Faculty of Engineering
School of Photovoltaic and Renewable Energy Engineering

Solcore Workshop – Silicon Tandem Cell Computer Modelling

Sungkyunkwan University, 1 – 3 August 2023

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www.qpvgroup.org

EkinsNed

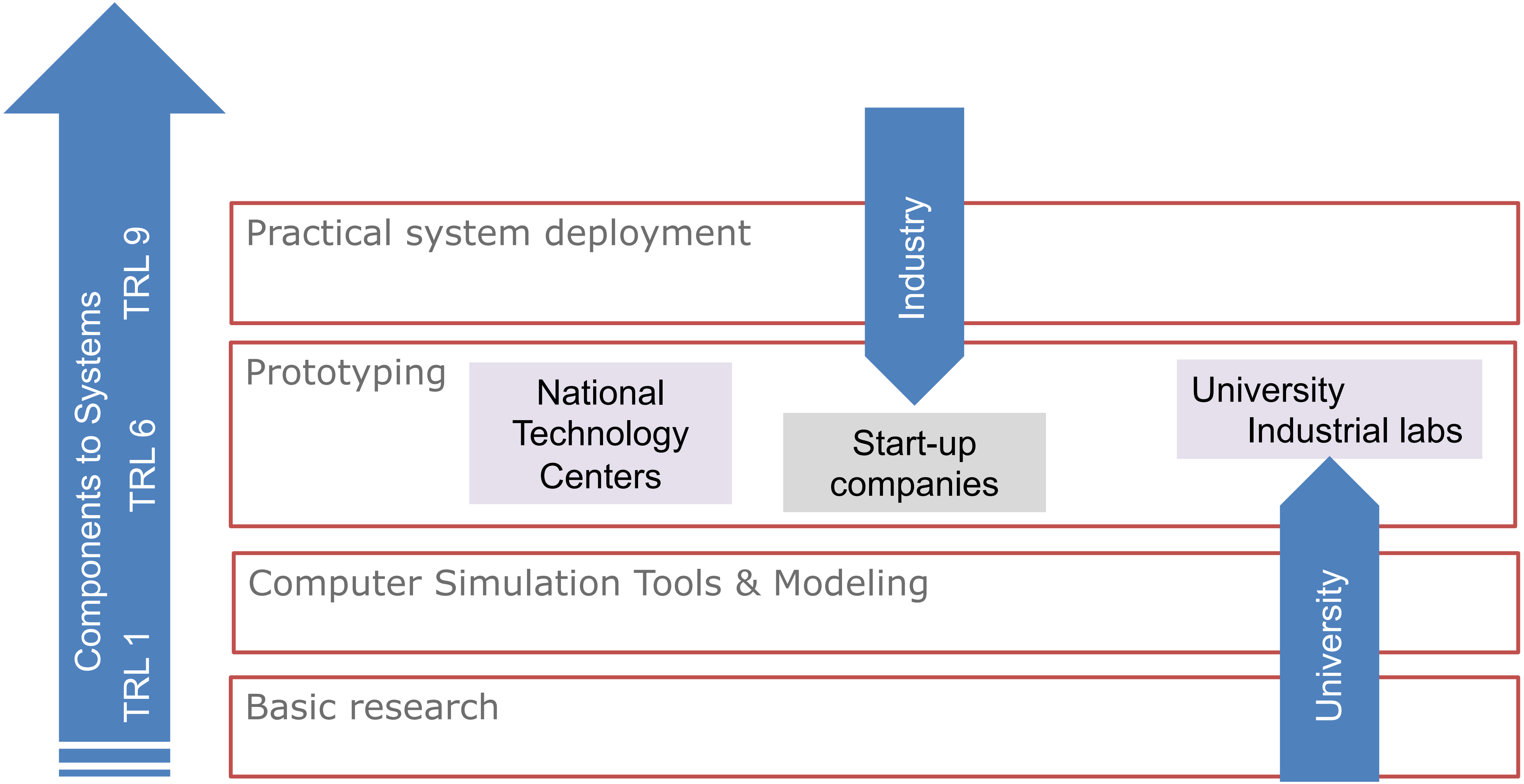
Faculty of Engineering
School of Photovoltaic and Renewable Energy Engineering

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

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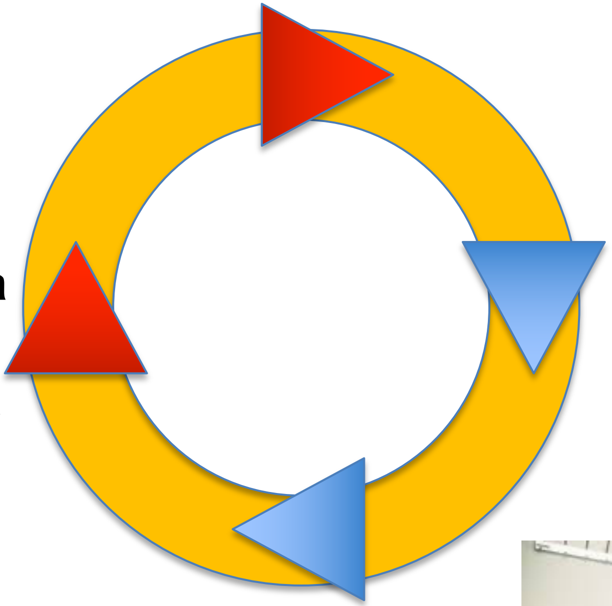
The Present Value of Computer Modelling in Research & Development

**Design aided by
a computer (TCAD):**

**Evaluate data
through
fitting of data**



**Device
Fabrication**

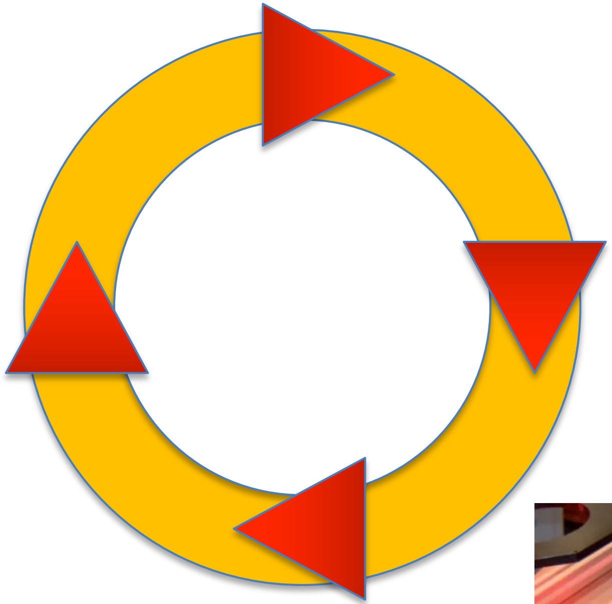
Device Test

The Future Value of Computer Modelling in Research & Development

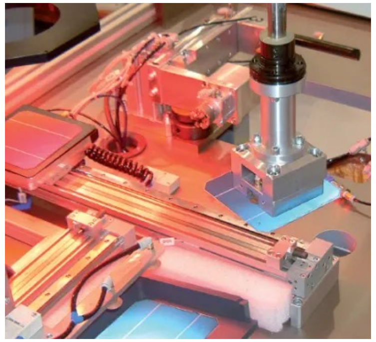
Design aided by a computer (TCAD):

Robot Device Fabrication

AI assisted fitting of test data

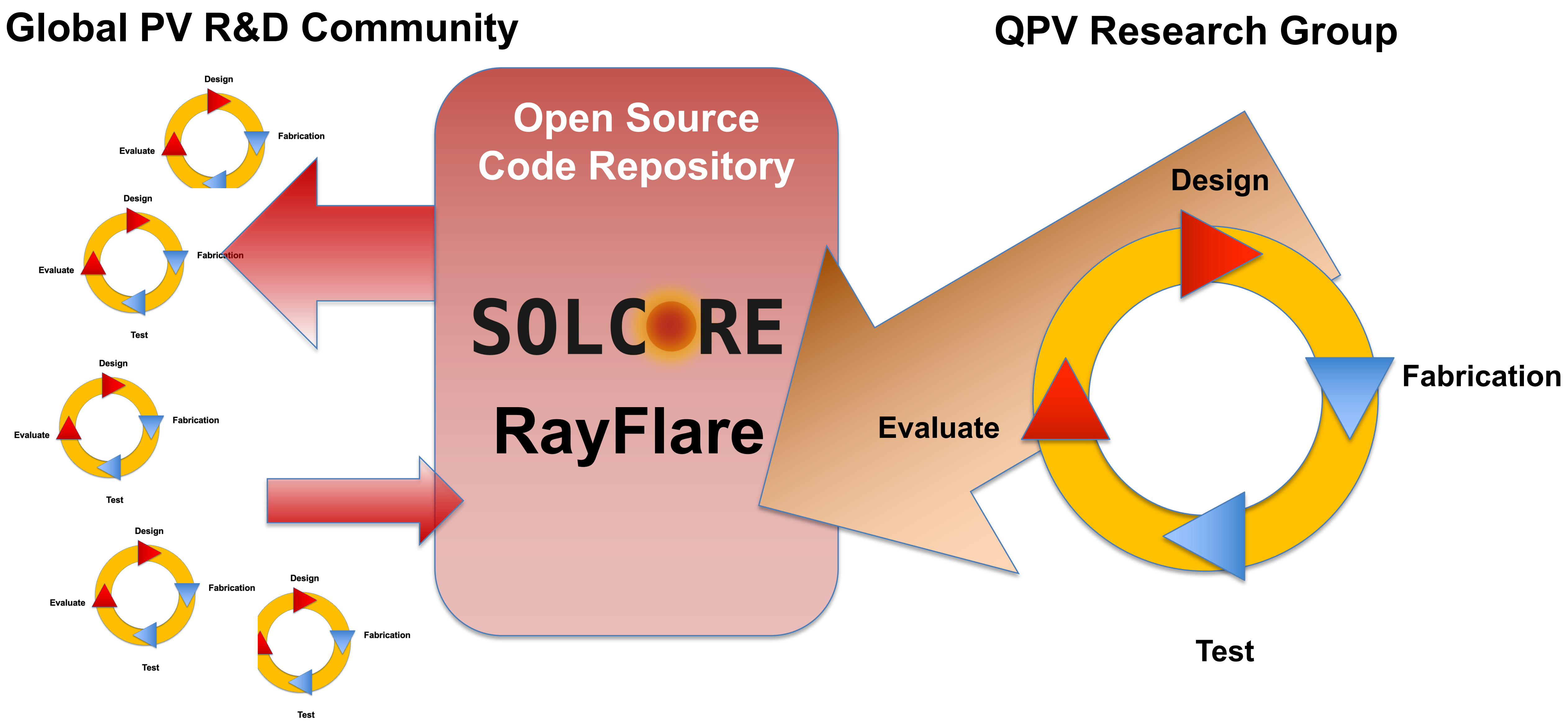


Automated Device Test

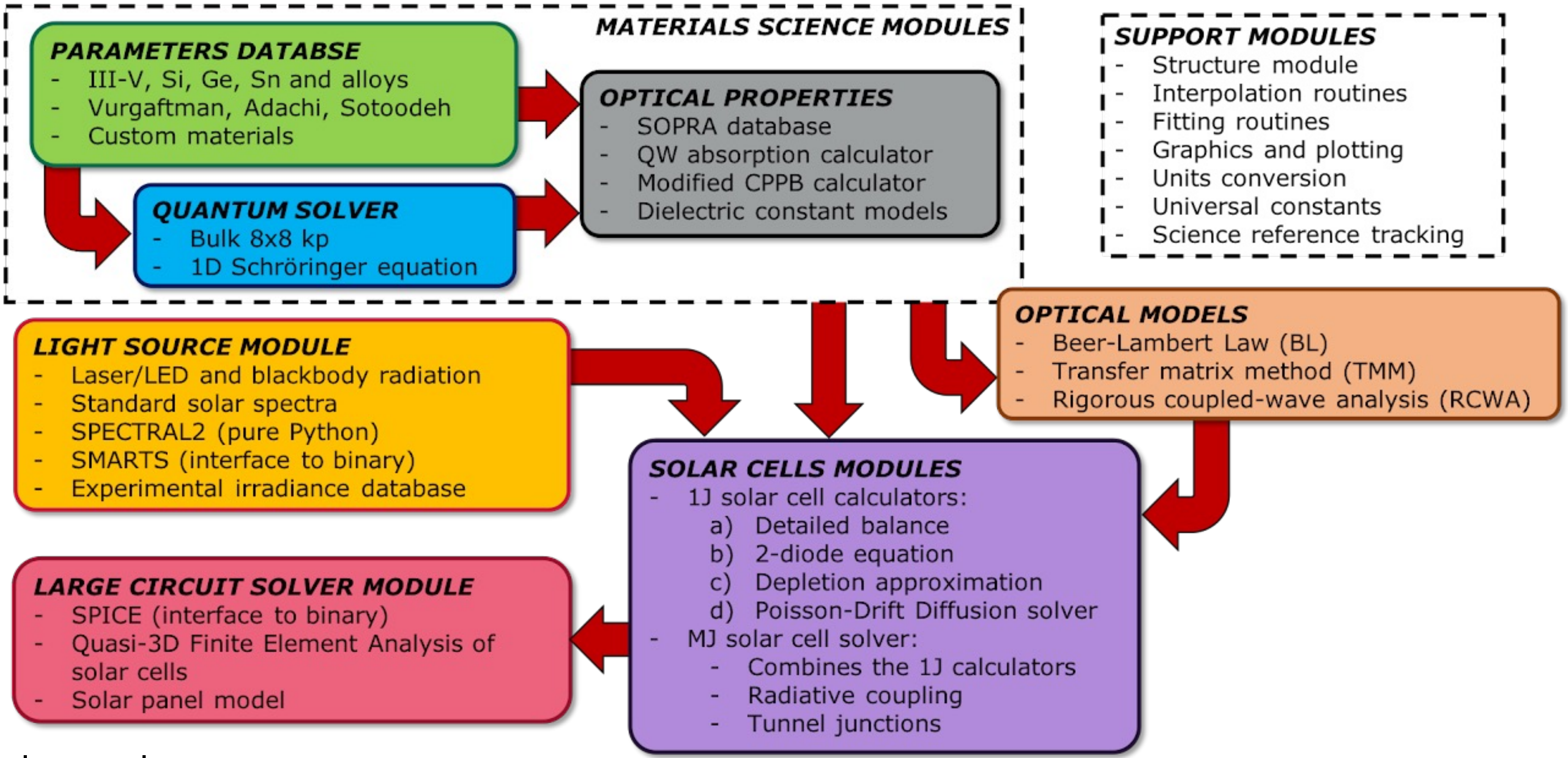


Rachel Kurchin, Giuseppe Romano, & Tonio Buonassisi,. 'Bayesim: A tool for adaptive grid model fitting with Bayesian inference'. Computer Physics Communications, (2019)

Development Process for our Computer Code:



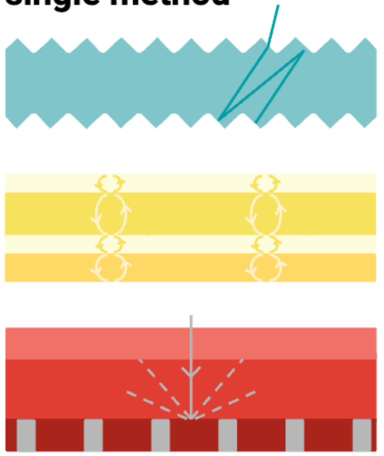
Solcore capabilities



www.solcore.solar

RayFlare capabilities

Simulations using a single method



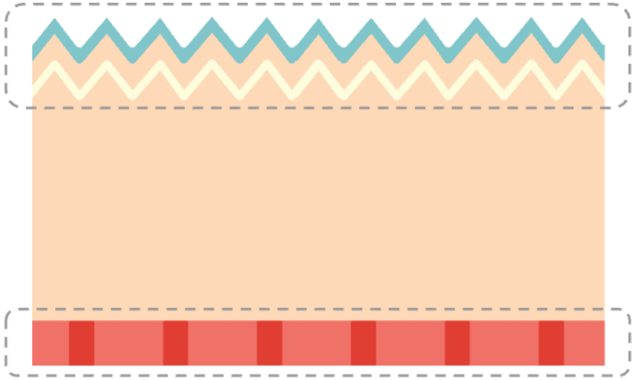
Ray-tracing: Geometric optics for large-scale textures without diffraction effects

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

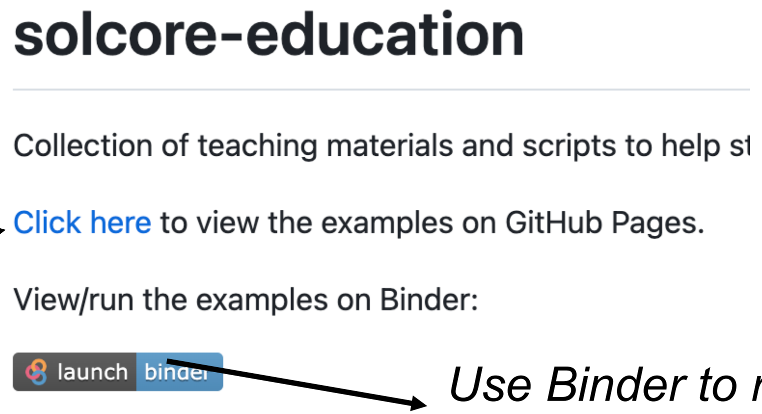
- Free, open source
- Anyone can contribute
- Modular
- Documented

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), and then:

