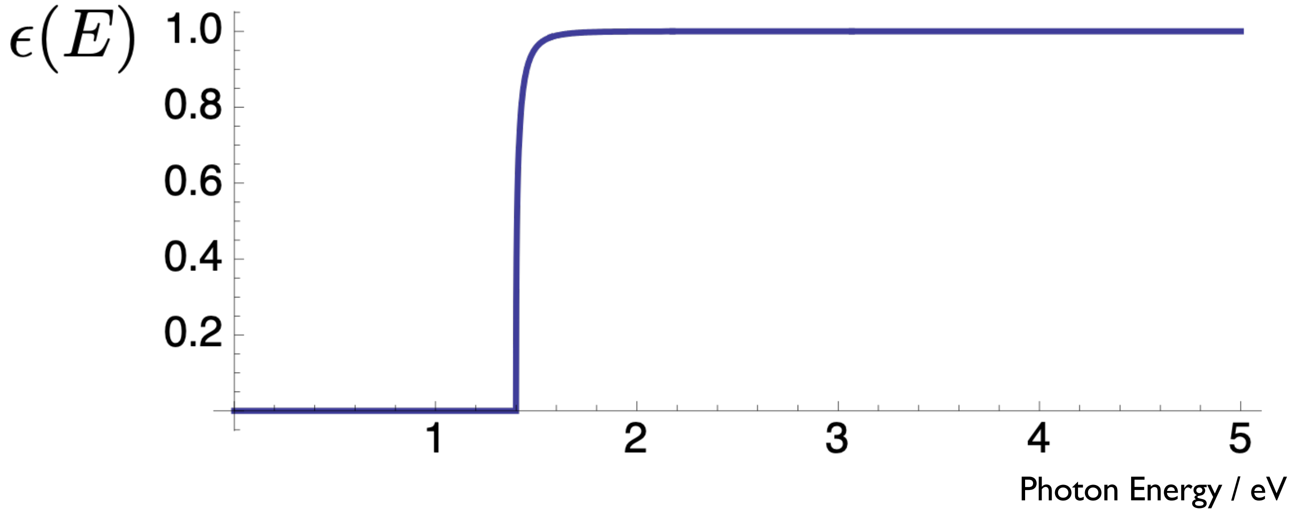
$$\epsilon(E) = 1$$

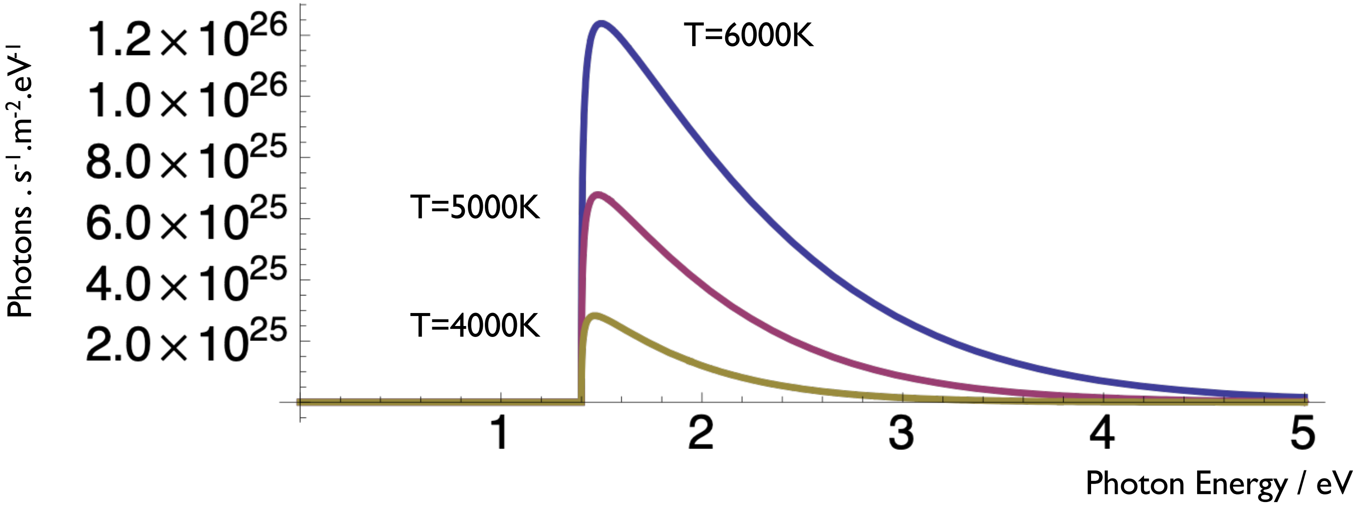


Semiconductors are “Grey” bodies

$$n(E) = \epsilon(E)\frac{2\pi}{c^2h^3}\frac{E^2}{e^{\frac{E-\mu}{kT}}-1}$$

$\mu = 0$
$T > 300K$

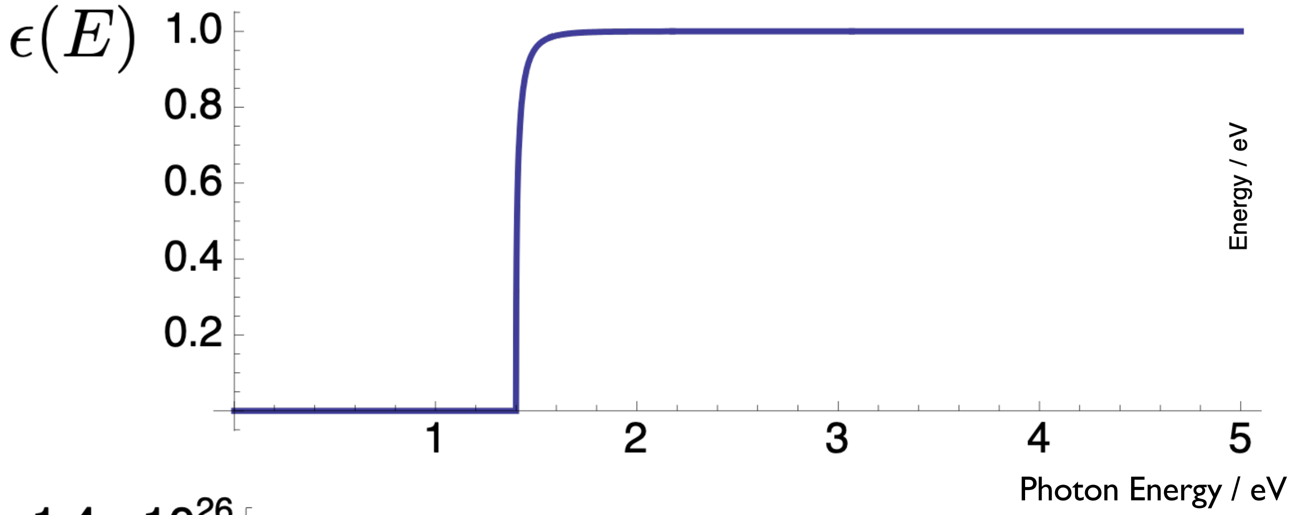


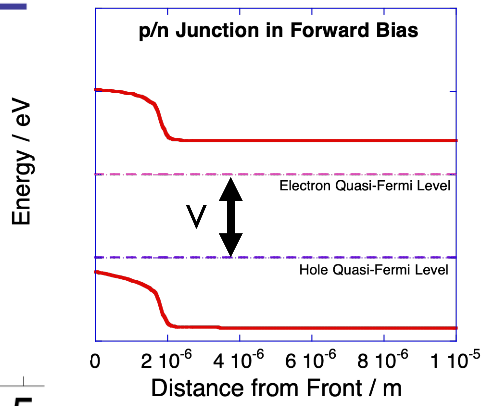


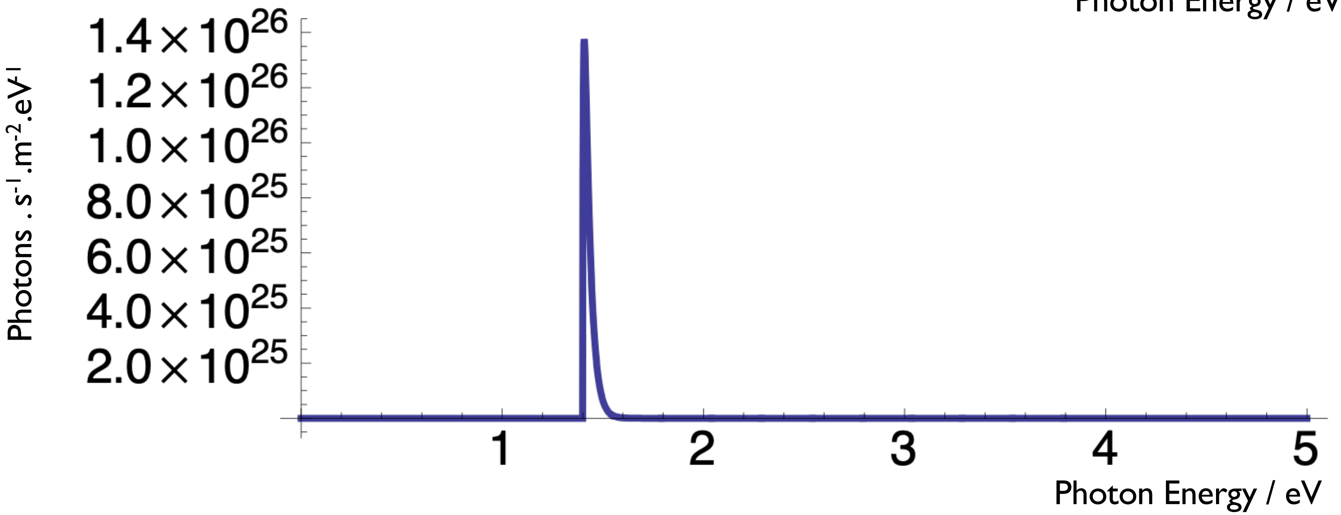
Electroluminescence

$$n(E) = \epsilon(E)\frac{2\pi}{c^2h^3}\frac{E^2}{e^{\frac{E-\mu}{kT}}-1}$$

$$\mu = 1.35V$$
$$T = 300K$$







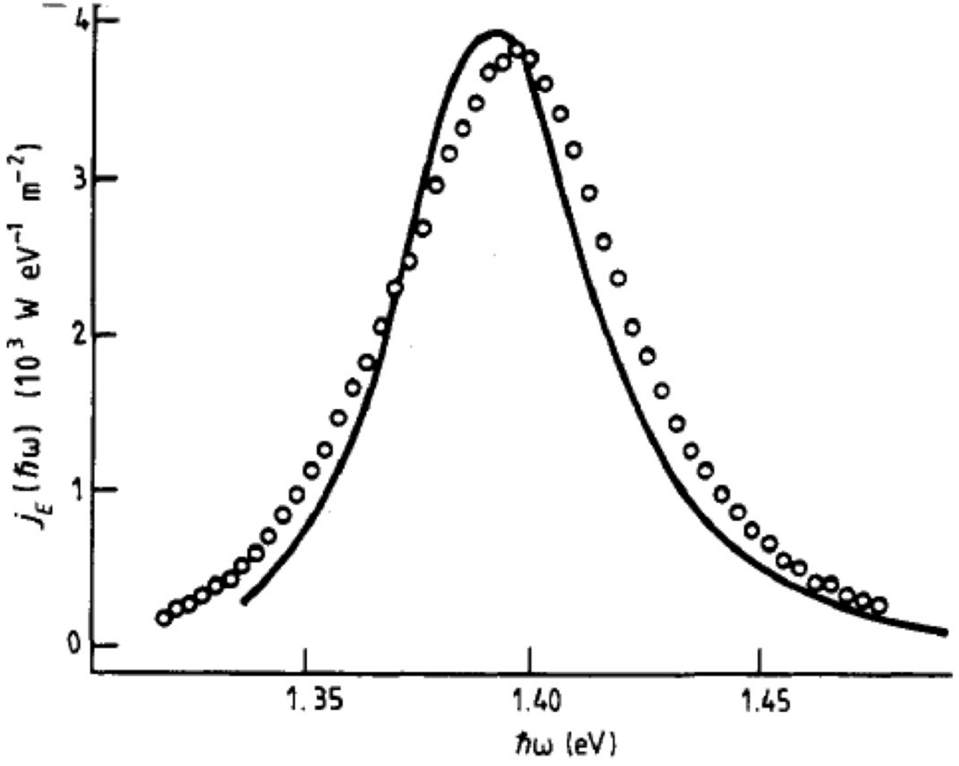
Verification of the Generalised Planck Expression

$$n(E) = \epsilon(E)\frac{2\pi}{c^2h^3}\frac{E^2}{e^{\frac{E-\mu}{kT}}-1}$$

$$\mu = 1.206V$$

$$T = 296K$$

GaAs p/n diode

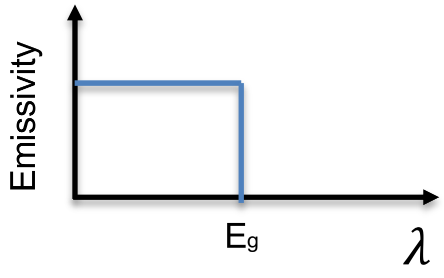


J.Phys: Condens.Matter 2 (1990) p.3803

Radiative limit to J_0

$$\dot{N} = \int_{Eg}^{E_{top}} \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1} dE$$

- Assume F(E) Boltzmann approximation
- Bands are infinite ($E_g \rightarrow \infty$)

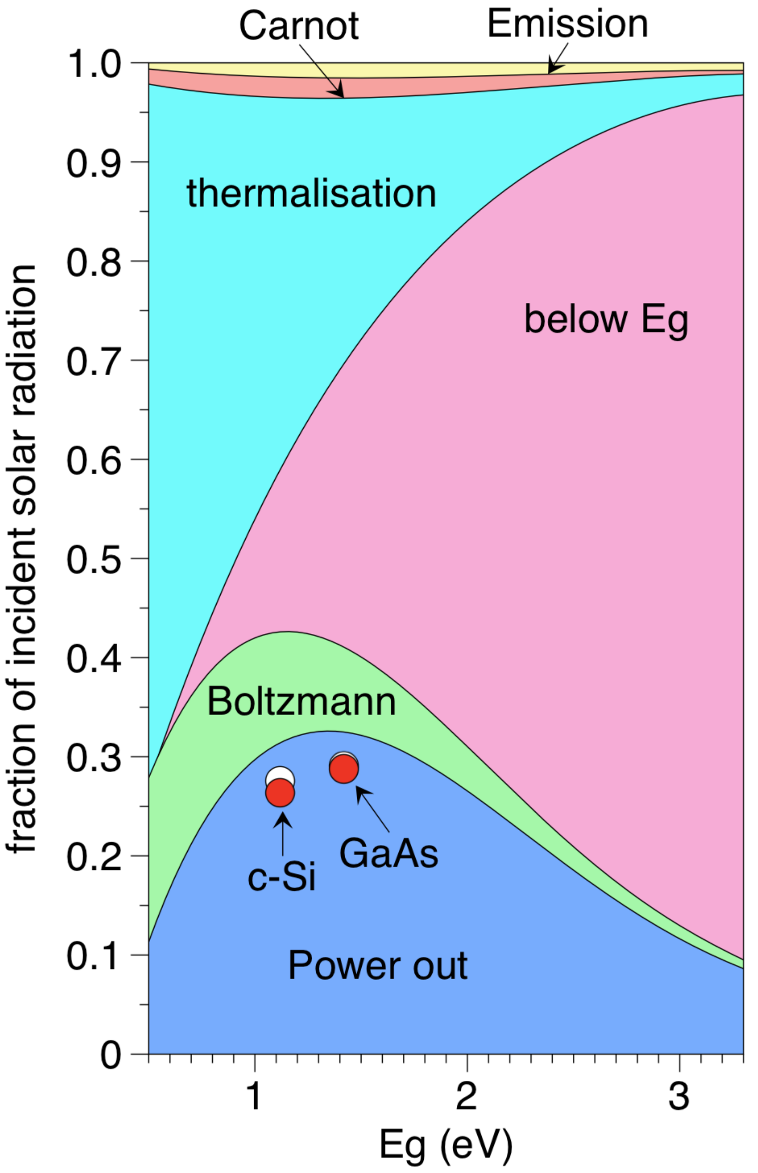


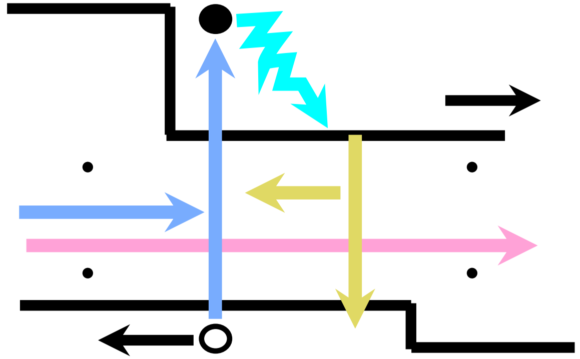
$$\begin{aligned}\dot{N} &= \int_{Eg}^{\infty} \epsilon(E) \frac{2\pi}{c^2 h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}}} dE \\ &= \underbrace{(\epsilon kT(Eg^2 + 2EgkT + 2k^2T^2)e^{\frac{-Eg}{kT}})}_{\frac{J_0}{q}} e^{\frac{\mu}{kT}}\end{aligned}$$

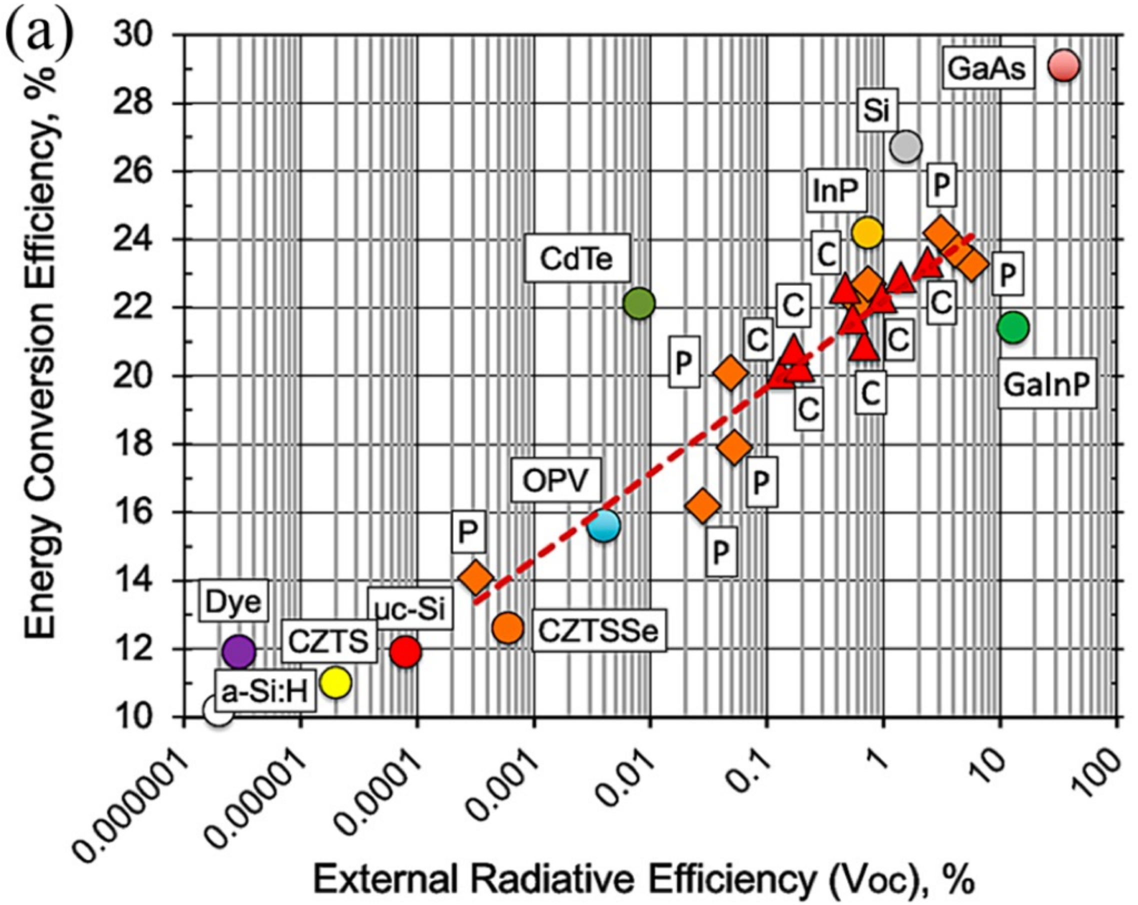
$$\mu = qV$$

$$J = J_0 e^{\frac{qV}{kT}}$$

Unpacking the Shockley Queisser Efficiency limit:







L. Hirst & N.J.Ekins-Daukes, Progress in Photovoltaics, (2011) 19: p286 ,
M.A. Green, & A.W.Y. Ho-Baillie, ACS Energy Letters, 4(7) (2019) 1639

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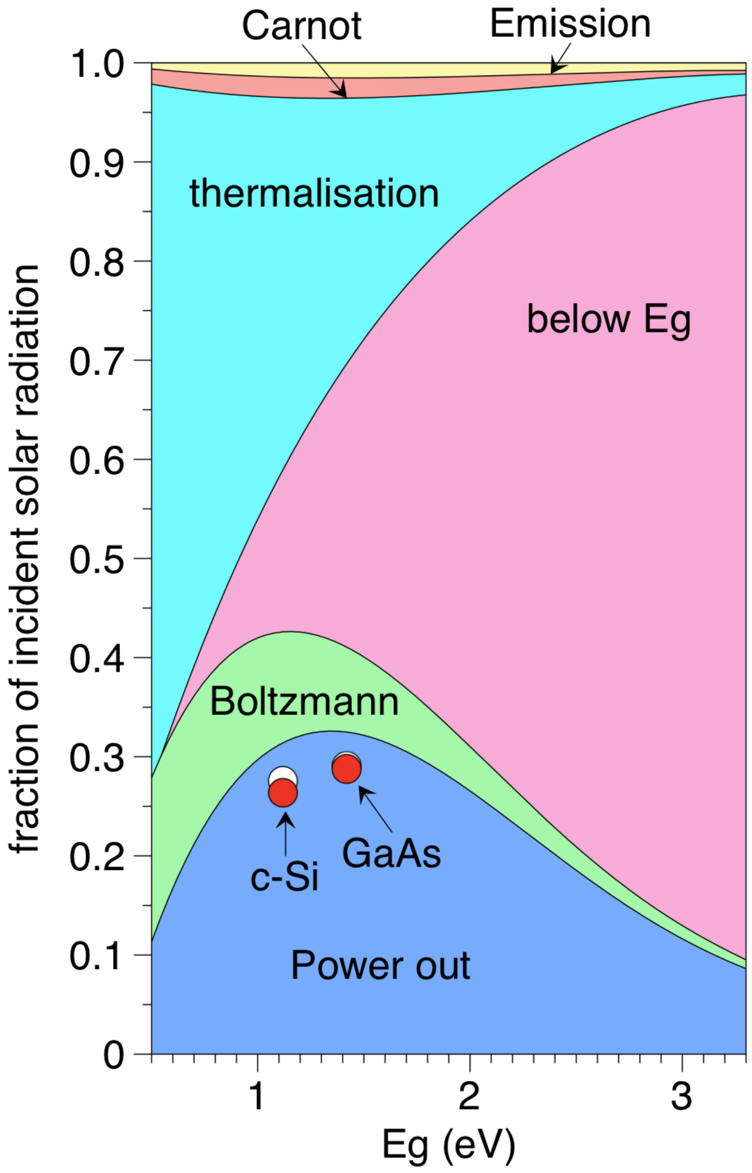
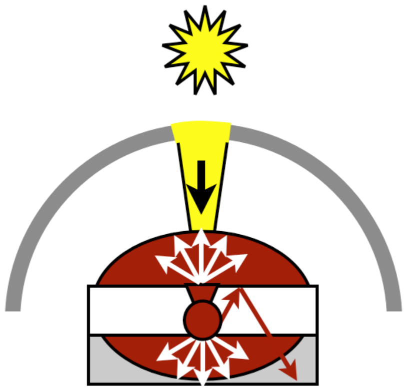
Understanding the effect of solar concentration



$$qV_{max} = E_g - E_g\frac{T_A}{T_s} - kT_A \ln\left(\frac{\Omega_{emit}}{\Omega_{abs}}\right)$$

Boltzmann loss

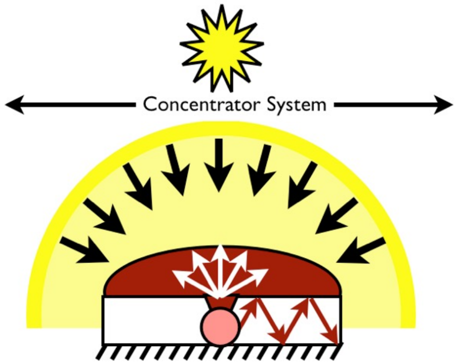
Conventional solar cell



$\Omega_{emit} >> \Omega_{abs}$

Significant Boltzmann loss!