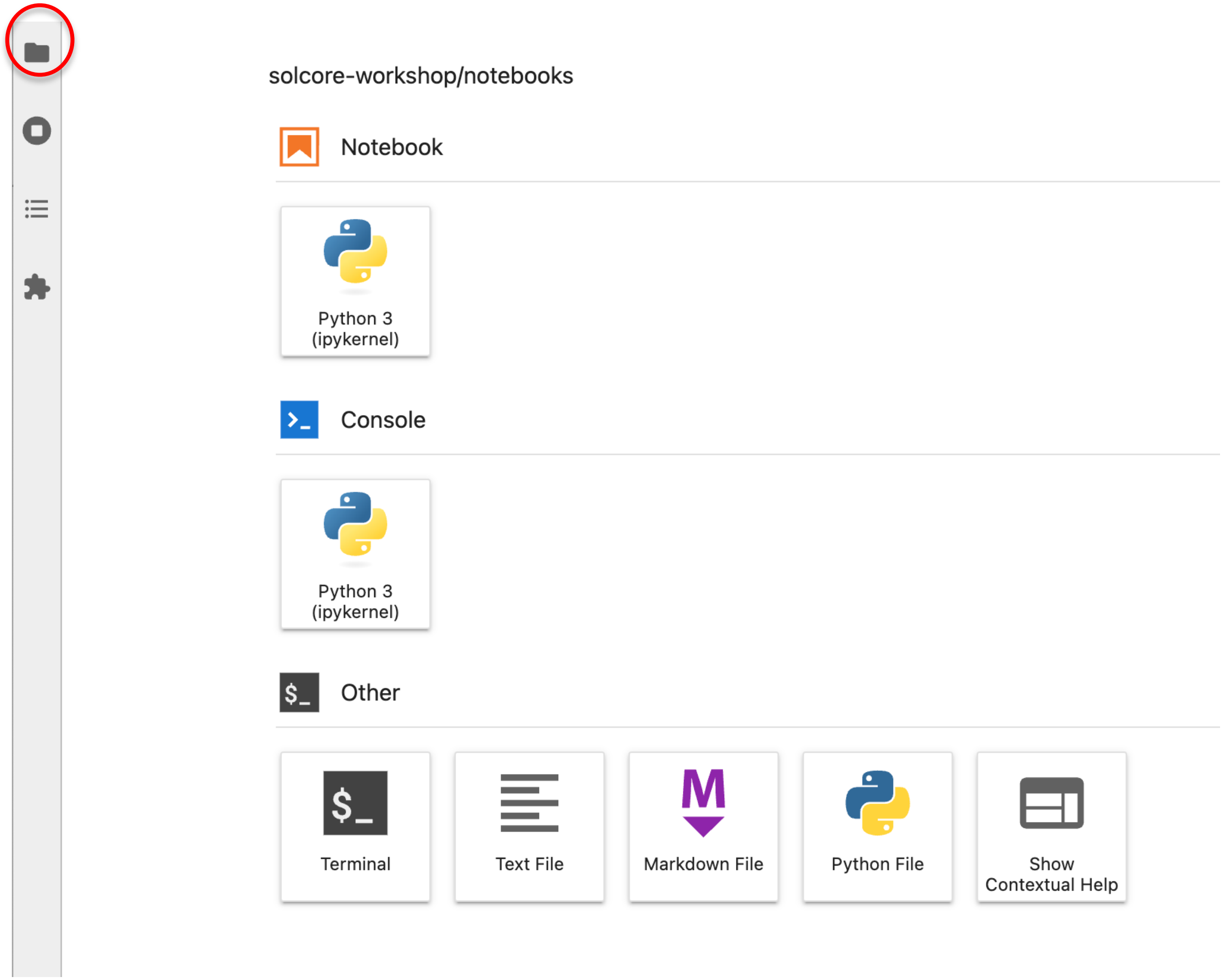
pip install solcore rayflare seaborn

Recommendations for installing Python:

- 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)

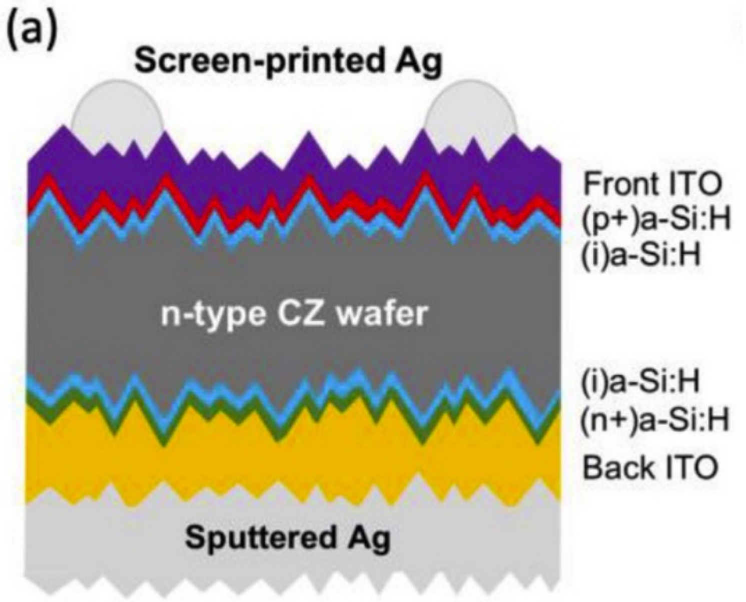
Binder

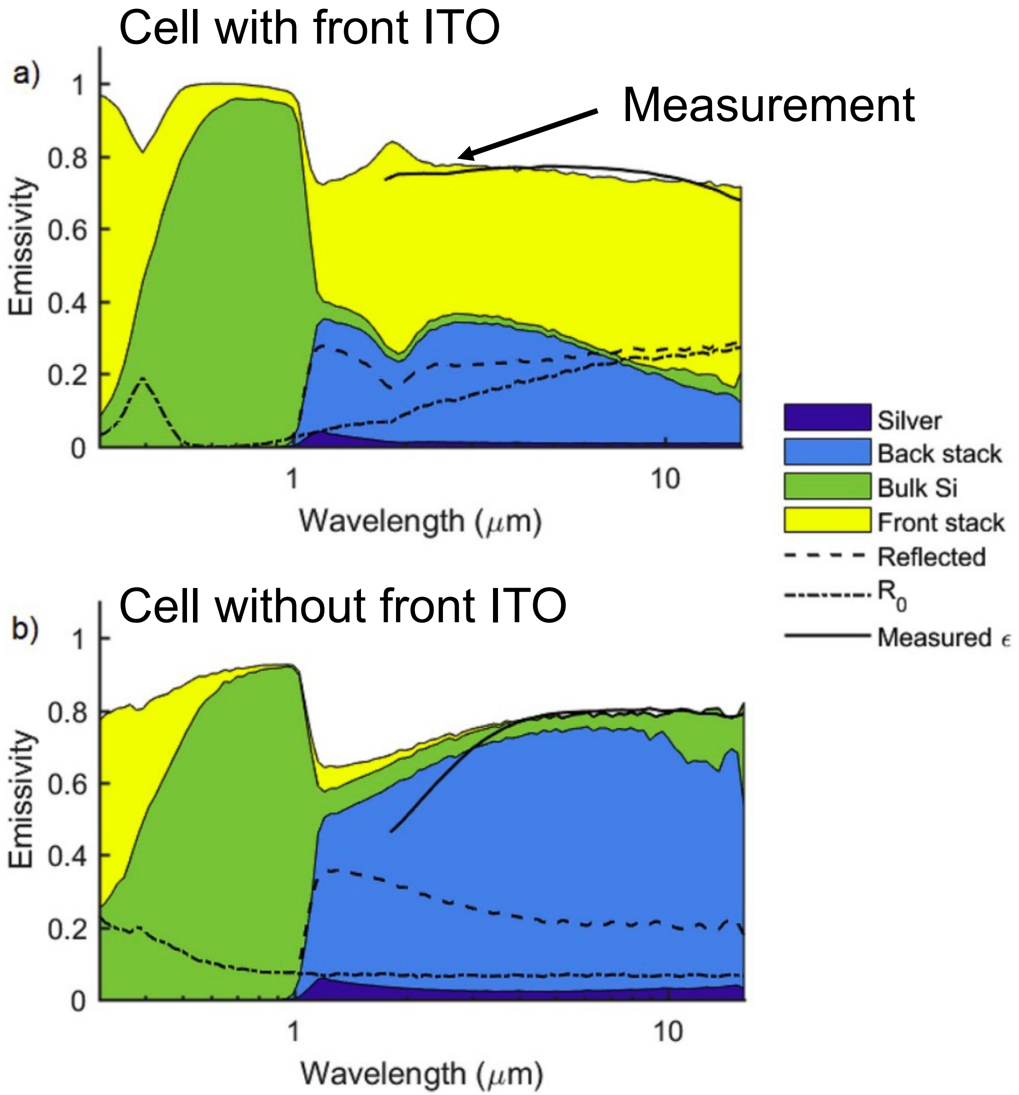
- Binder may take a long time (~ 10 minutes) to load, so please click the link to 'Launch Binder' now



After loading, it should look like this – click circled icon to open the examples

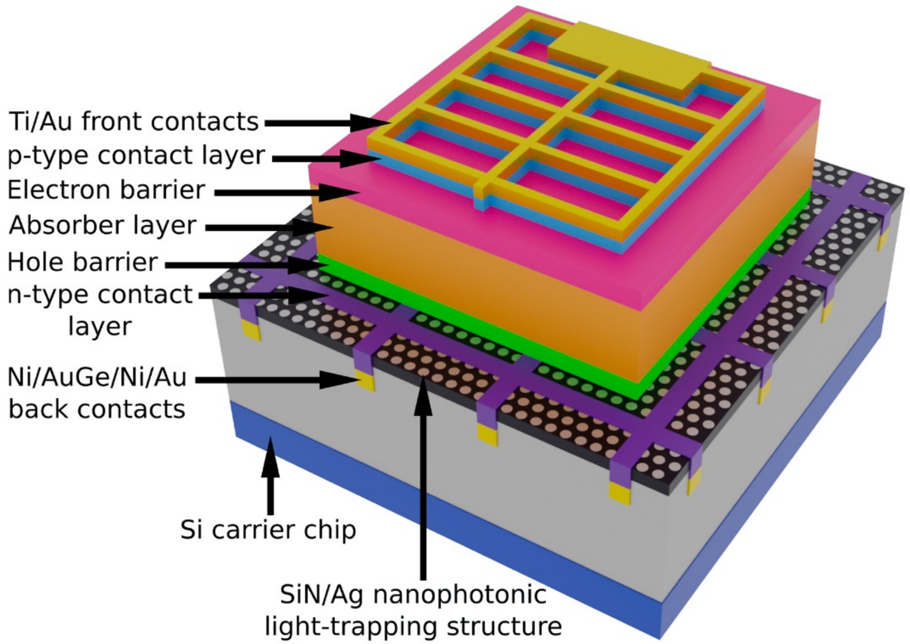
Example: Si cell emissivity

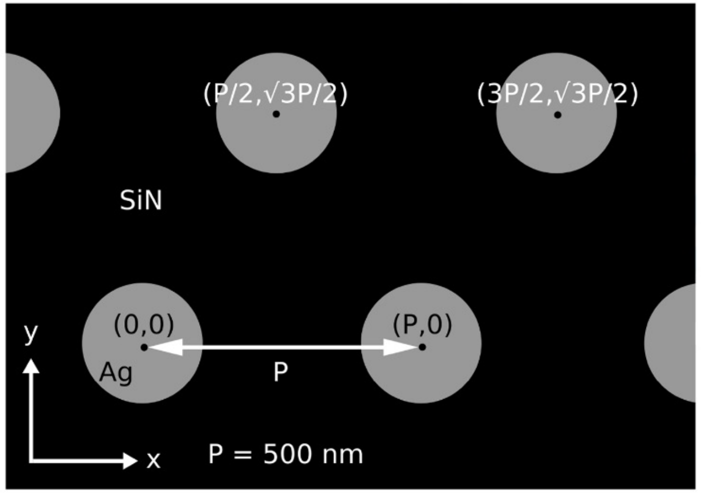


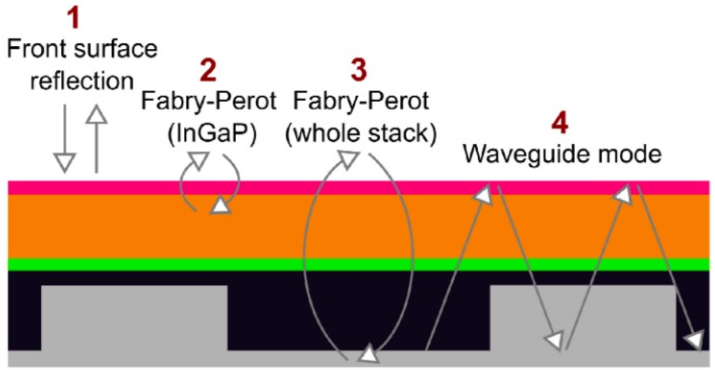


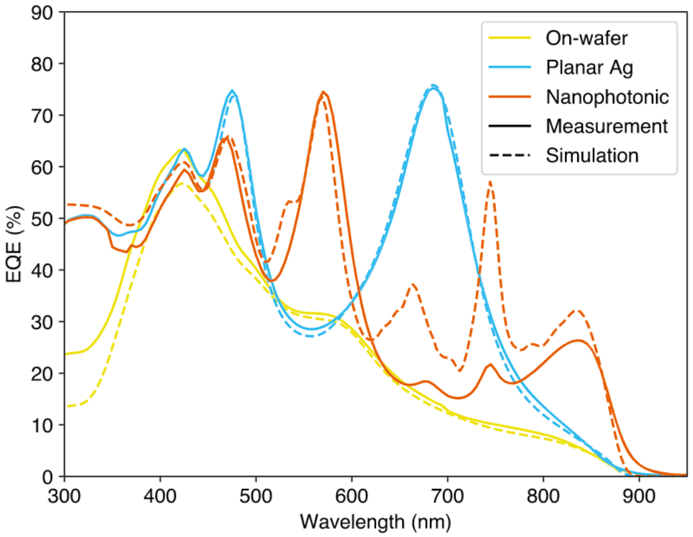
Simulations & measurement of cell absorptivity (emissivity) between 300 nm and 20 µm. This is relevant for the operating temperature of the cell. Due to free-carrier absorption in doped layers and very good light-trapping, the cell absorbs well even at wavelengths far beyond the bandgap.

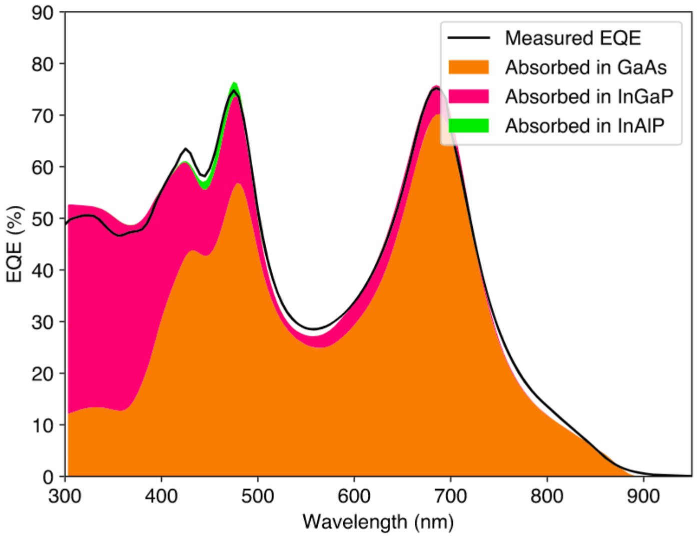
Example: ultra-thin GaAs cell





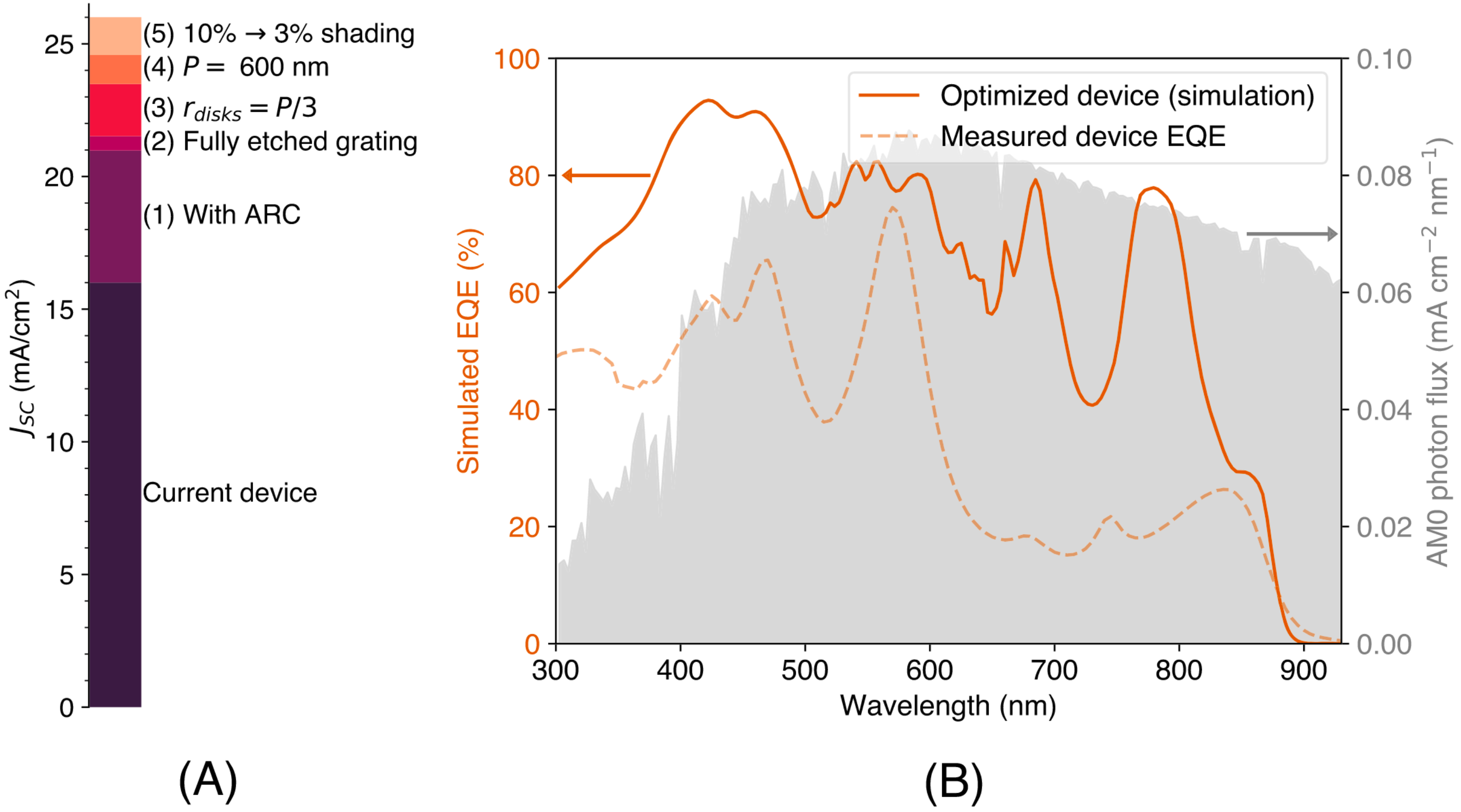




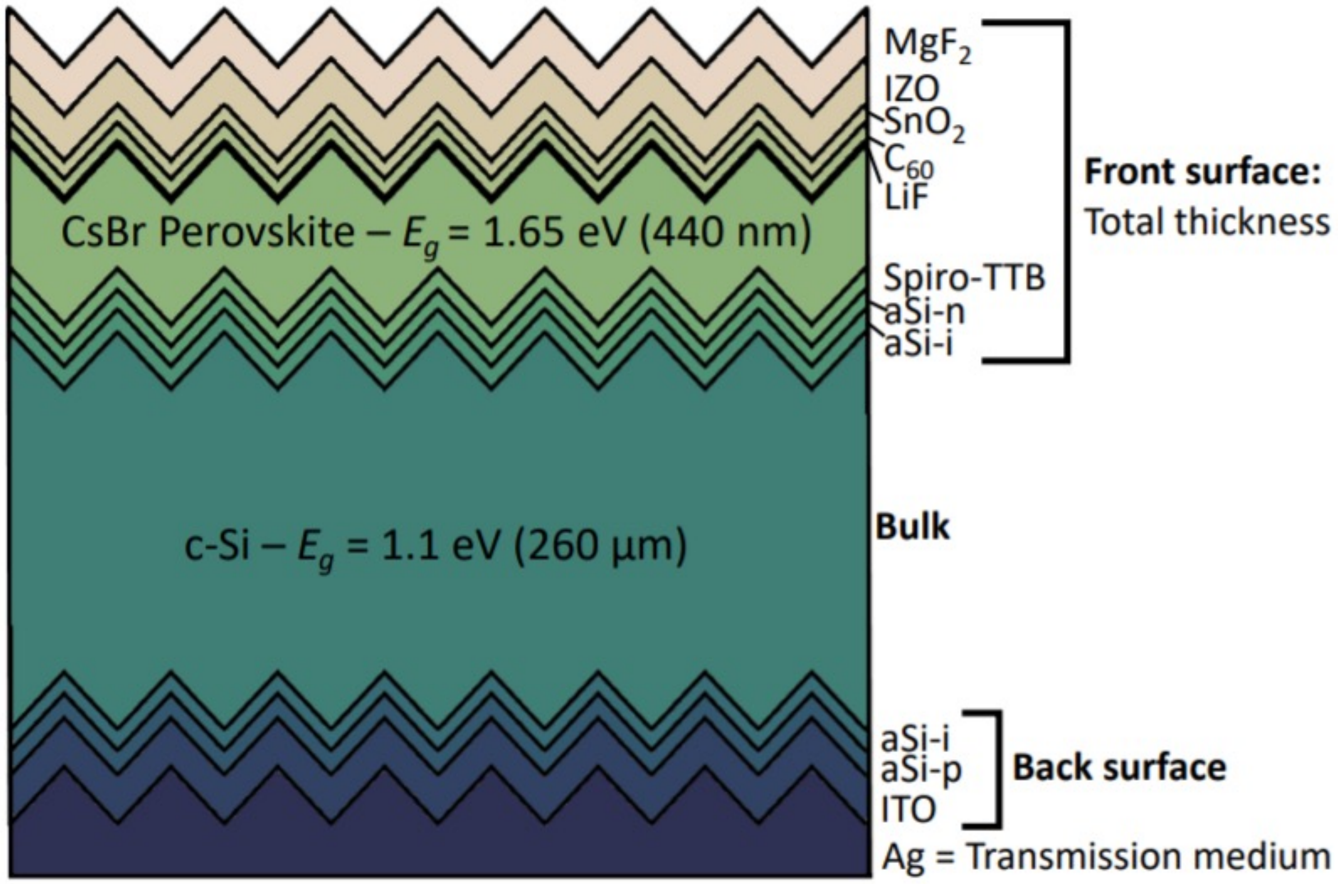


[1] L. Sayre *et al.*, 'Ultra-thin GaAs solar cells with nanophotonic metal-dielectric diffraction gratings fabricated with displacement Talbot lithography', *Progress in Photovoltaics*, vol. 30, no. 1, pp. 96–108, Jan. 2022, doi: 10.1002/pip.3463.

Example: ultra-thin GaAs cell (cont.)

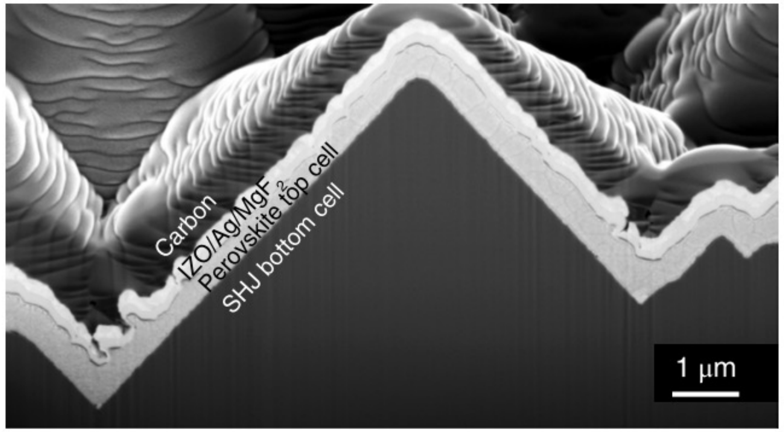


Example: Perovskite/Si tandem cell



Perovskite on silicon heterojunction (SHJ) tandem cell

Perovskite is deposited conformally on standard etched Si pyramid texture

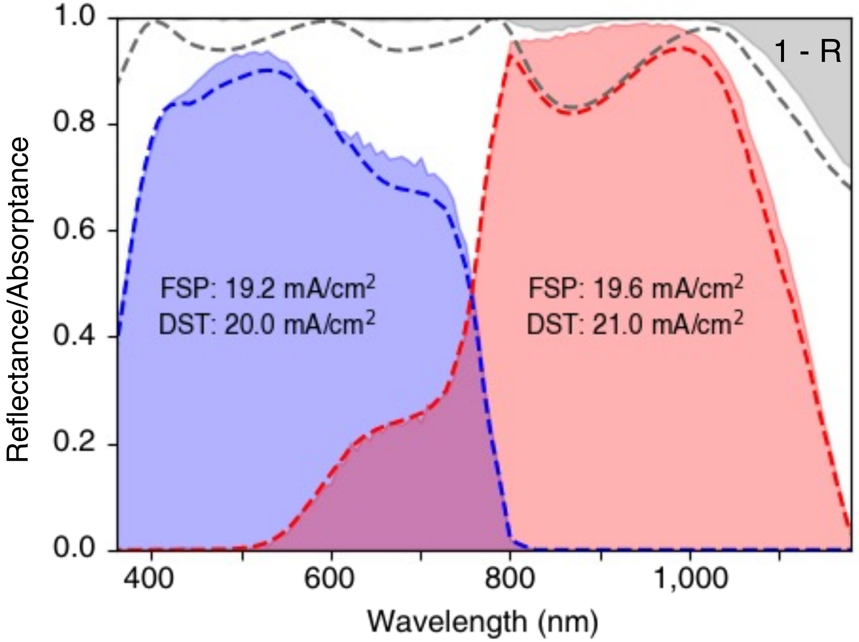


From [1]

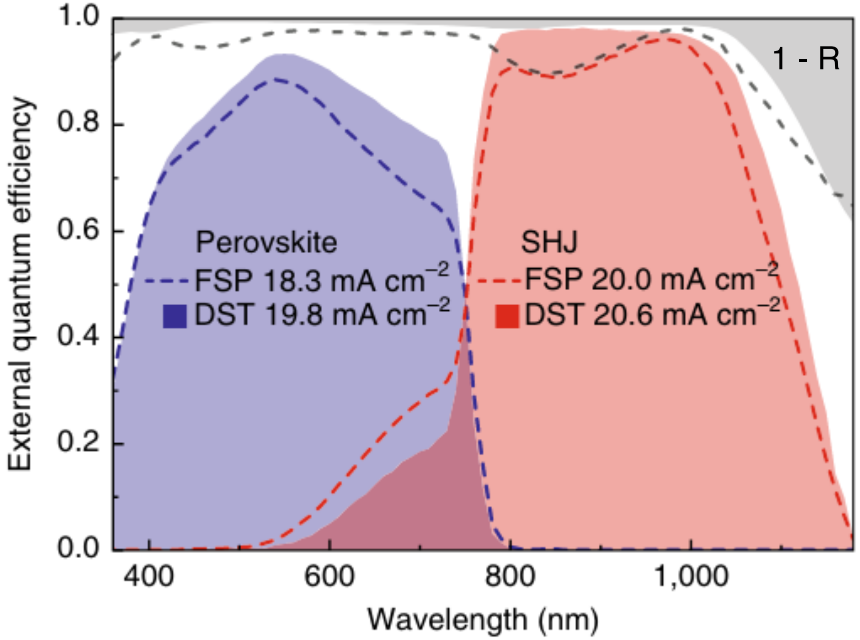
[1] Sahli, F., Werner, J., et al. (2018) 'Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency', *Nature Materials*. Springer US, 17(9), pp. 820–826.

Example: Perovskite/Si tandem cell (cont.)

RayFlare simulation

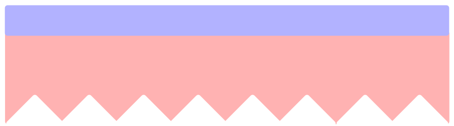


EQE measurement

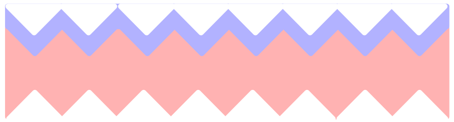


From [1]

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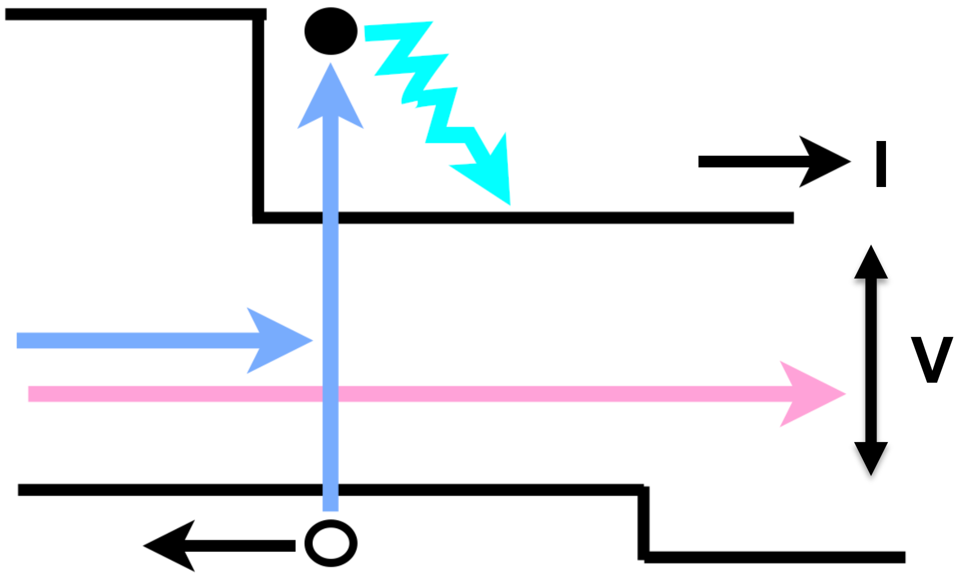
Session 2: Hands-on exercise
Using SolCore to calculate the Shockley-Queisser Efficiency limit

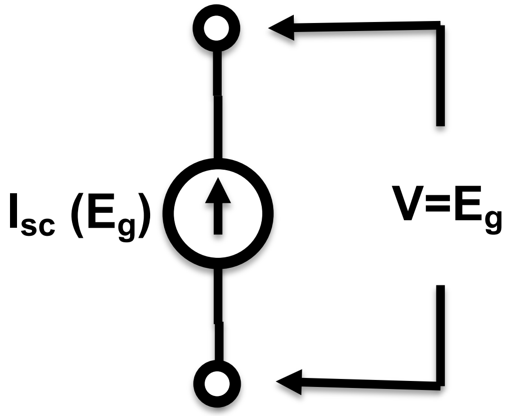
1 August 2023

Ned Ekins-Daukes, Phoebe Pearce

What is the Maximum Efficiency of a Solar Cell?

Trivich-Flynn Limit (1955)