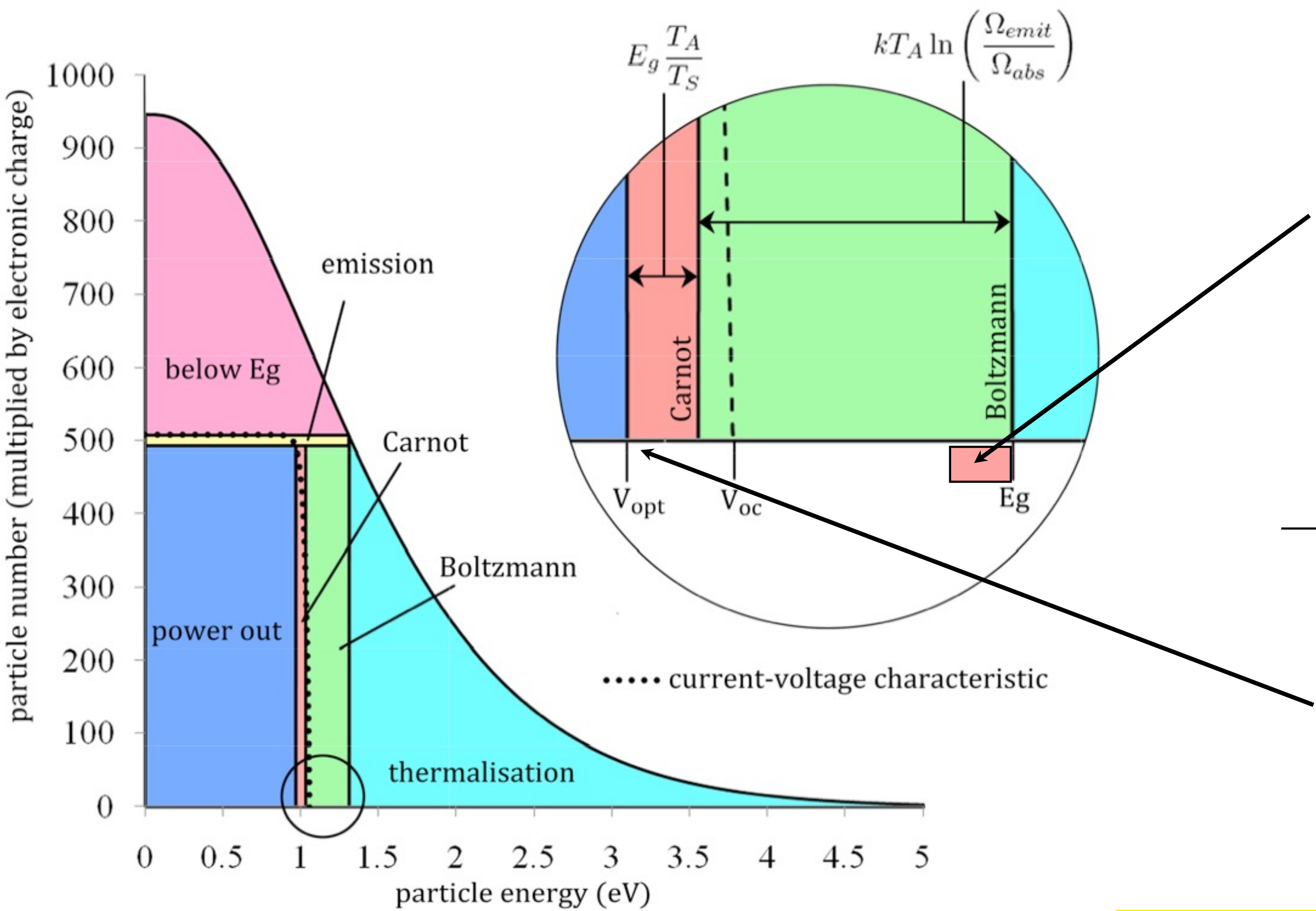
Maximum concentration

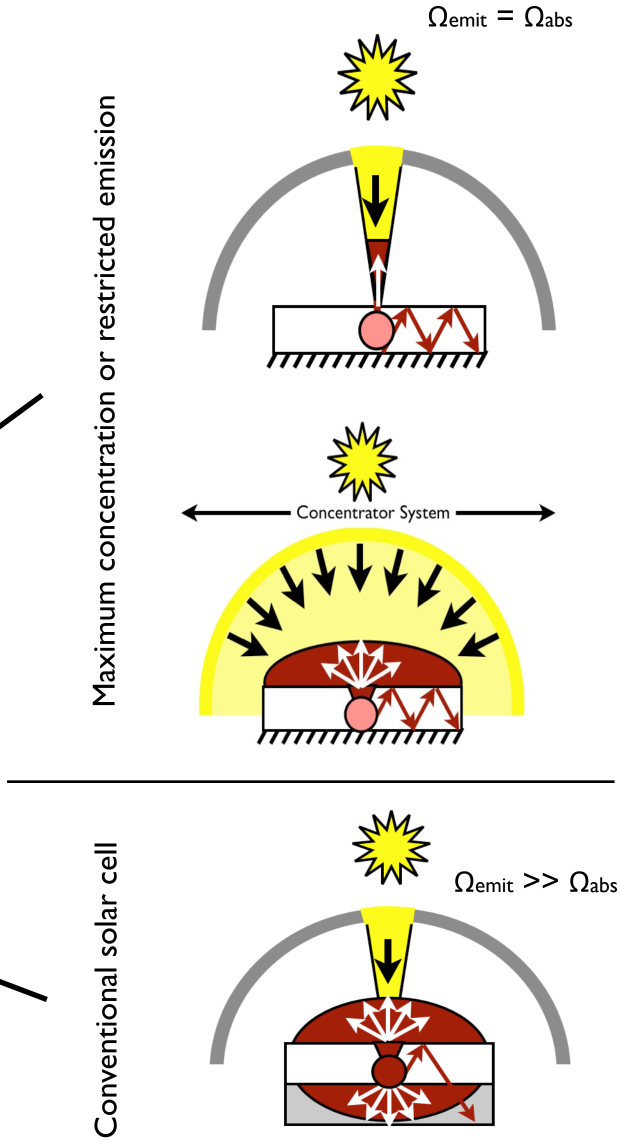


$\Omega_{emit} = \Omega_{abs}$

Zero Boltzmann loss.

Understanding the effect of solar concentration :





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Session 5: Simple Si and GaAs cells using the depletion approximation

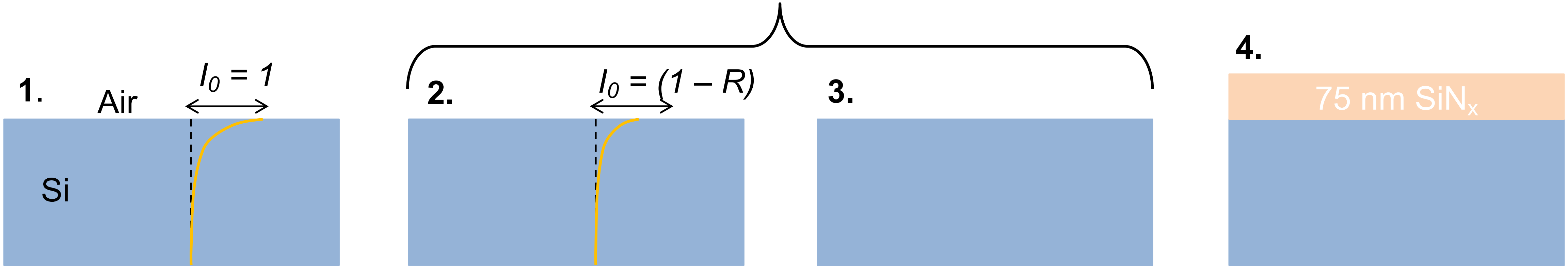
2nd August 2023

Ned Ekins-Daukes, Phoebe Pearce

Example 5a: Simple Si cell

Si is considered infinitely thick, with 200 μm of absorbing thickness (ignore back-surface reflection)

Calculate same result in this case!



Beer-Lambert absorption:
$I(z) = I_0 \, e^{-\alpha(\lambda) z}$

$I_0 = 1$

Fresnel eqn + Beer-Lambert absorption:
$I(z) = I_0(\lambda) \, e^{-\alpha(\lambda) z}$

$I_0(\lambda) = 1 - R(\lambda)$

Transfer matrix method
(Si treated *incoherently*)

Add ARC, Transfer-matrix method

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Sessions 6 & 7: Transfer-matrix method

2nd August 2023

Ned Ekins-Daukes, Phoebe Pearce

Transfer-matrix method (TMM) in Solcore

Defining structures

Materials $Ga_{0.51}In_{0.49}P$ = GaInP | In = 0.49

with optical properties (n(λ), k(λ)) retrieved from database

Layers 500 nm of InGaP

Stacks / Structures

Stack = [500 nm of InGaP
+ 1500 nm of GaAs
+ 70 nm of AlAs
+ …]

calculate RAT of Stack with AM0 spectrum

Modelling optics

Transfer-matrix method (TMM)

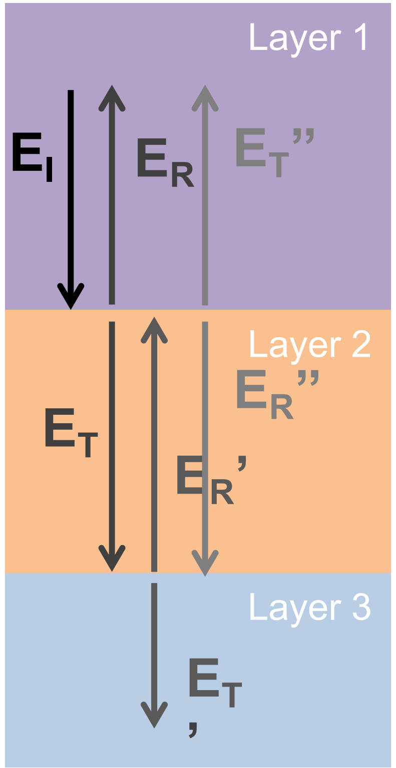
Efficiently handles **planar multilayer** stacks (including thin film interference effects)

$\mathbf{M}_{\text{Layer 1}}$

$\mathbf{M}_{\text{Layer 2}}$

Relates waves entering and exiting layer 2 (both directions)

$\mathbf{M}_{\text{Layer 3}}$



R, A, T of stack

$$\mathbf{M}_{\text{stack}} = \mathbf{M}_{01} \times \mathbf{M}_{\text{Layer 1}} \times \mathbf{M}_{\text{Layer 2}} \times \mathbf{M}_{\text{Layer 3}} \times \ldots$$

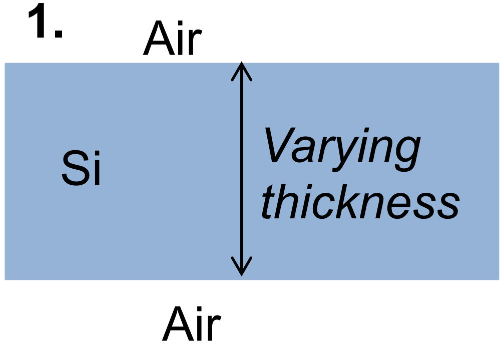
Solcore integrates & streamlines the **tmm** Python package

TMM: S. J. Byrnes, “Multilayer optical calculations.” *arXiv*, Dec. 30, 2020

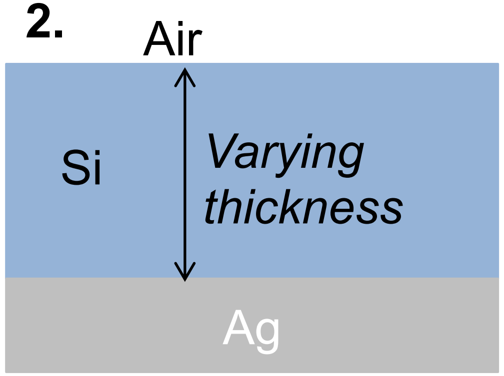
Example 6a: More exploration of TMM

No longer ignore back-surface reflection. Explore effect of different assumptions about coherency, the incidence angle, and the polarization of the incident light

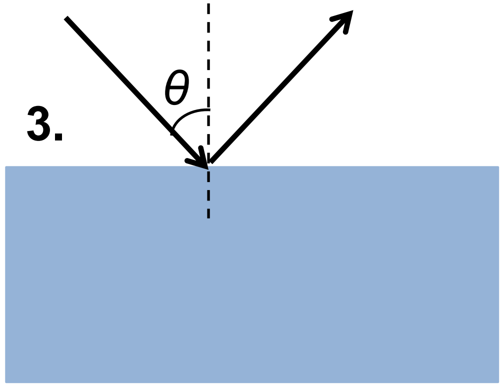
1.



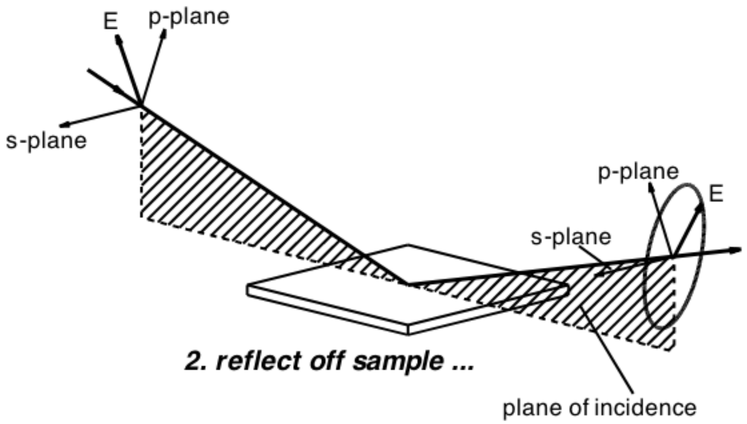
2.



3.



Varying angle of incidence and polarization

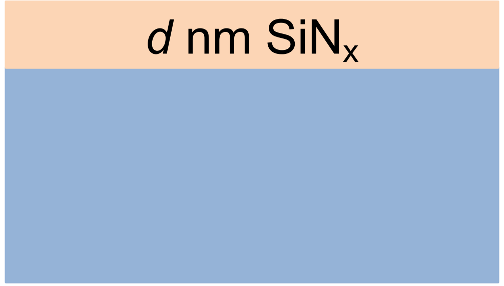


Treating a layer **incoherently** means **discarding the phase information** inside that layer; no **Fabry-Perot/thin-film interference**. The absorption profile is assumed to follow the Beer-Lambert law.