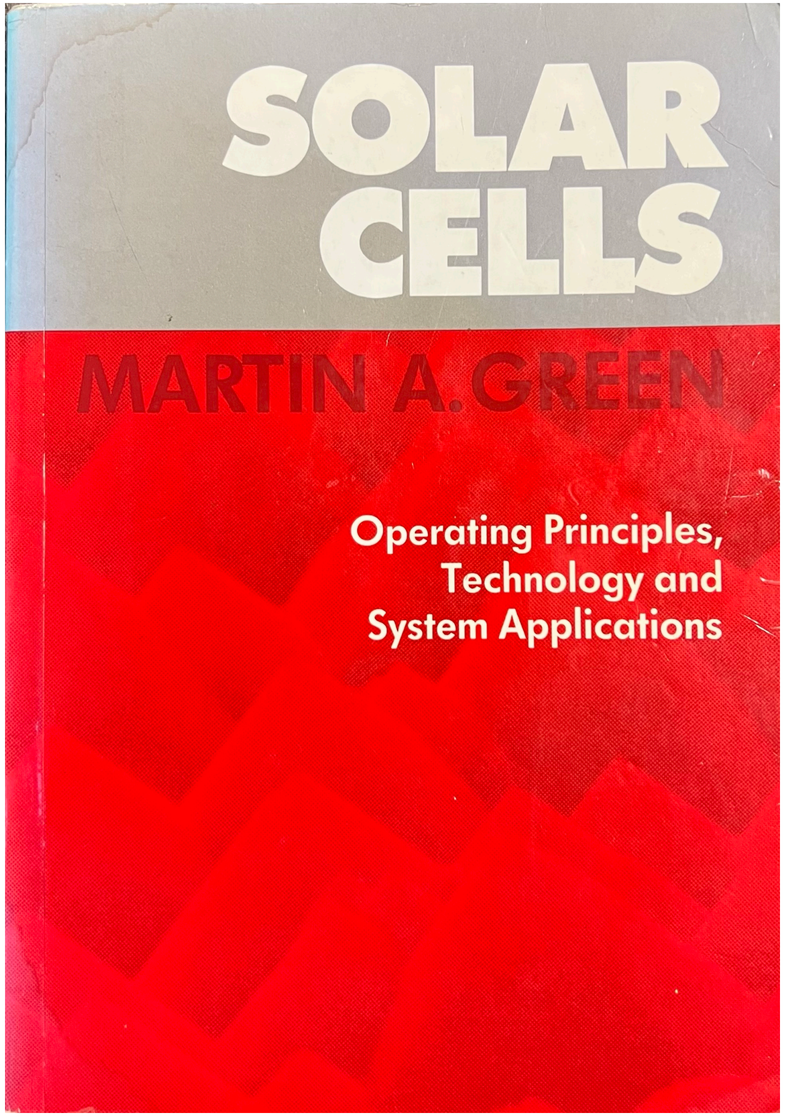


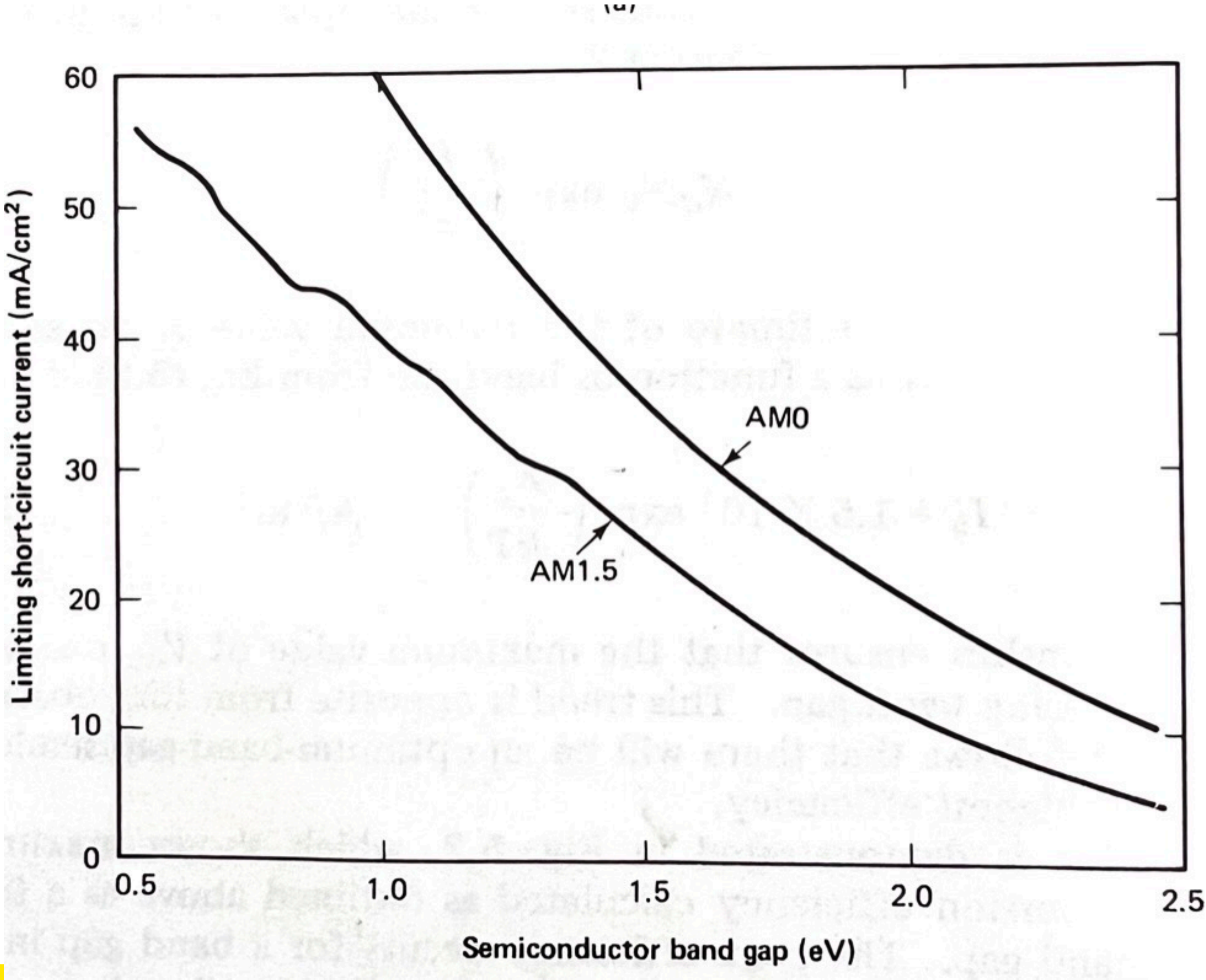
Warning : Limit is invalid for T > 0K !

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

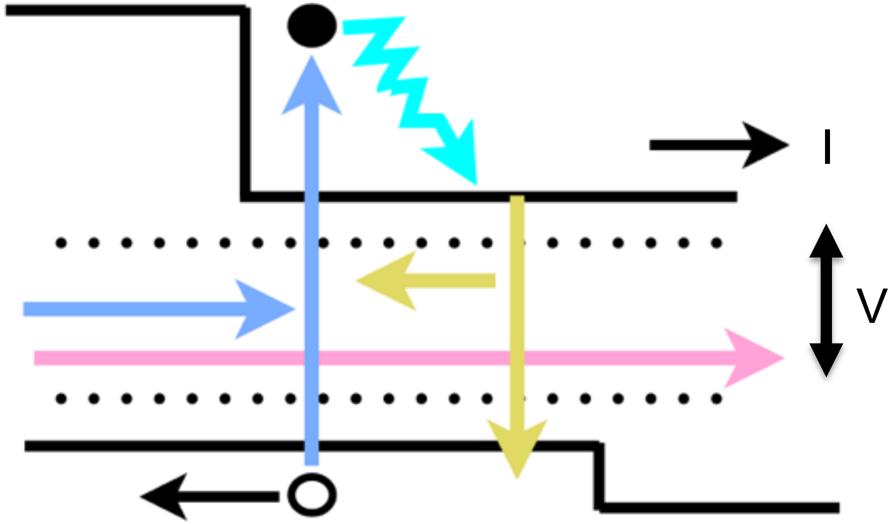
Limit to the Short-Circuit Current

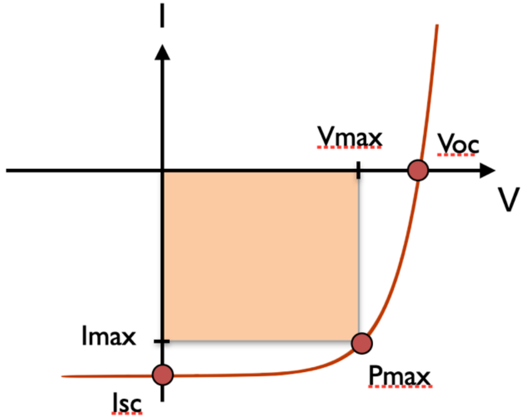


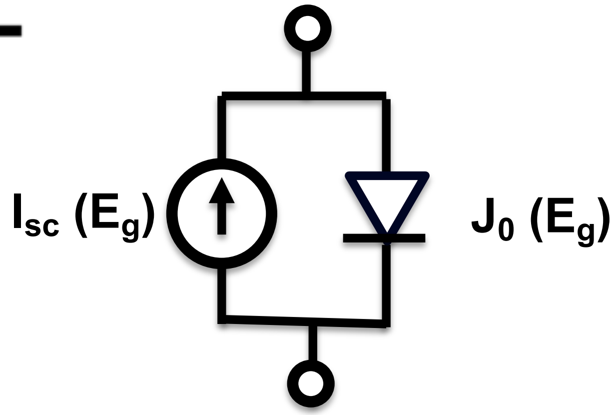


What is the Maximum Efficiency of a Solar Cell?

Shockley Queisser limit (1961)







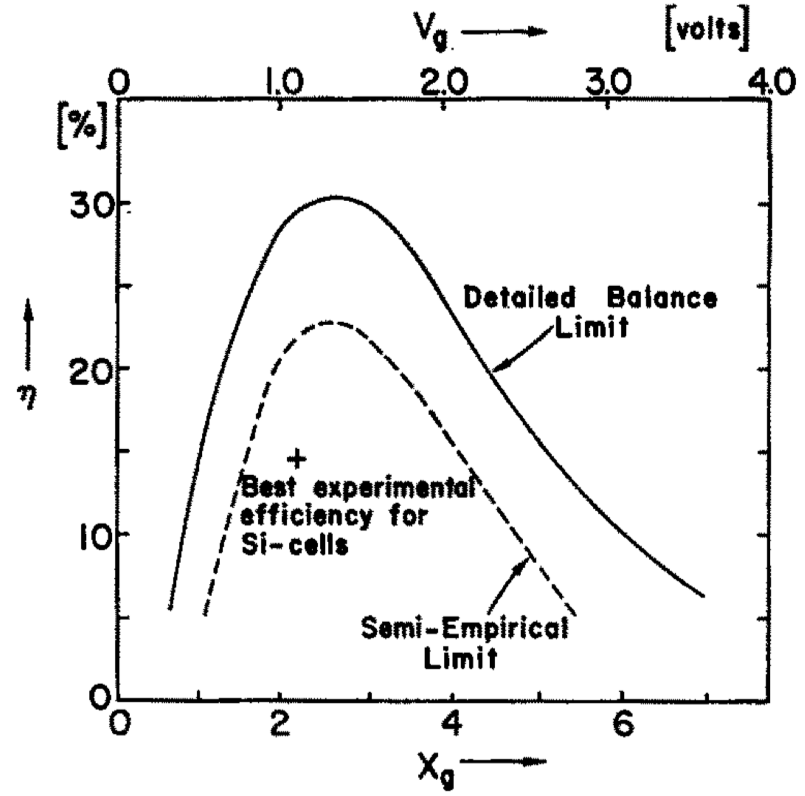


FIG. 1. Comparison of the "semiempirical limit" of efficiency of solar cells with the "detailed balance limit," derived in this paper. + represents the "best experiment efficiency to date" for silicon cells. (See footnote 6.)

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

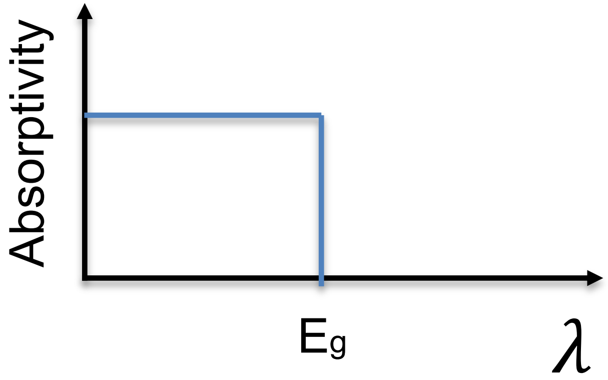
Ned Ekins-Daukes, Phoebe Pearce

Optical Models for PV Devices

Fundamental

Shockley-Queisser (Detail Balance)

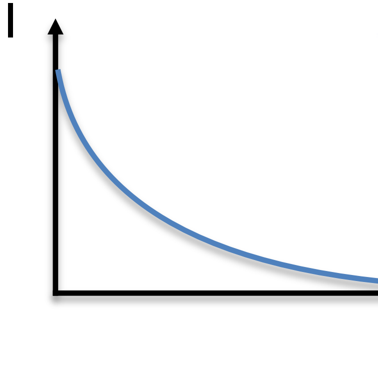
Complete absorption to band-gap energy Eg

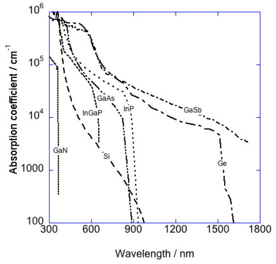


Beer Lambert Law

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

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

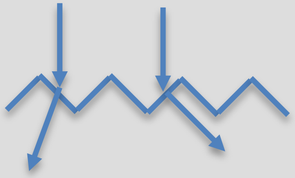




Ray Optics

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

Surface texture of a silicon solar cell

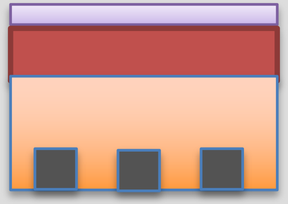


Wave Optics

Sub-wavelength structures $\ll \lambda$

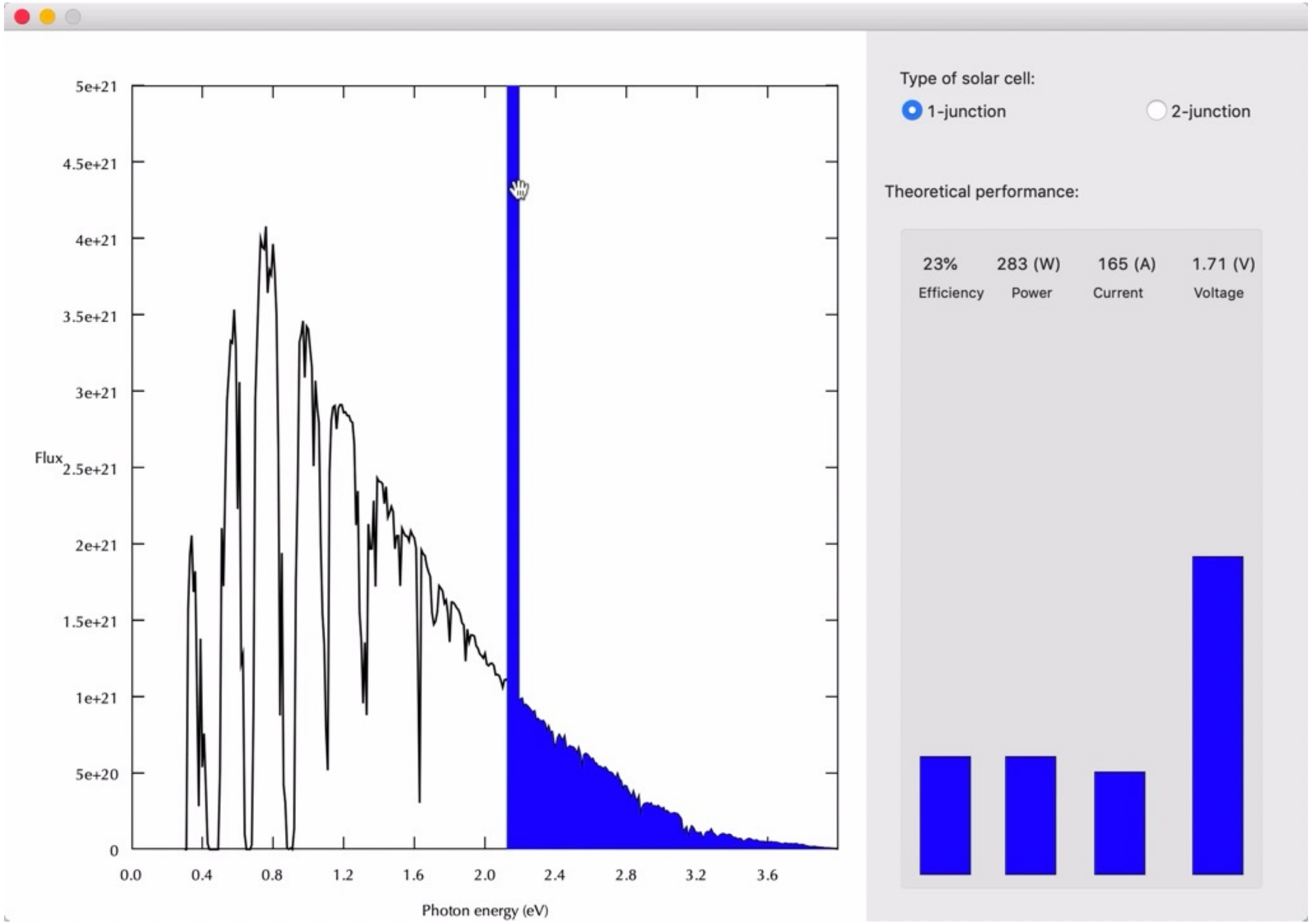
Anti-reflection coating
90nm p-doped layer

800nm n-doped layer

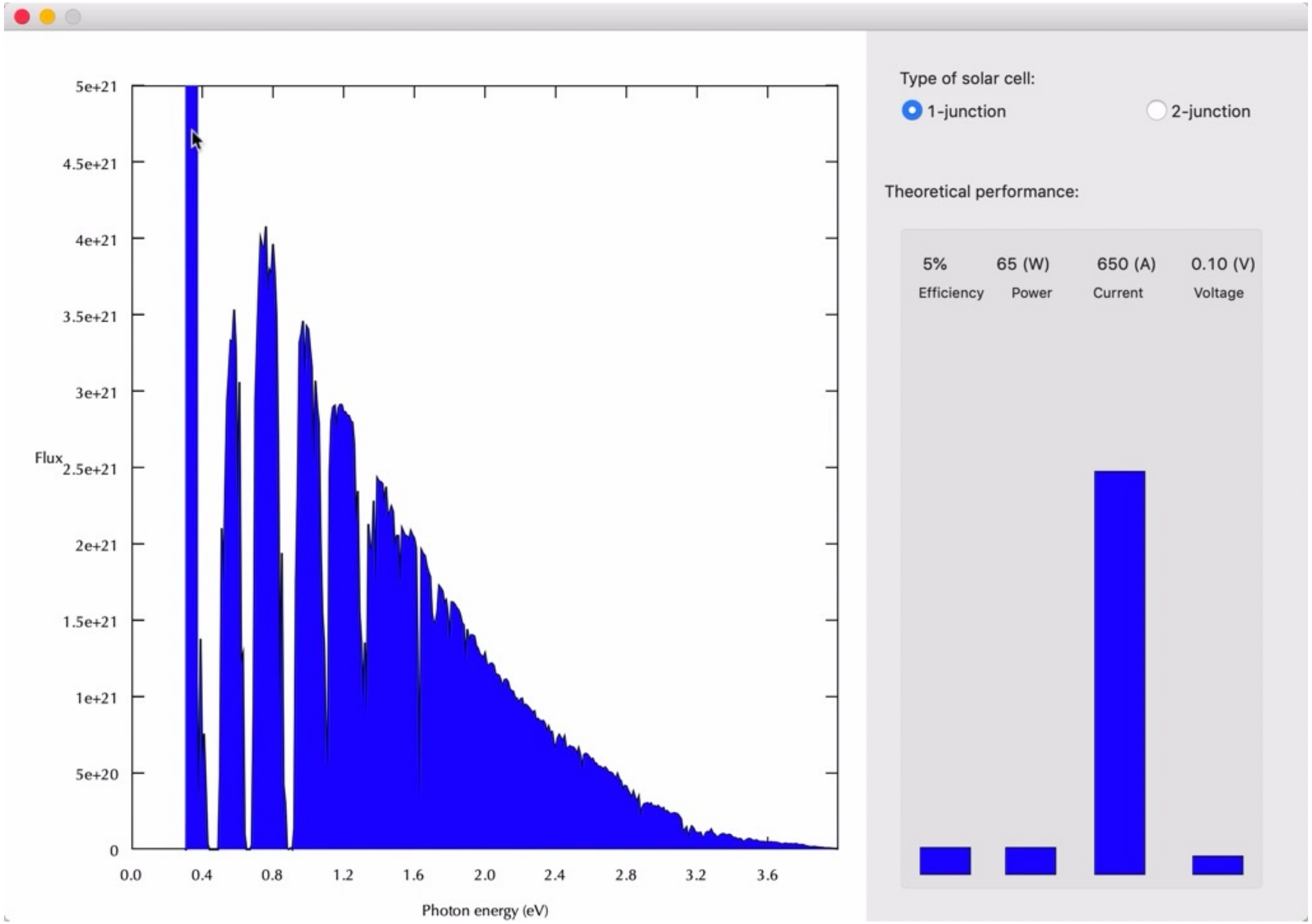


Diffractive grating on rear side.

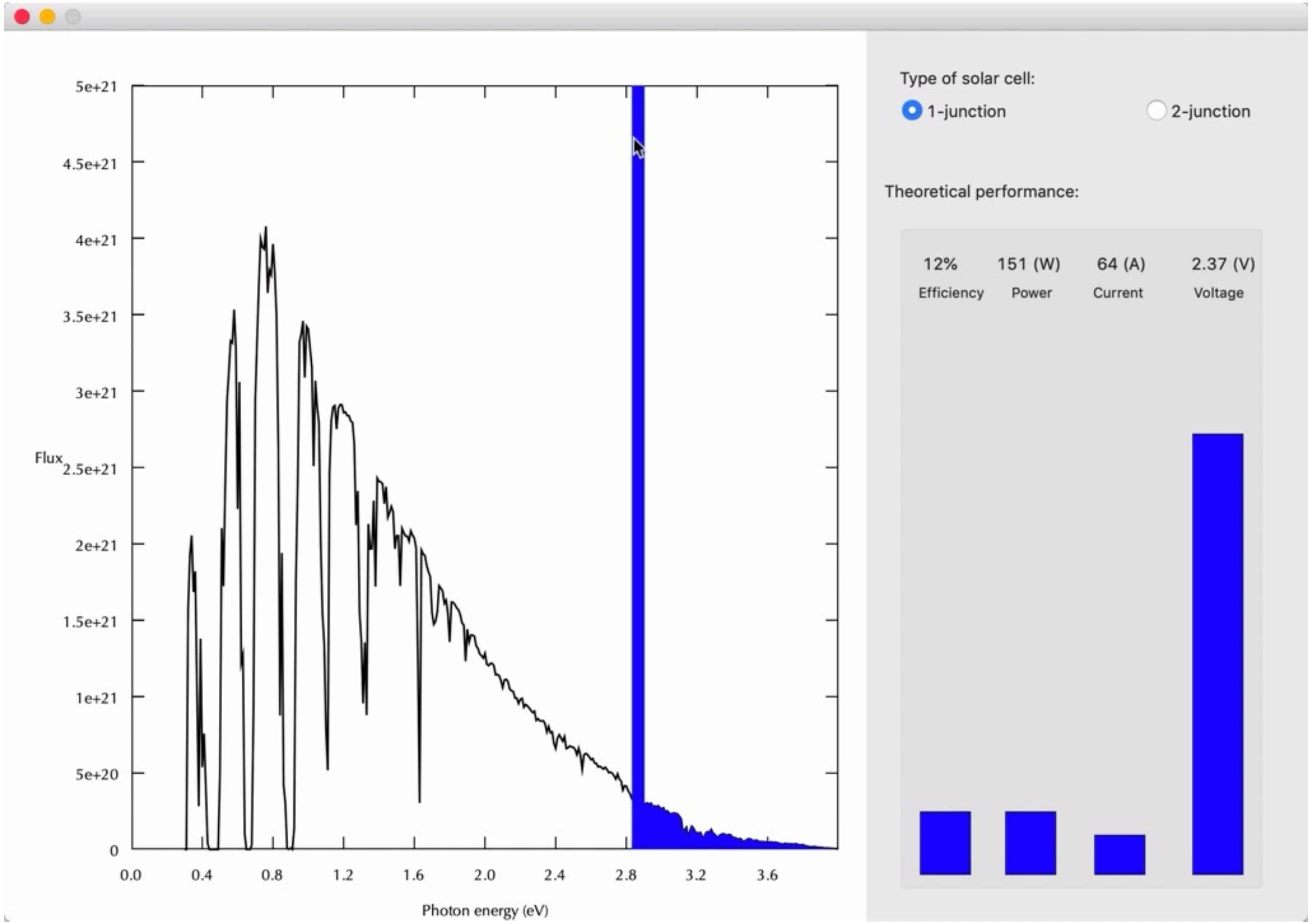
Current, Voltage, Power & Efficiency vs Eg



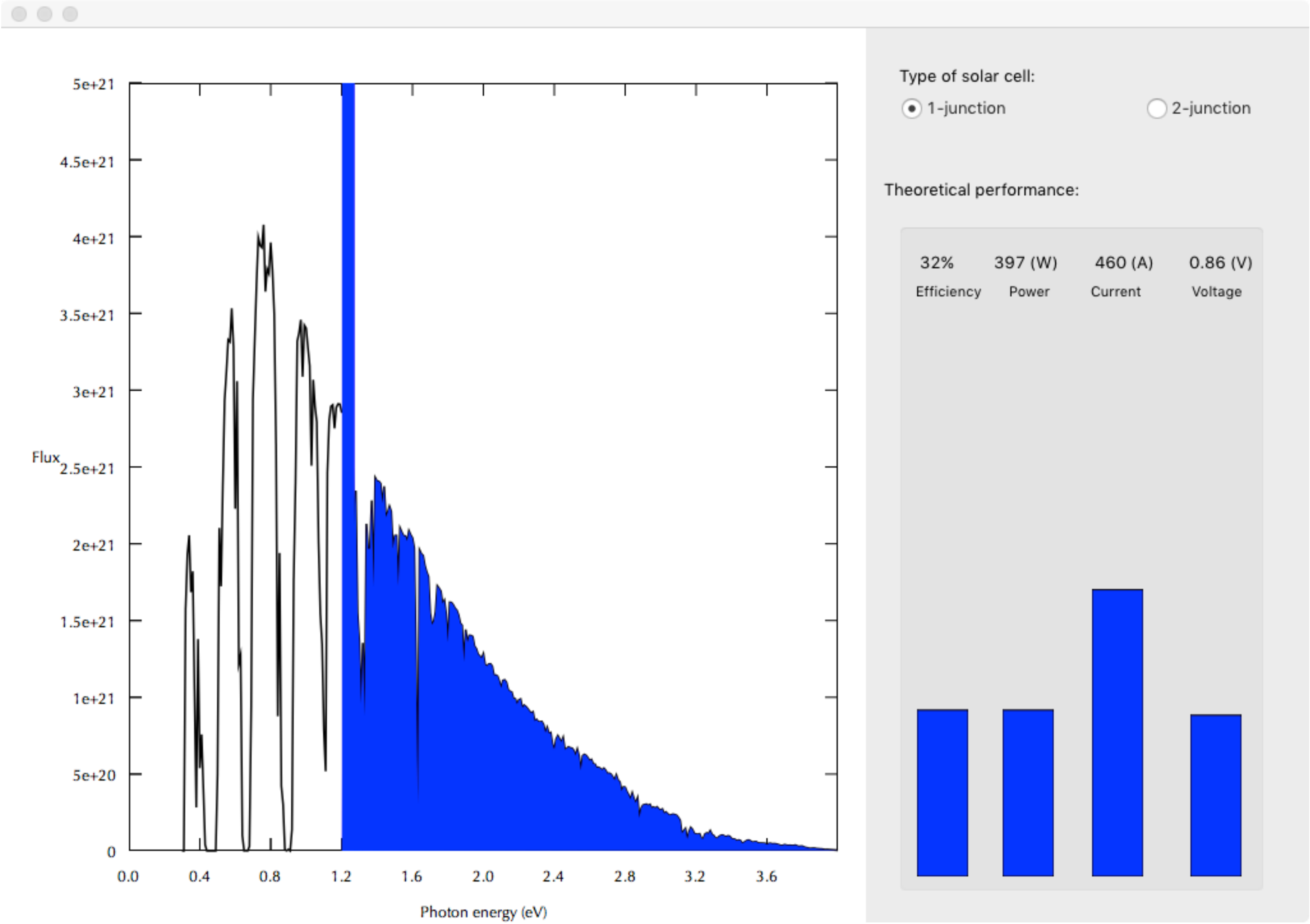
Current, Voltage, Power & Efficiency vs Eg



Current, Voltage, Power & Efficiency vs Eg



Current, Voltage, Power & Efficiency vs Eg

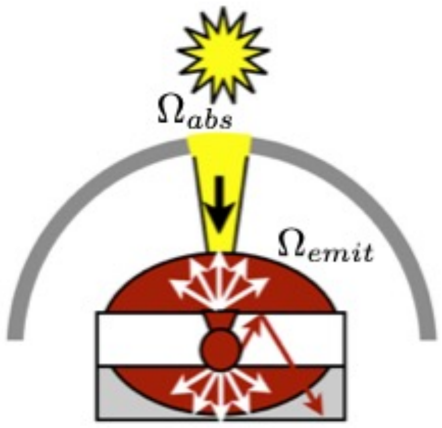


Electrical Models for PV Devices

Fundamental

Shockley-Queisser (Detail Balance)

Band-gap : Eg
Temperature : T

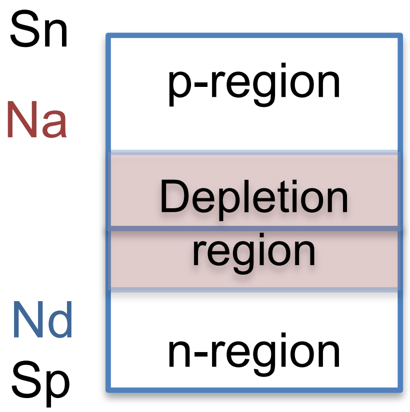


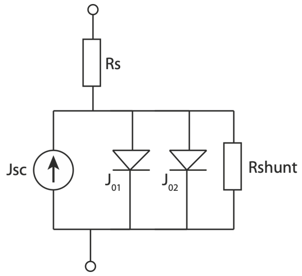
Depletion approximation

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



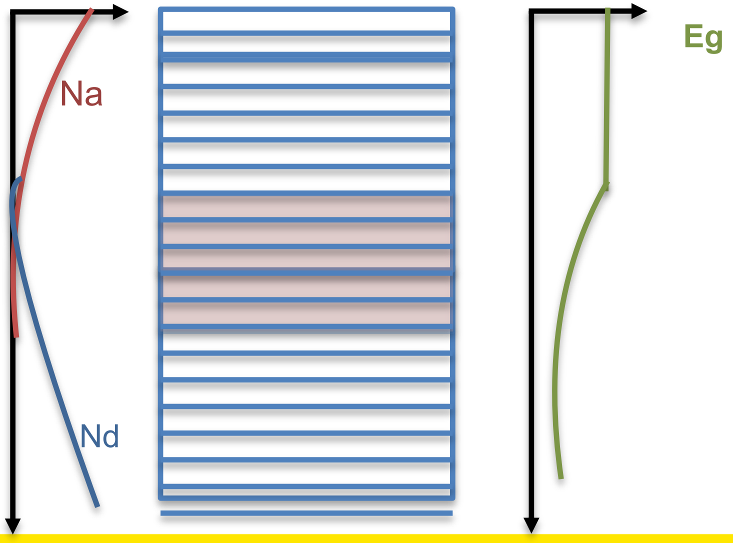


Drift-Diffusion

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)*



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General Form of the Planck Equation

Stove

900K

Tungsten-Halogen light bulb

2800K

Sun

5800K

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

Photon modes

Occupation probability

Encapsulates the electronic density of states.

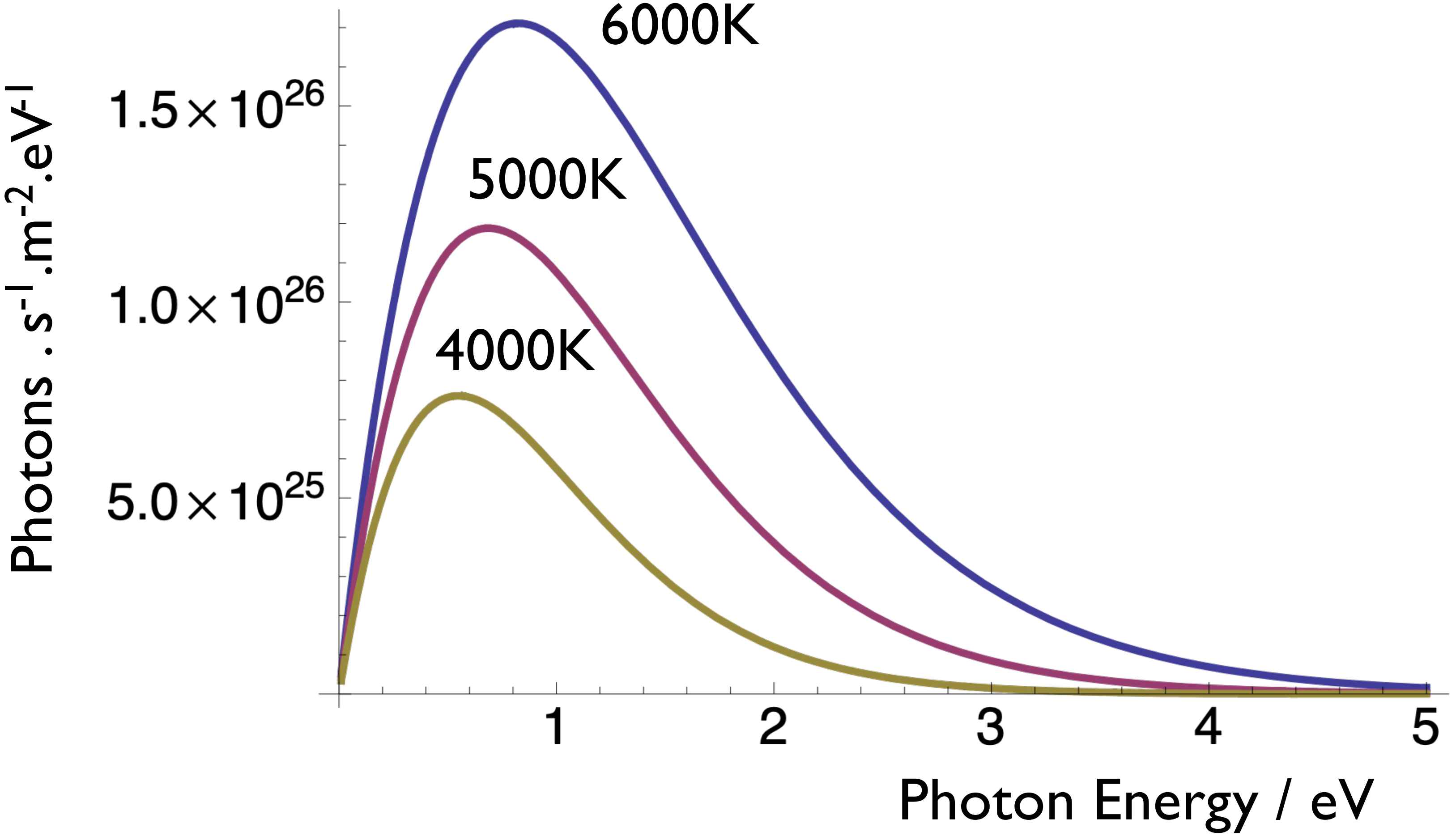
Generalised Planck Equation: P.Würfel, J.Phys C, Vol 15, 18(1982) p.3967