Example 6b: Simple ARC optimization

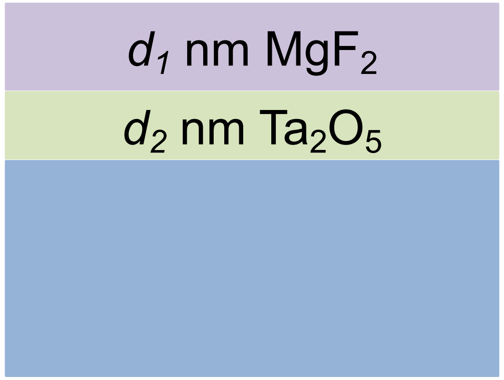
Find ARC layer thicknesses which minimize reflectance

1.



Vary d

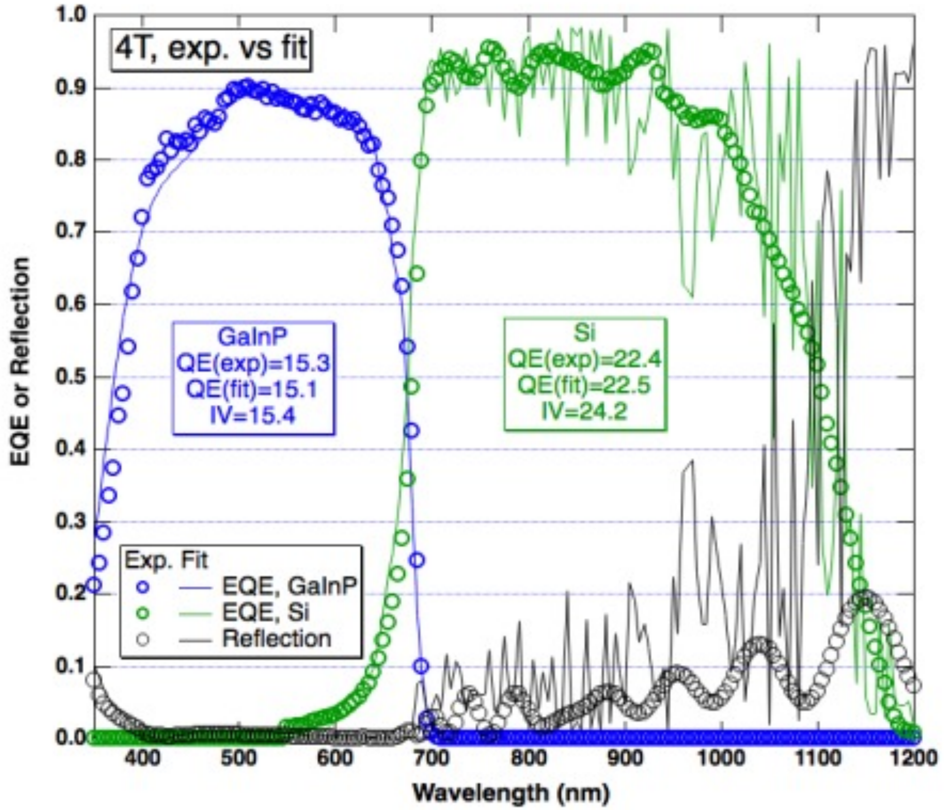
2.



Vary d_1 and d_2

Example 7: Planar GaInP/Si cell (2-terminal vs. 4-terminal)

Material	Thickness (nm)	Contrib. to j_{sc}
air	0	0
MgF_2	97	0
ZnS	41	0
n-$Al_{0.52}In_{0.48}P$	17 (20)	0
n-$Ga_{0.5}In_{0.5}P$	950 (1000)	0.91
p-$Al_{0.27}Ga_{0.26}In_{0.47}P$	200	0
p-$Al_{0.5}Ga_{0.5}As$	500	0
ZnS	82	0
epoxy	10,000	0
glass, n=1.56	1,000,000	0
epoxy	10,000	0
PECVD SiO_x	100	0
SiN_x, n=1.91	70	0
SiN_x, n=2.4	15	0
n,p-Si	357,000 (150,000)	1
Al_2O_3	15	0
SiN_x, n=1.91	120	0
Al	10,000	0



Note: the paper uses a textured Si bottom cell, while we assume all interfaces are planar. We will discuss the use of textures in III-V/Si and perovskite/Si tandem cells tomorrow.

https://doi.org/10.1109/PVSC40753.2019.9198960

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Sessions 8 - 10: Advanced optical modelling

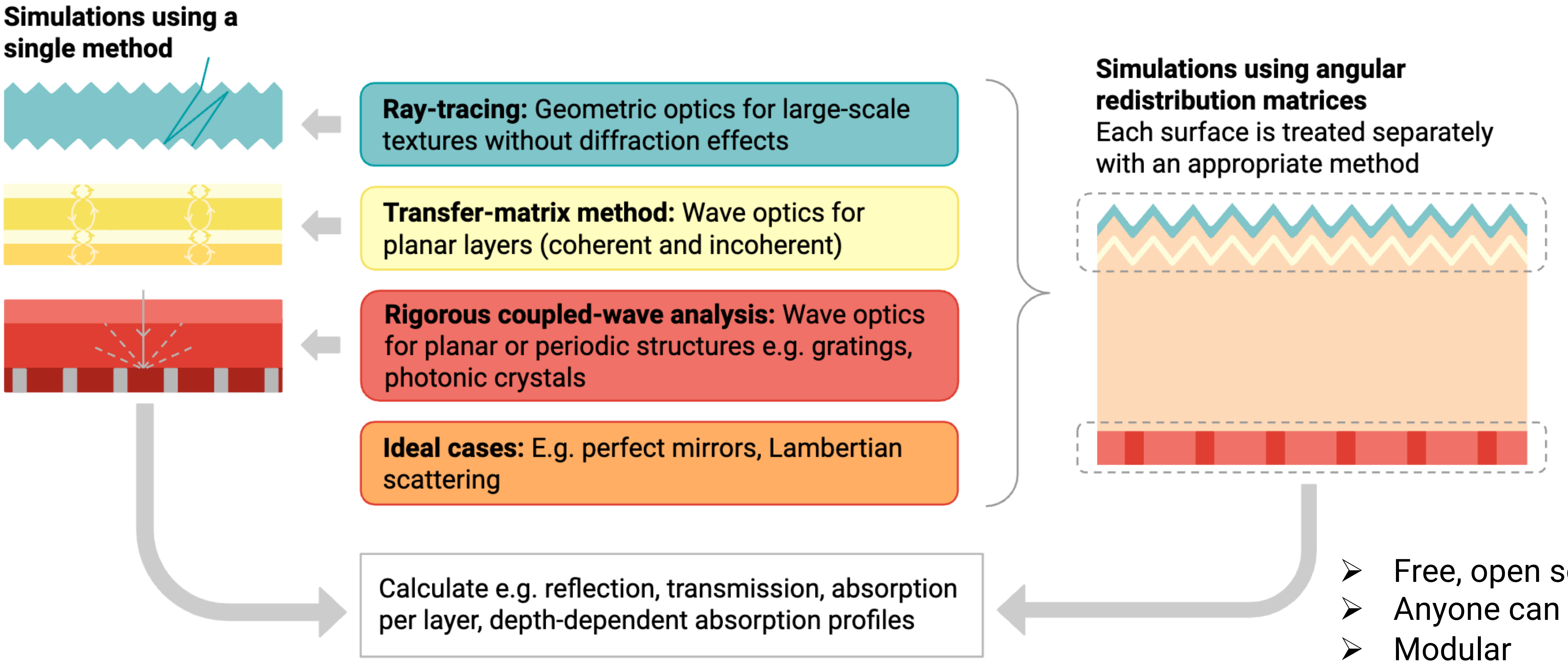
3rd August 2023

Ned Ekins-Daukes, Phoebe Pearce

RayFlare installation

- Previously, we have used **Solcore** for all the examples.
  - Solcore has quite a lot of optics capabilities, but **it cannot do ray-tracing**
  - **RayFlare** is our dedicated optics package; it can reproduce what Solcore does, but also adds new functionality:
    - Ray-tracing
    - Angular redistribution matrix method (ARMM)
- Please go to **rayflare.readthedocs.io** and read the installation instructions
  - Basic installation: **pip install rayflare**
  - This will install everything except RCWA functionality (for diffraction gratings/2D periodic structures)
  - Installation instructions for RCWA functionality can be found in the documentation. Unfortunately, it does not work on Windows (but all other RayFlare functionality does work!)

RayFlare capabilities



- Free, open source
- Anyone can contribute
- Modular
- Documented

P. Pearce, 'RayFlare: flexible optical modelling of solar cells', *Journal of Open Source Software*, vol. 6, no. 65, p. 3460, 2021, doi: 10.21105/joss.03460.

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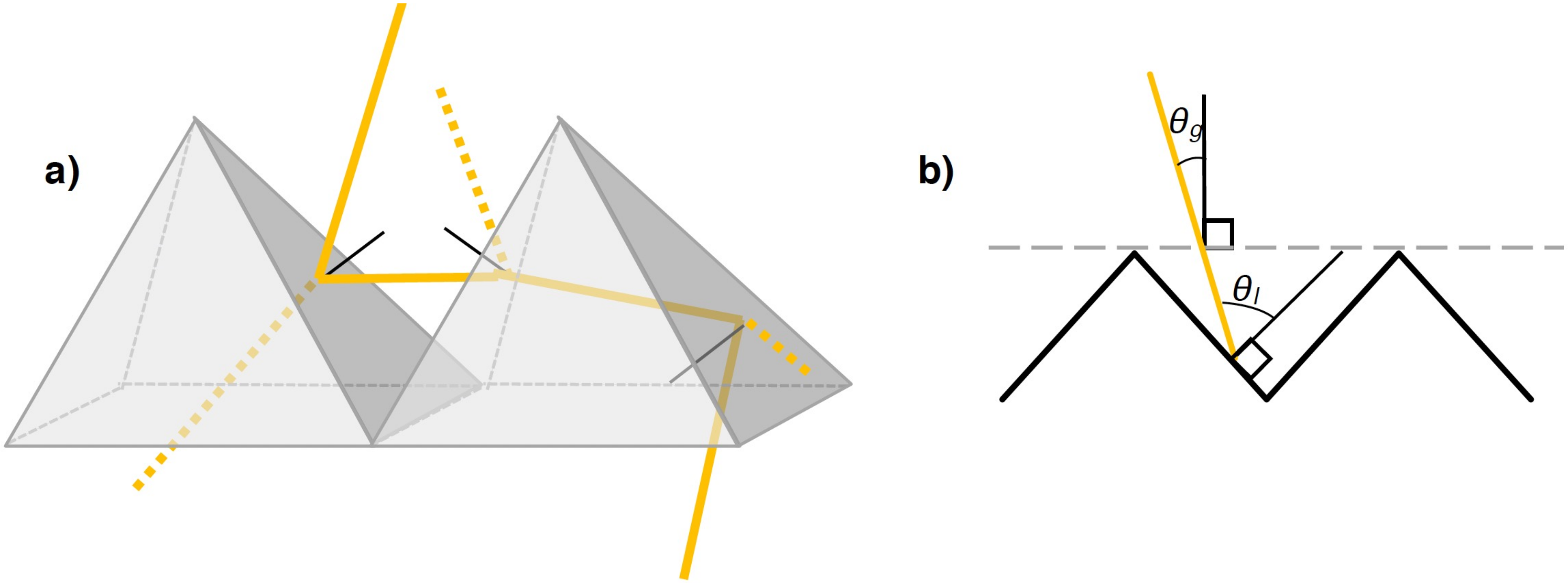
Ray-tracing



Reflection and transmission probabilities can be calculated using the Fresnel equations (for simple interfaces) or TMM (for interface with thin layers). If using TMM, can also calculate absorption per layer (and absorption profiles)

Rigorous coupled-wave analysis (RCWA)

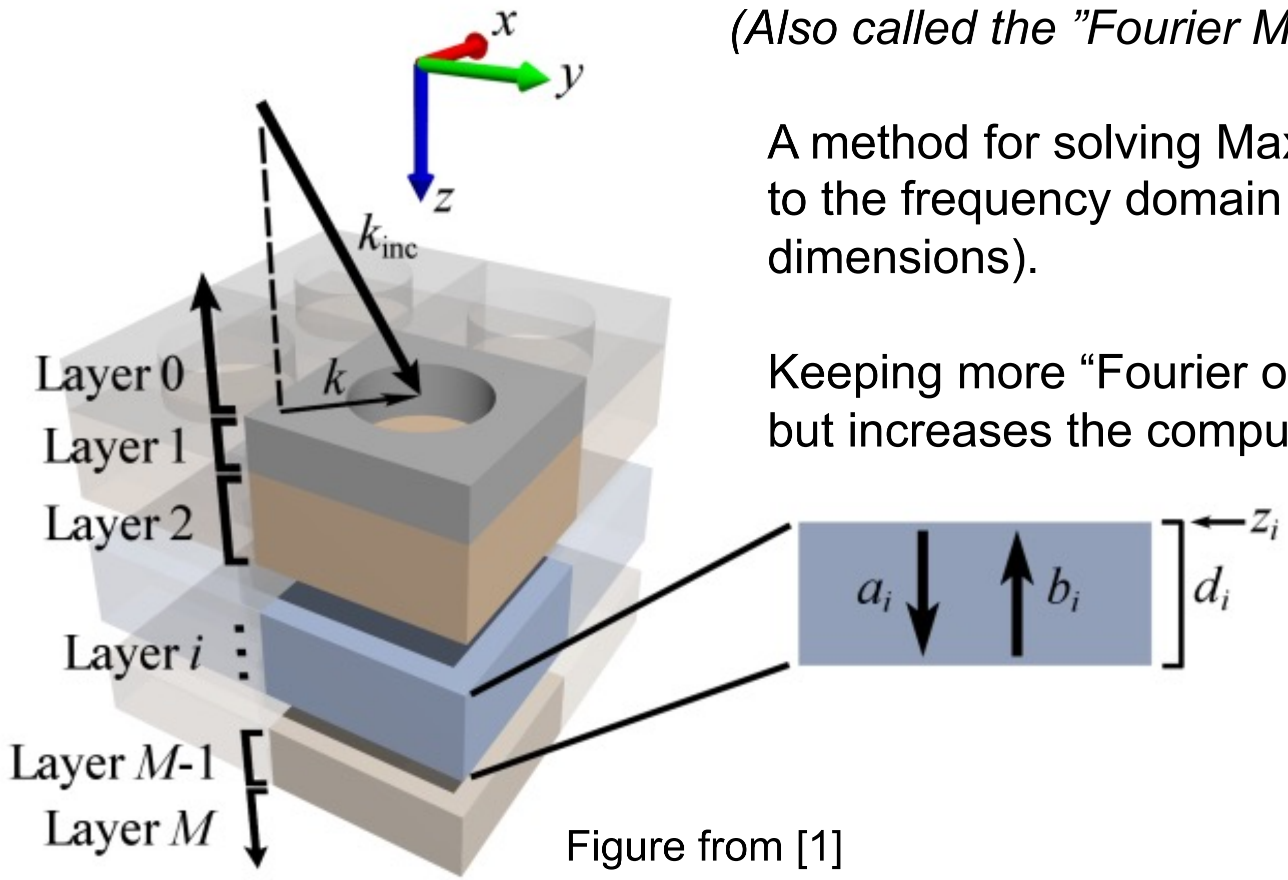


Figure from [1]

(Also called the "Fourier Modal Method")

A method for solving Maxwell's equations, which transforms the problem to the frequency domain (for structures which are periodic in two dimensions).

Keeping more "Fourier orders" should make the solution more accurate, but increases the computation time

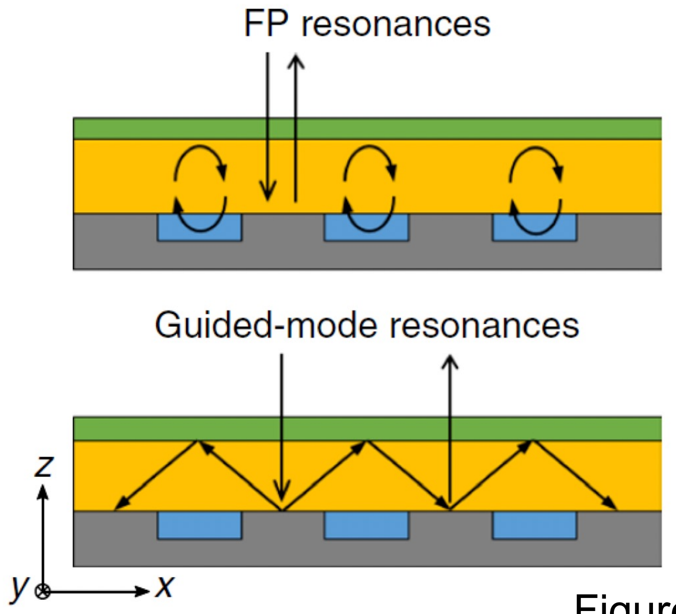
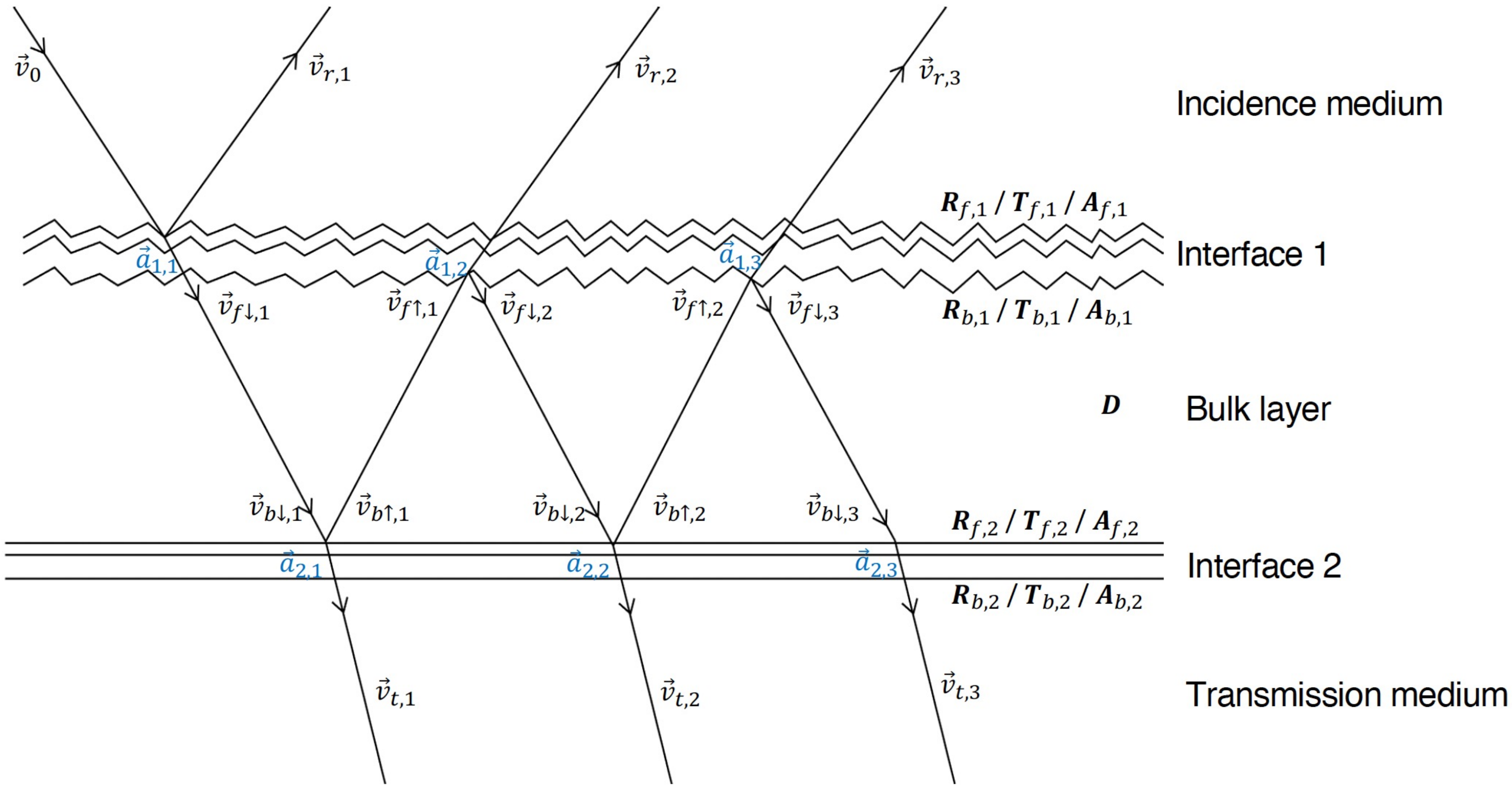