Blackbody Emission

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

$$\mu = 0$$

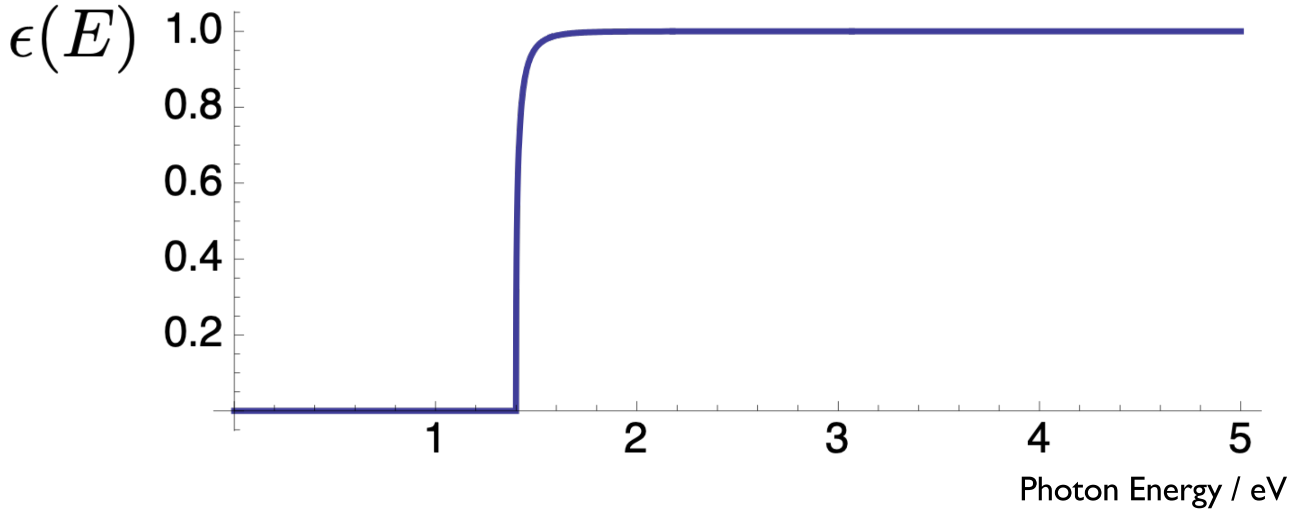
$$\epsilon(E) = 1$$

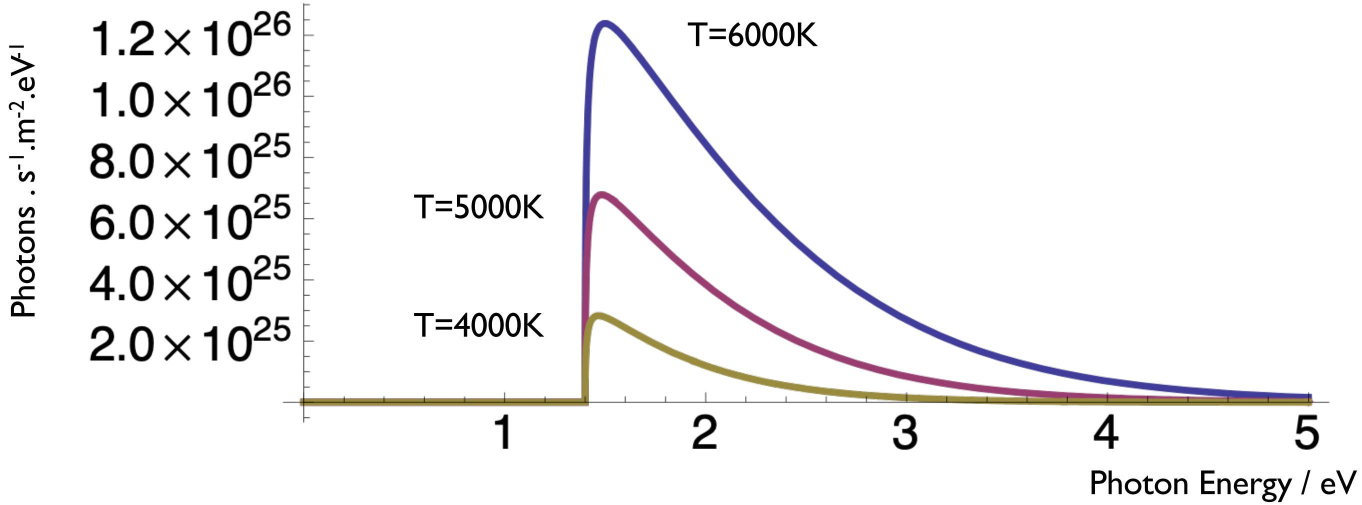


Semiconductors are "Grey" bodies

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

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

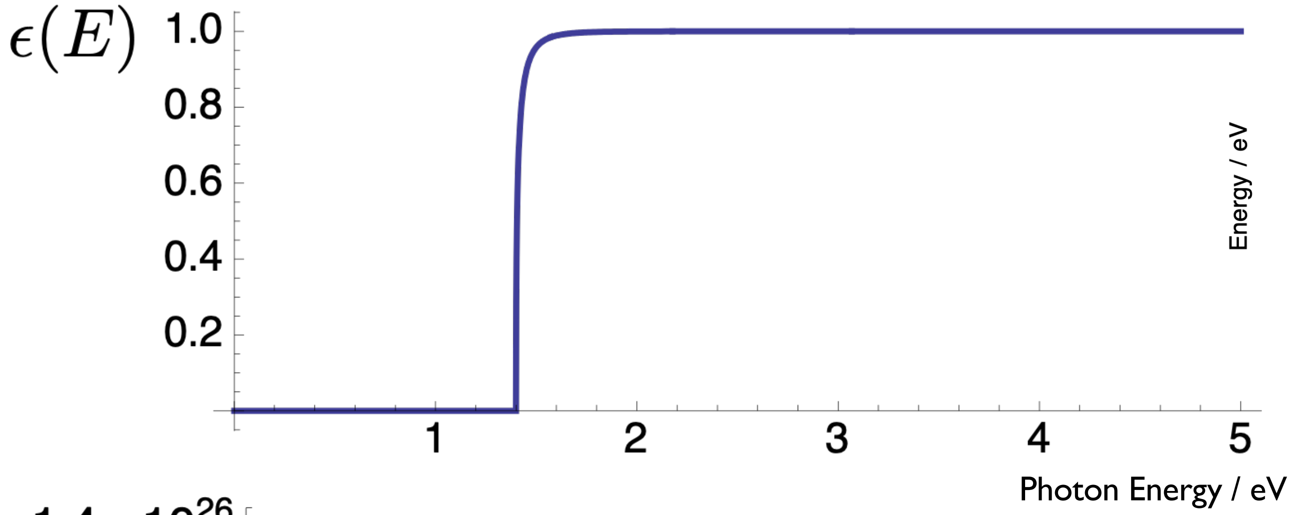


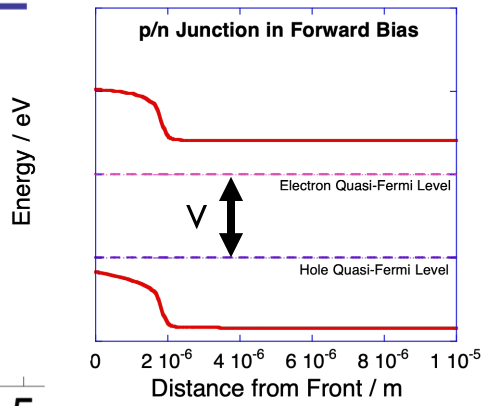


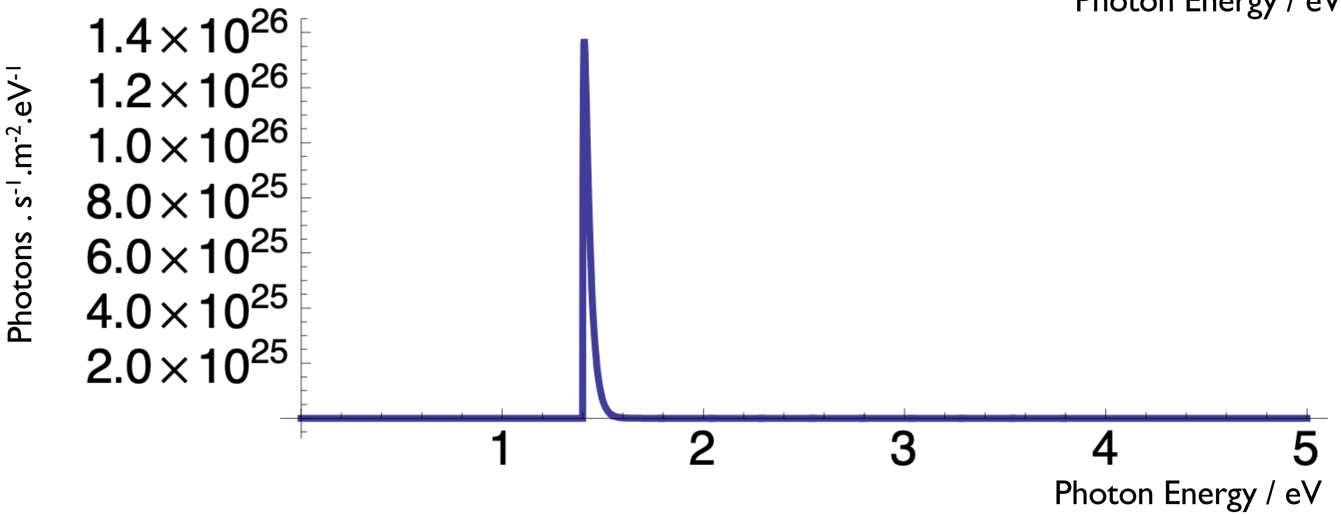
Electroluminescence

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

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





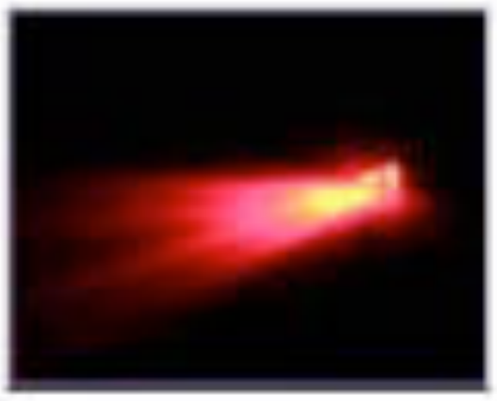


Verification of the Generalised Planck Expression

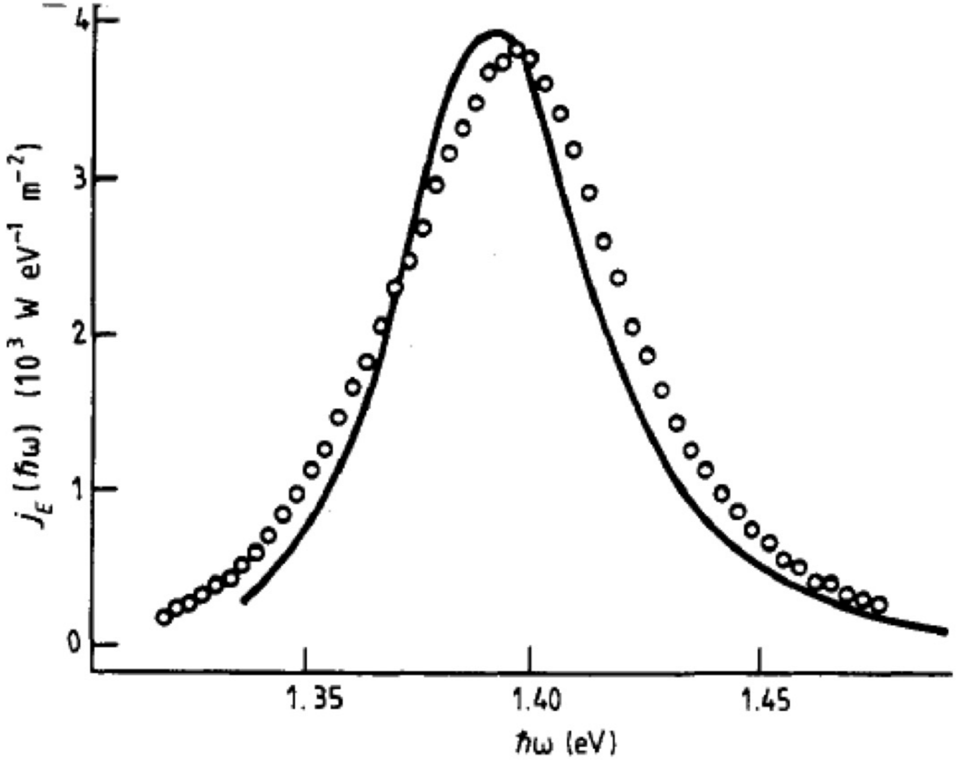
$$n(E) = \epsilon(E)\frac{2\pi}{c^2h^3}\frac{E^2}{e^{\frac{E-\mu}{kT}}-1}$$

$$\mu = 1.206V$$

$$T = 296K$$



GaAs p/n diode

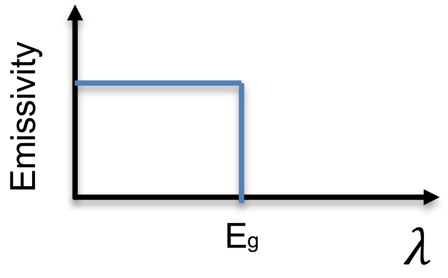


J.Phys: Condens.Matter 2 (1990) p.3803

Radiative limit to J_0

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

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

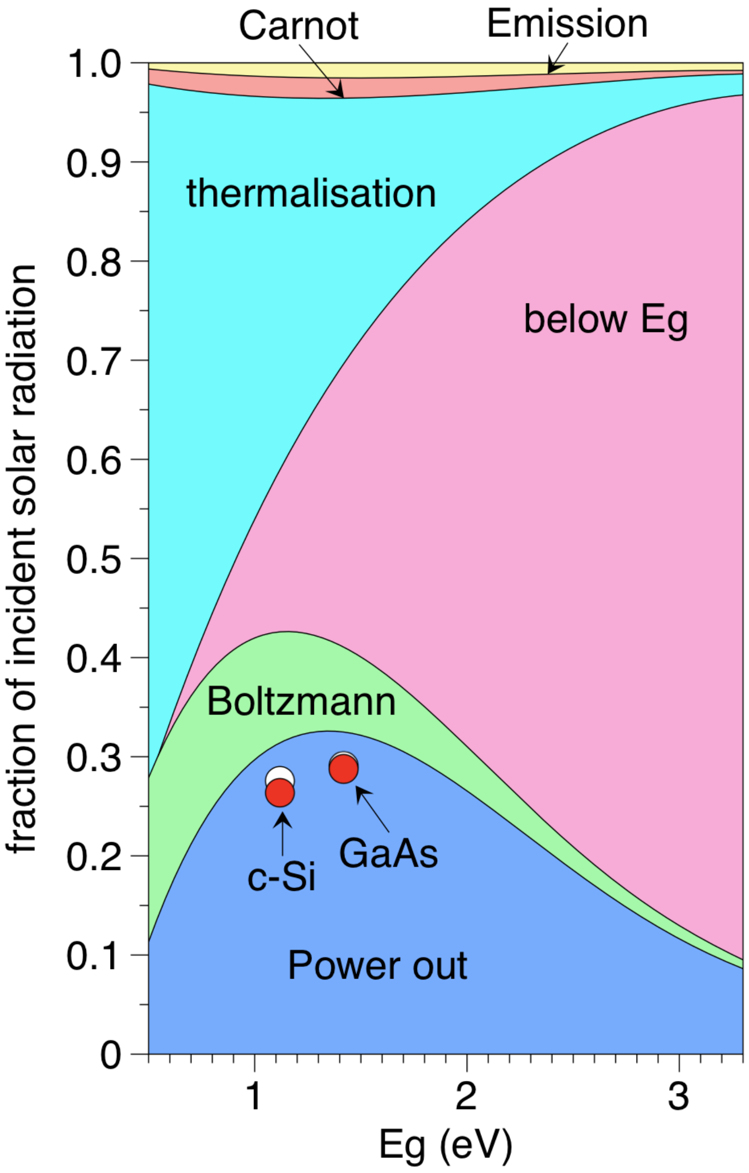


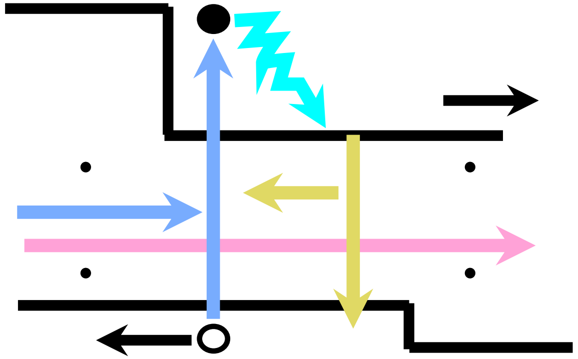
$$\begin{aligned} \dot{N} &= \int_{Eg}^{\infty} \epsilon(E) \frac{2\pi}{c^2h^3} \frac{E^2}{e^{\frac{E-\mu}{kT}}} dE \\ &= \underbrace{(\epsilon kT(Eg^2 + 2EgkT + 2k^2T^2)e^{\frac{-Eg}{kT}})}_{\frac{J_0}{q}} e^{\frac{\mu}{kT}} \end{aligned}$$