Figure from [2]

[1] H.-L. Chen *et al.*, *Nature Energy*, vol. 4, no. September, 2019, doi: 10.1038/s41560-019-0434-y.
[2] https://web.stanford.edu/group/fan/S4

Angular Redistribution Matrix Method



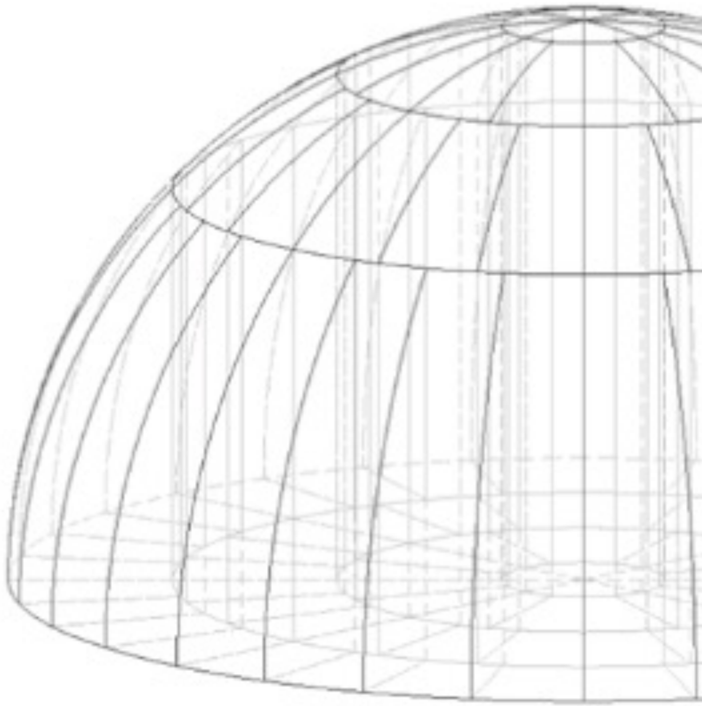
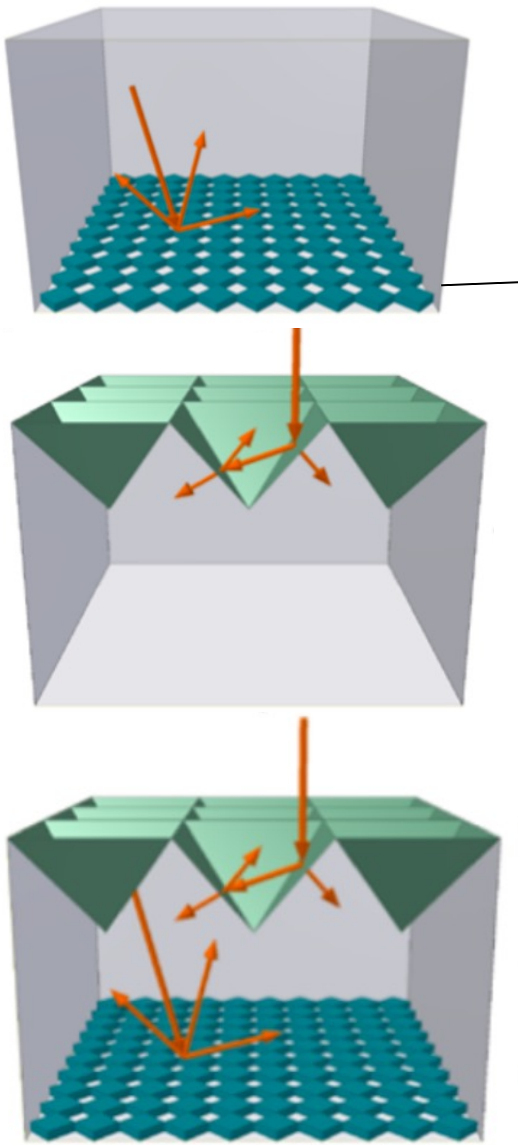


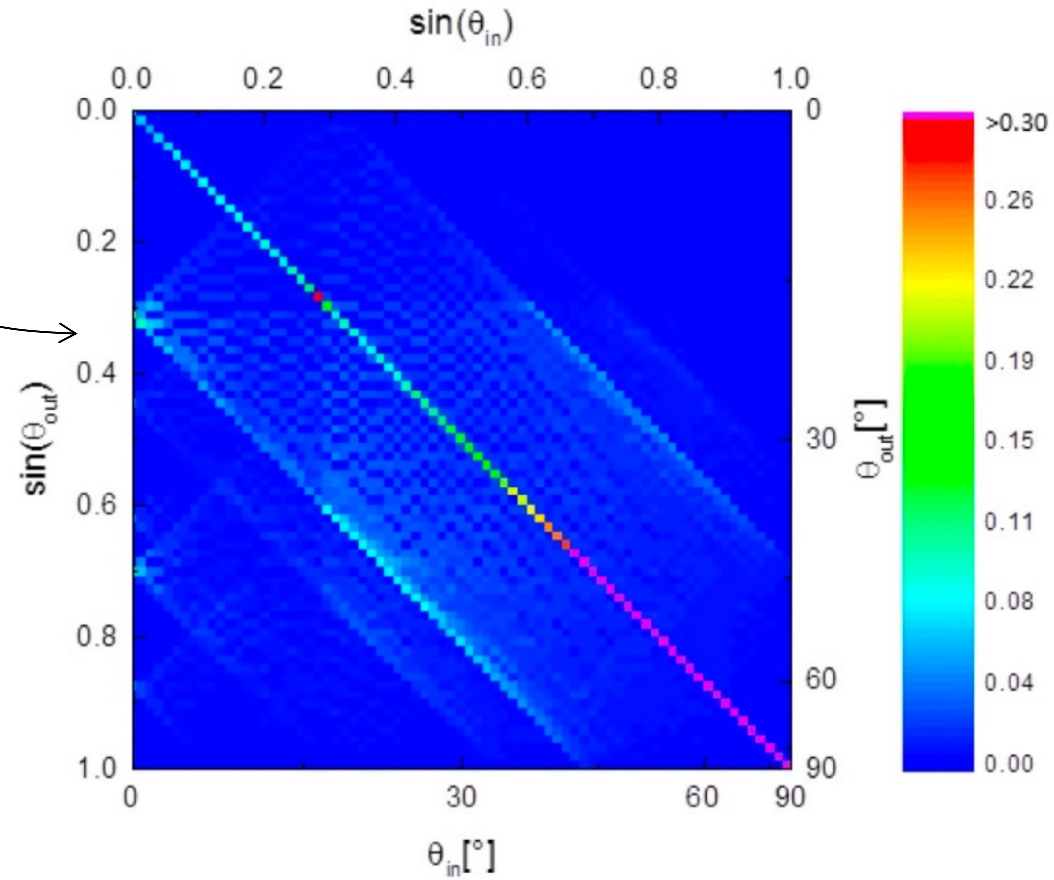
Image from [1]

[1] N. Tucher *et al.*, *Optics Express*, vol. 23, no. 24, p. A1720, 2015, doi: 10.1364/OE.23.0A1720.

Further reading: https://rayflare.readthedocs.io/en/latest/Theory/theory.html

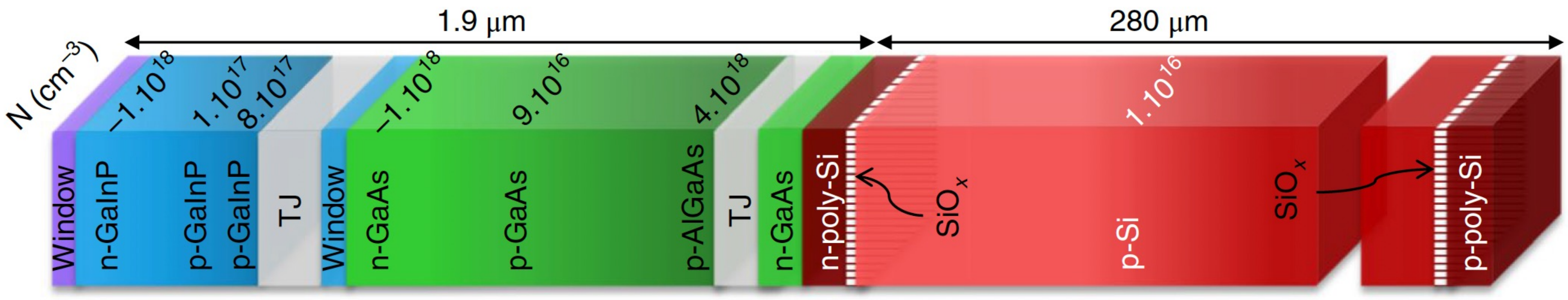
8. Textured Si: pyramids/grating

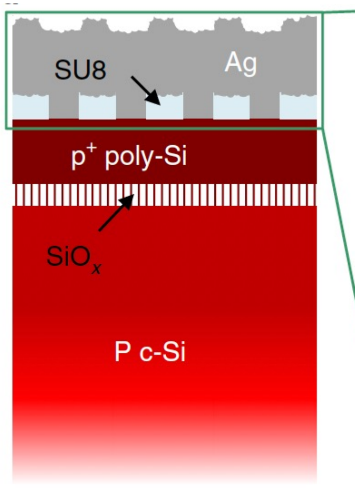


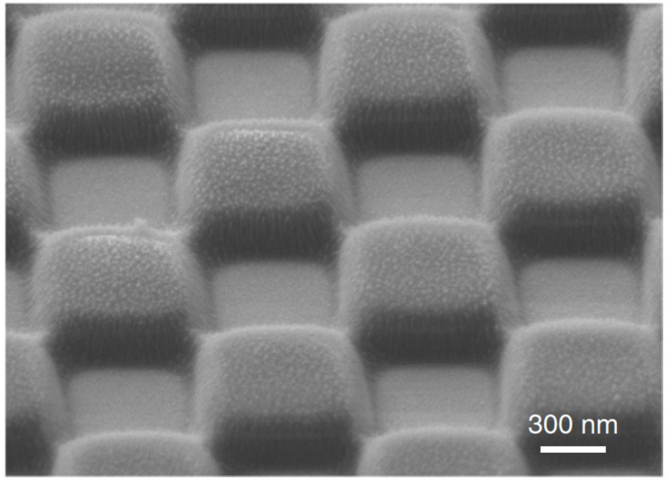


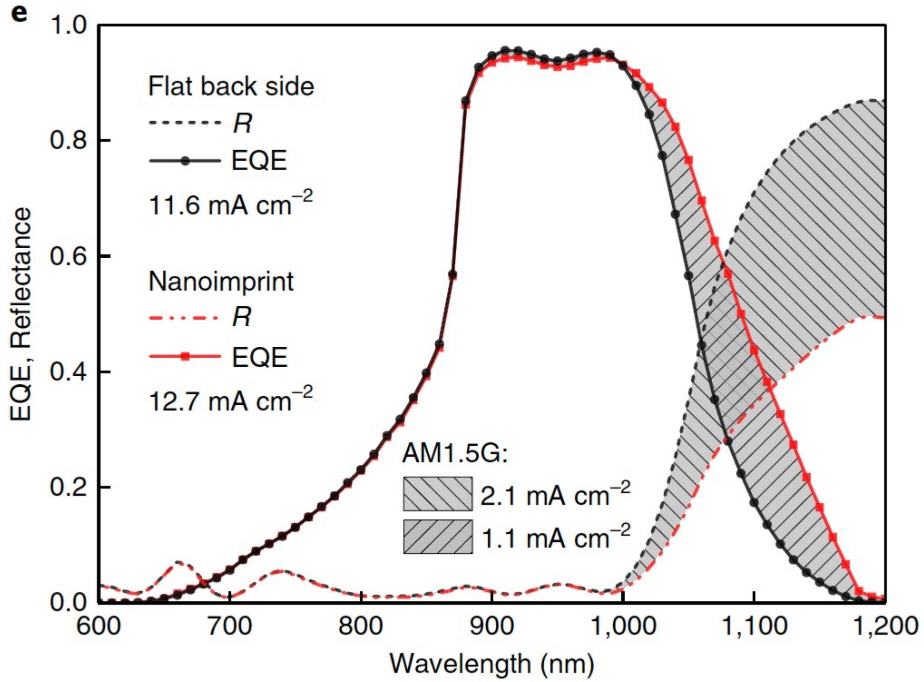
Figures from: https://doi.org/10.1364/OE.23.0A1720

9a. III-V on Si, planar vs. rear grating





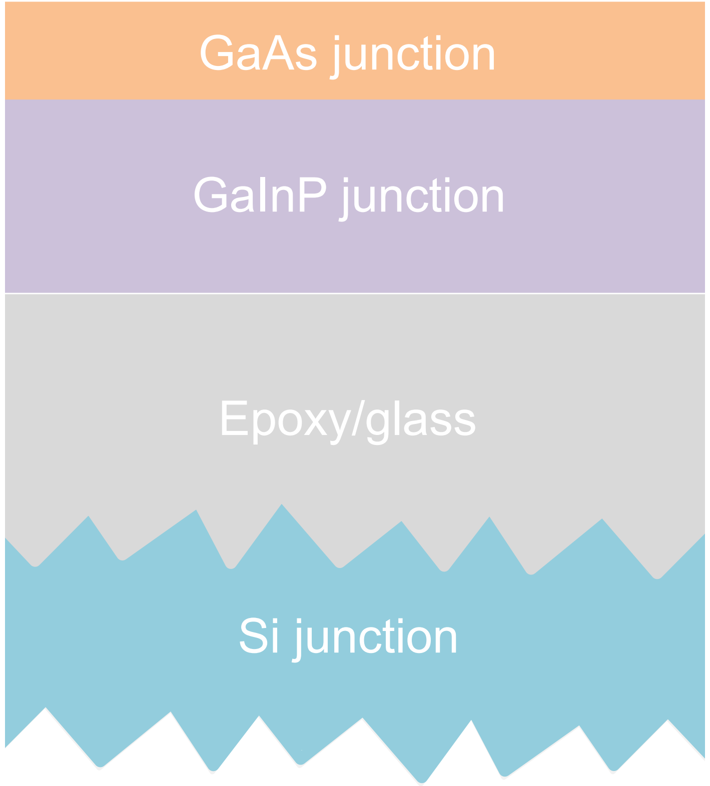




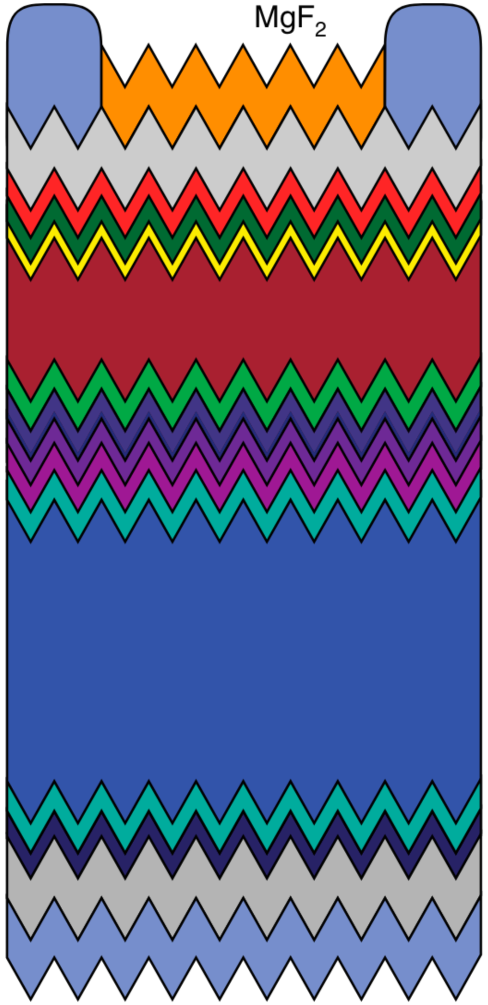
https://doi.org/10.1038/s41560-018-0125-0

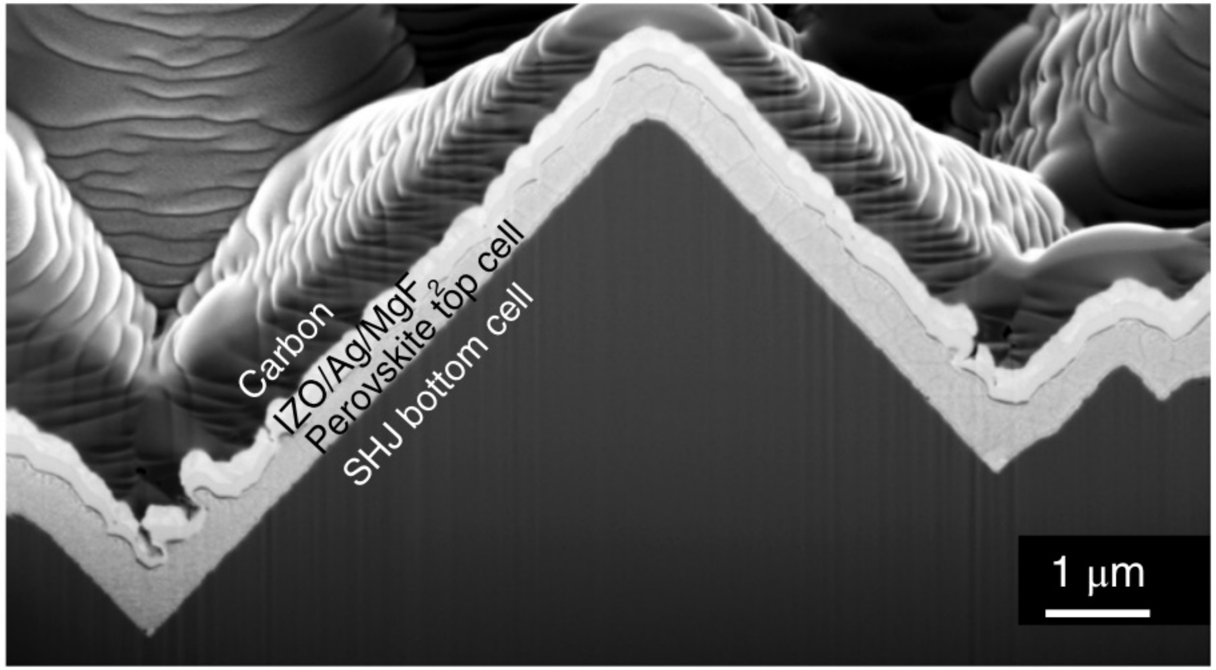
9b. III-V on Si, planar vs. pyramidal Si texture

Use same III-V layer stack as previous example, but assume Si is pyramidally textured on both sides, and epoxy/glass is used to mechanically connect the III-V layers to the Si.



10. Conformal perovskite on pyramidal Si texture





Figures from: https://doi.org/10.1038/s41563-018-0115-4