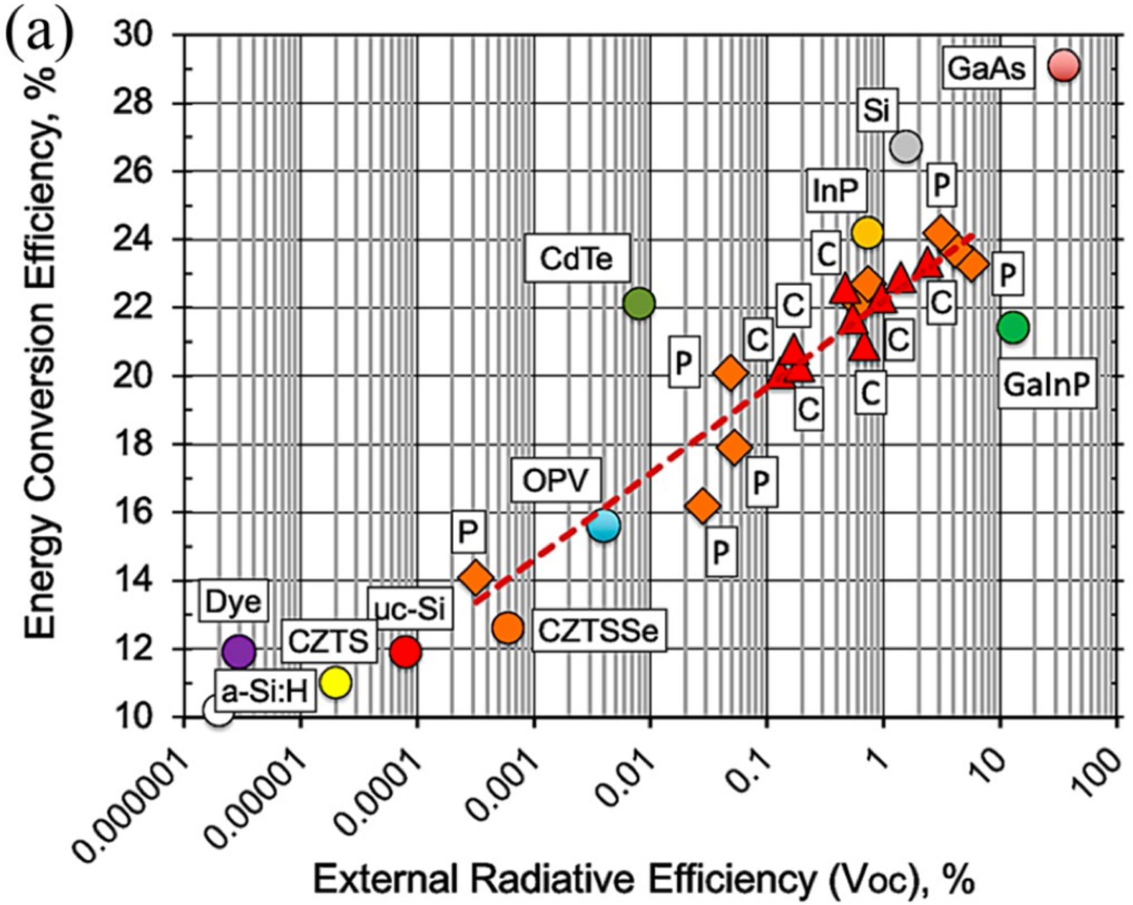
$$\mu = qV$$

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

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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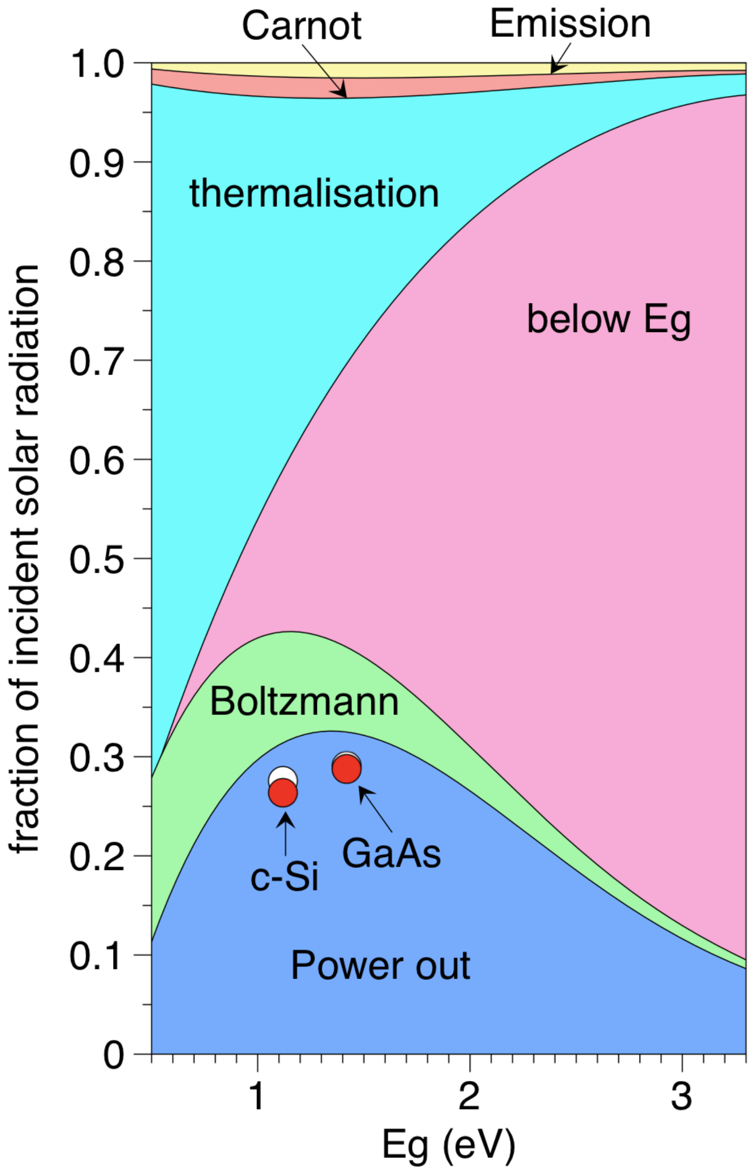
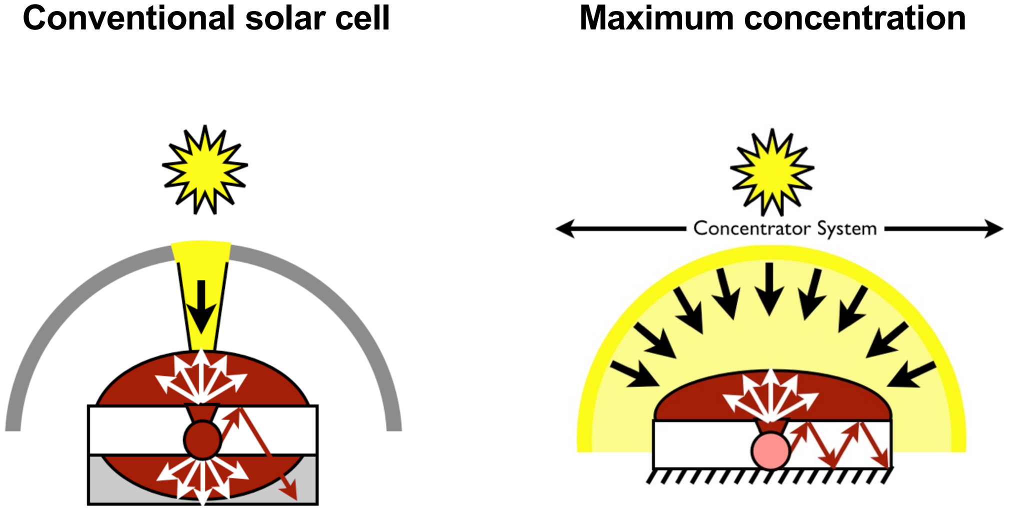
nse PV Module
Receiver
Receiver

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



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

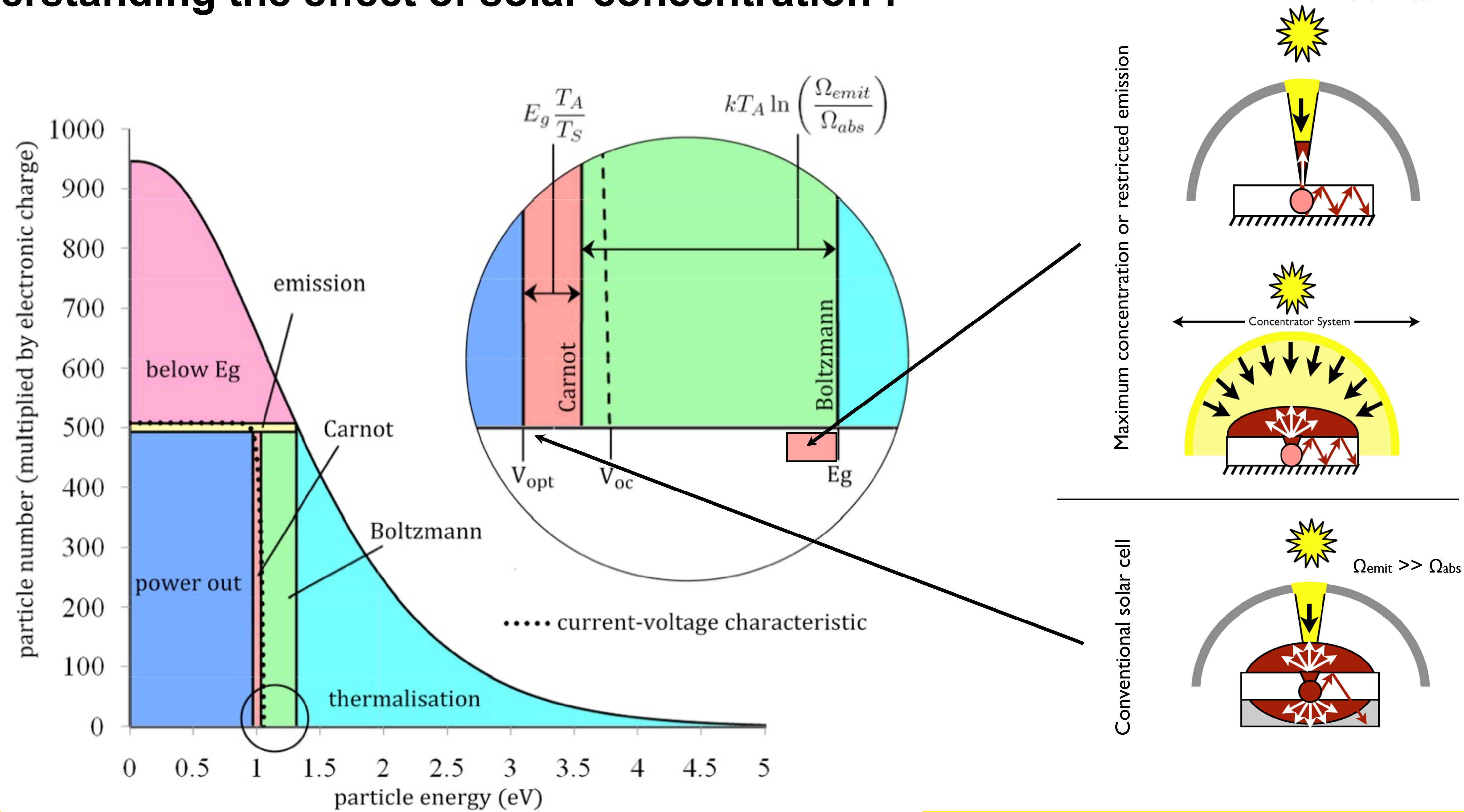
Significant Boltzmann loss!

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

Zero Boltzmann loss.

L. Hirst & N.J.Ekins-Daukes, Progress in Photovoltaics, (2011) 19: p286

Understanding the effect of solar concentration :



Faculty of Engineering
School of Photovoltaic and Renewable Energy Engineering

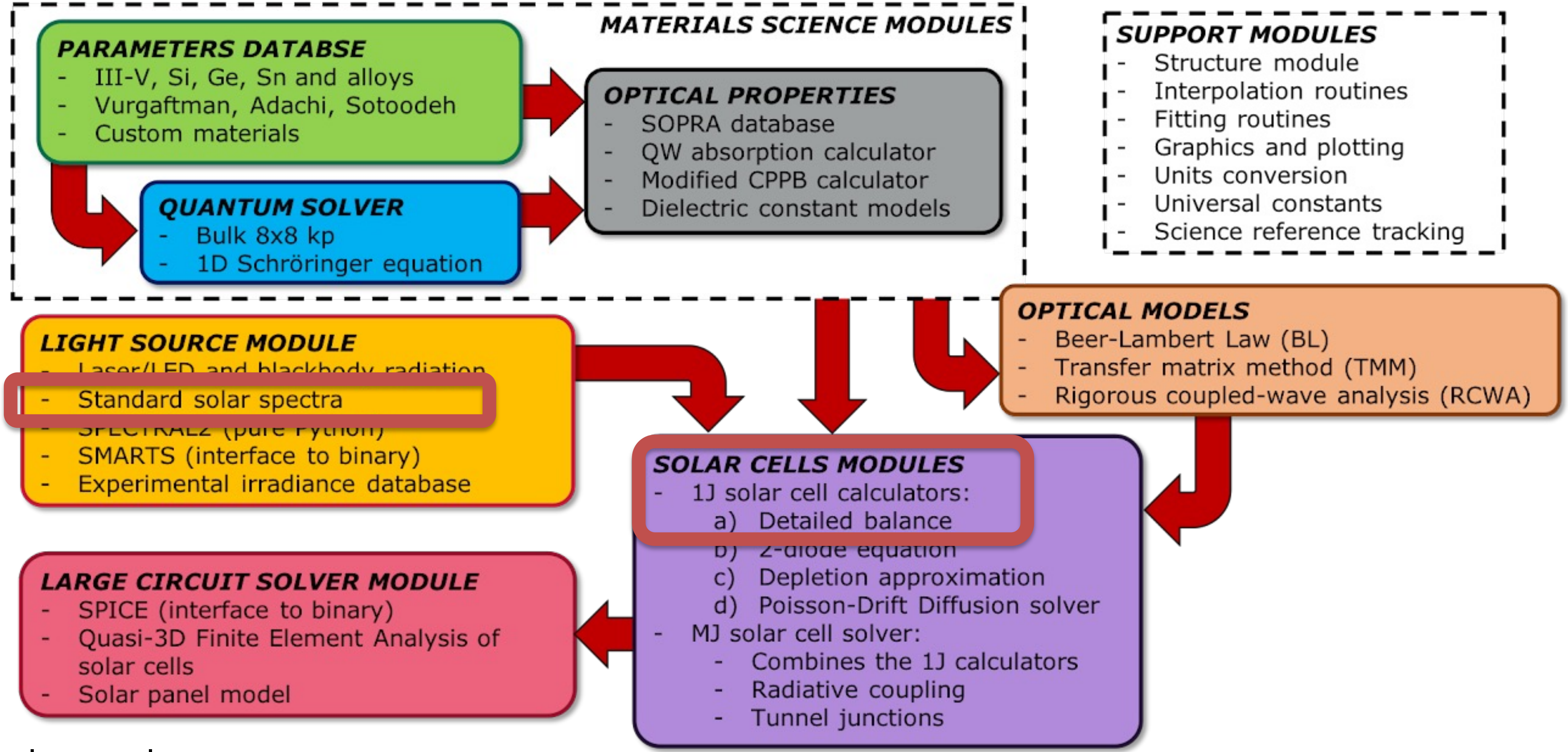
Day 2 Solcore Workshop – Silicon Tandem Cell Computer Modelling

Sungkyunkwan University, 1 – 3 August 2023

International Energy Joint R&D Project : Silicon / III-V Tandem solar cell to achieve over 40% efficiency.
Supported financially by KETEP (Korean Energy Technology Evaluation and Planning)

Ned Ekins-Daukes & Phoebe Pearce

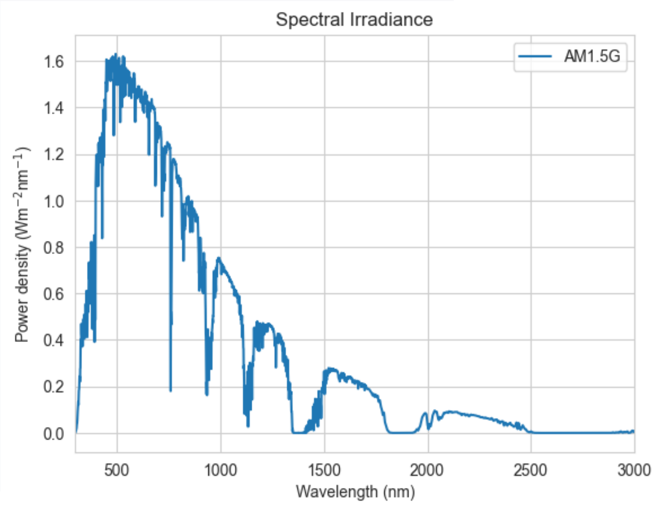
Summary of Day 1:



www.solcore.solar

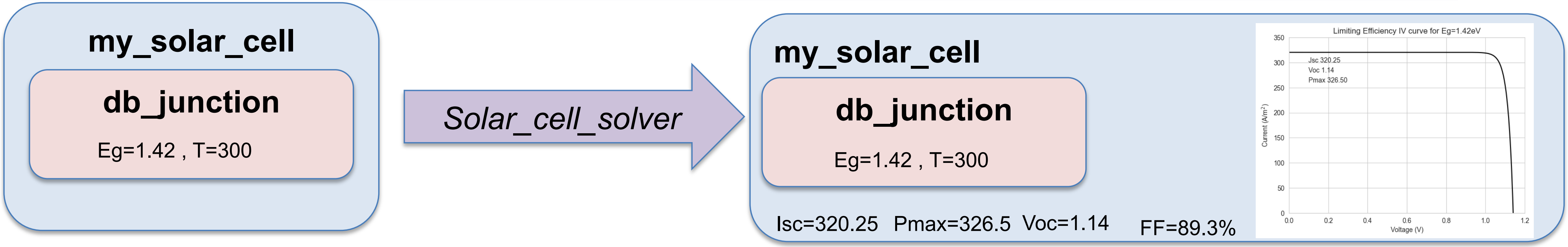
Importing the Solar Spectrum and Plotting

```python
import numpy as np
import matplotlib.pyplot as plt
from solcore.light_source import LightSource
import seaborn as sns

# Setup the AM1.5G solar spectrum
wl = np.linspace(300, 4000, 4000) * 1e-9    #wl contains the x-ordinate in wavelength
am15g = LightSource(source_type='standard', x=wl*1e9, version='AM1.5g')

plt.figure(1)
plt.title('Spectral Irradiance')
plt.plot(*am15g.spectrum(wl*1e9), label='AM1.5G')
plt.xlim(300, 3000)
plt.xlabel('Wavelength (nm)')
plt.ylabel('Power density (Wm$^{-2}$nm$^{-1}$)')
plt.legend()
```



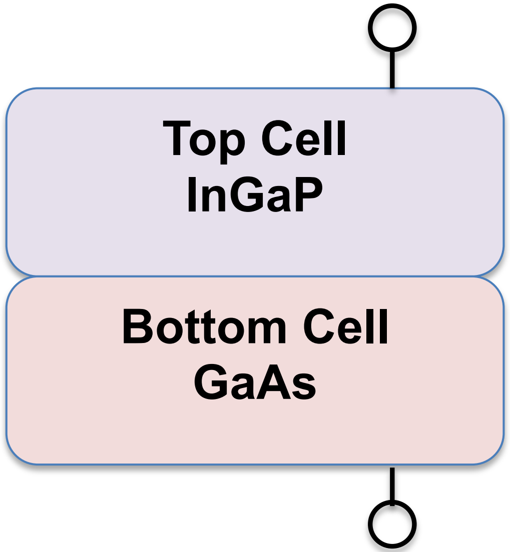
Calculating a Detailed-Balance IV curve in SolCore (Shockley-Queisser limit)

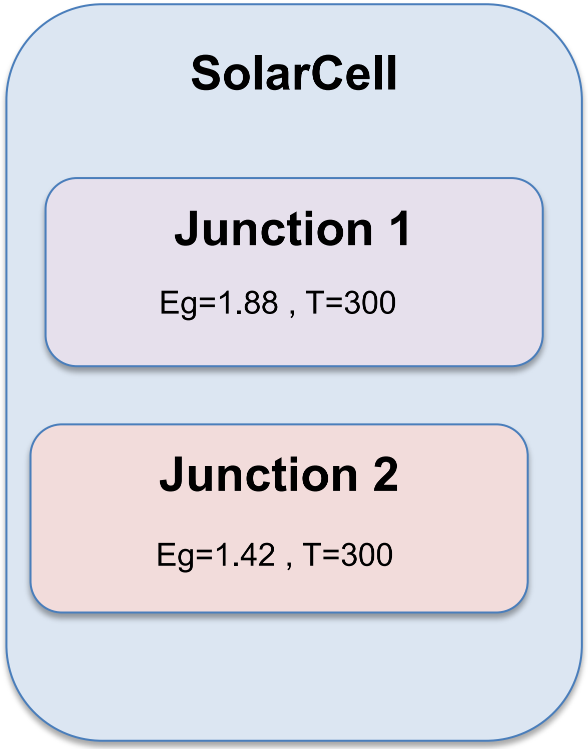
```
eg=1.42
V = np.linspace(0, 1.3, 500)
db_junction = Junction(kind='DB', T=300, Eg=eg, A=1, R_shunt=np.inf, n=1)
my_solar_cell = SolarCell([db_junction], T=300, R_series=0)

solar_cell_solver(my_solar_cell, 'iv',
                  user_options={'T_ambient': 300, 'db_mode': 'top_hat', 'voltages': V,
                   'light_iv': True,
                              'internal_voltages': np.linspace(0, 1.3, 400),
                               'wavelength': wl,
                              'mpp': True, 'light_source': am15g})
```



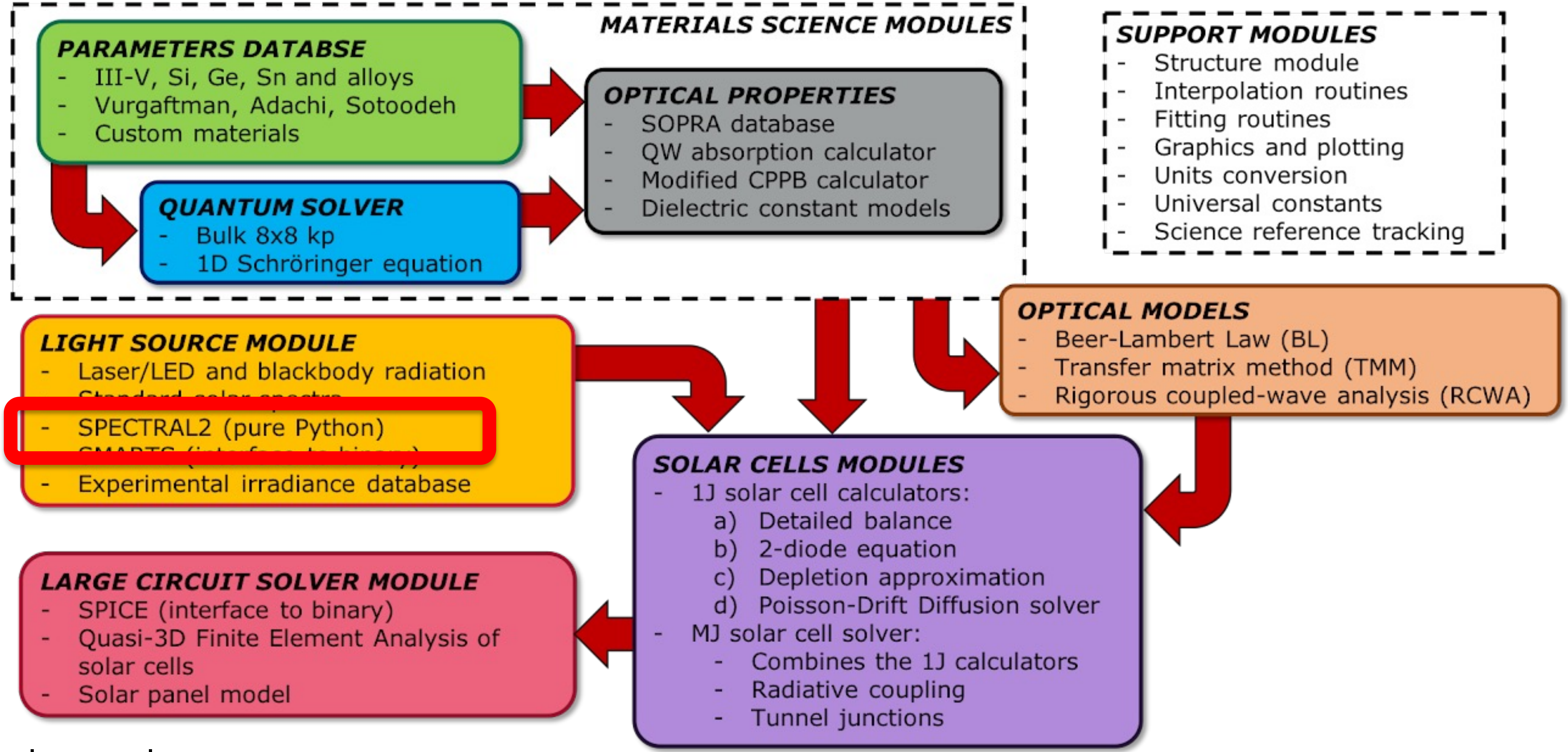

```
print (my_solar_cell.iv.Isc)
```

Detail Balance Double Junction Tandem Solar Cell



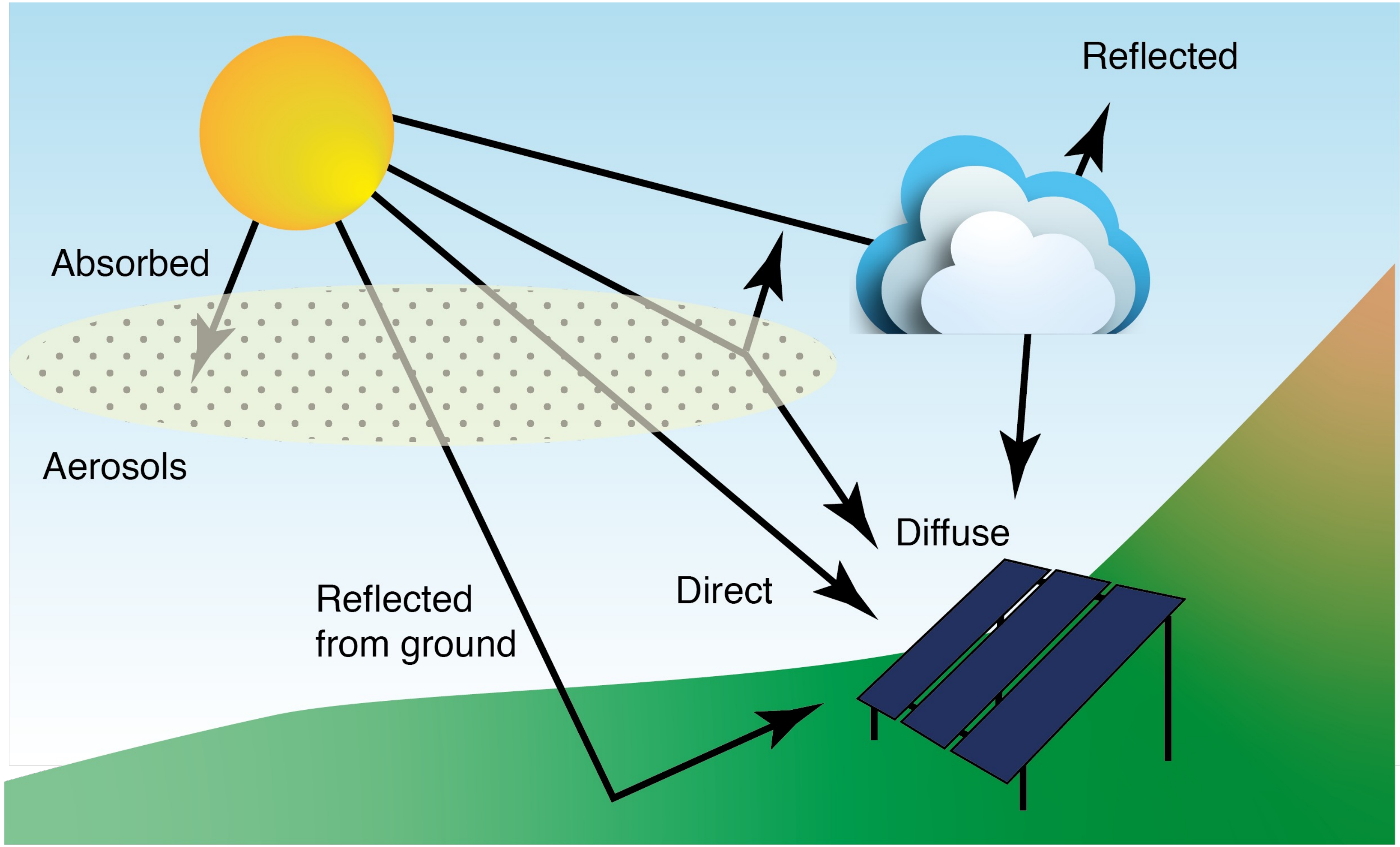


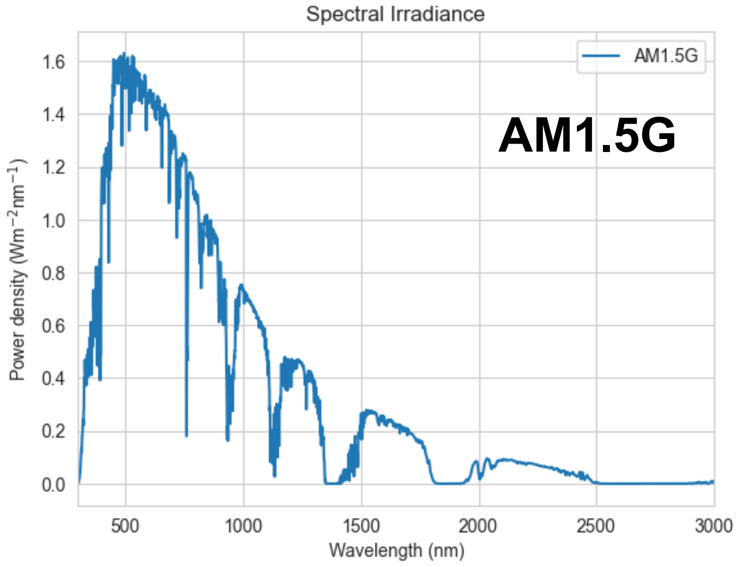
Summary of Day 1:

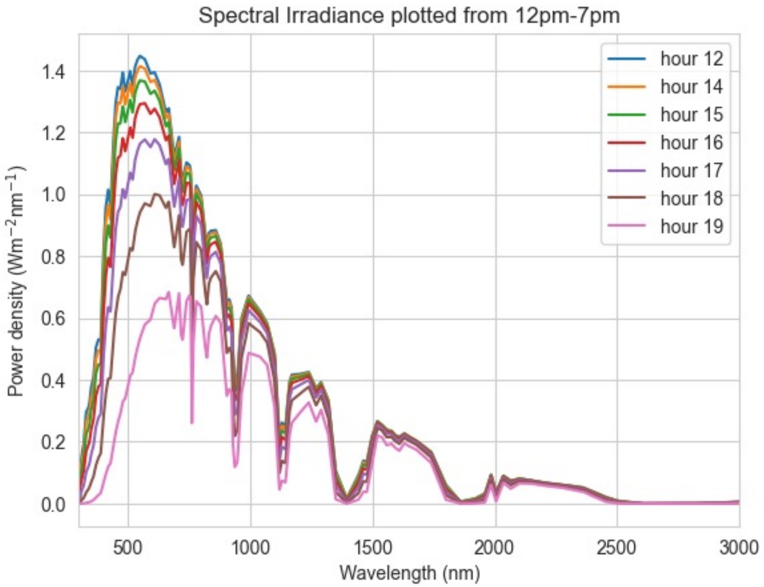


www.solcore.solar

Spectral Irradiance changes throughout the day:







Spectral Irradiance Models

SPCTRL2 | **SMARTS2** | **SBDart** | **MODTRAN** | **FASCODE**

Clear Sky AM1.5G standard

Clear Sky + Cloudy Conditions

Complexity / computational time

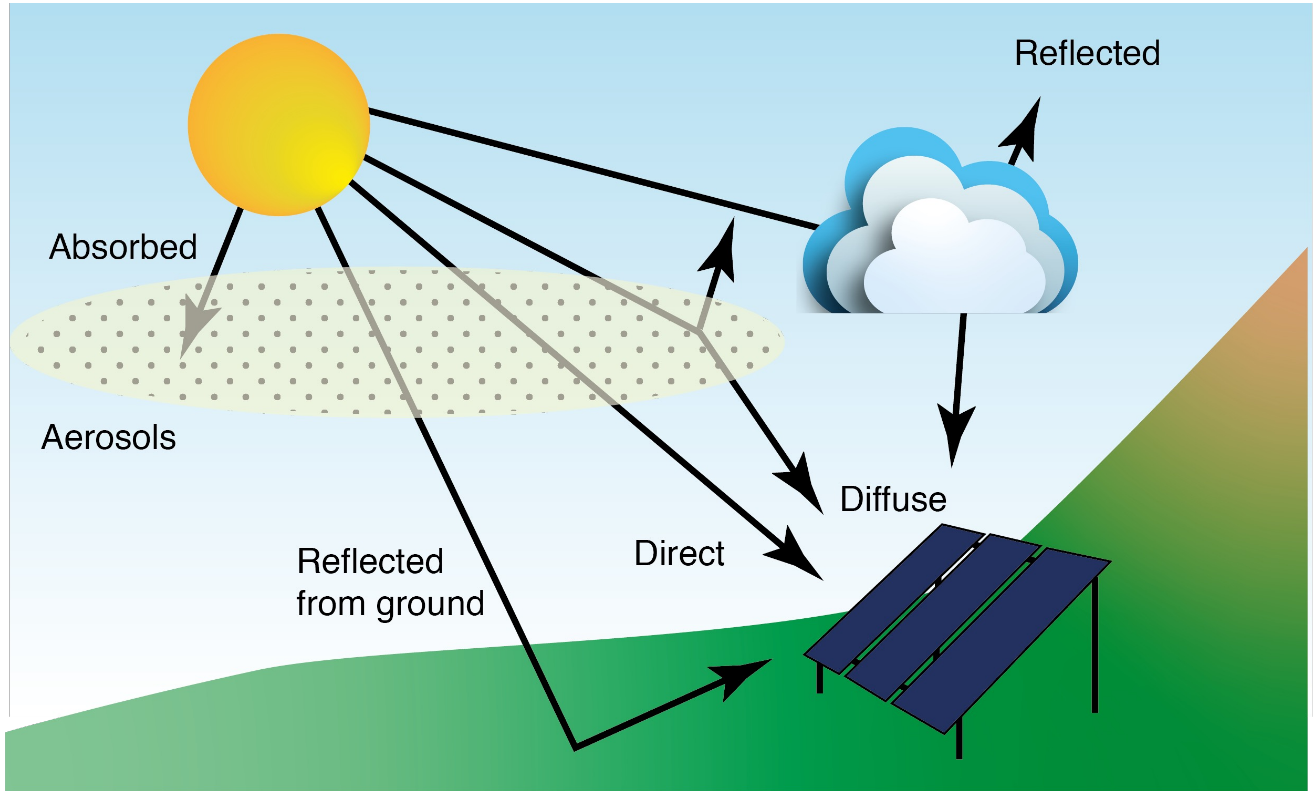
SPCTRL2	SMARTS2	MODTRAN	FASCODE
Empirical closed form transmission.	Parameterisation based on MODTRAN output.	band-model of HITRAN Database	HITRAN Database

Domain of solar system engineering

Domain of atmospheric physics

Implemented in SolCore

Spectral Irradiance changes throughout the day:



$$AOD = \beta \lambda^{-\alpha}$$

SPCTRL2	SMARTS2
Clear Sky	AM1.5G standard

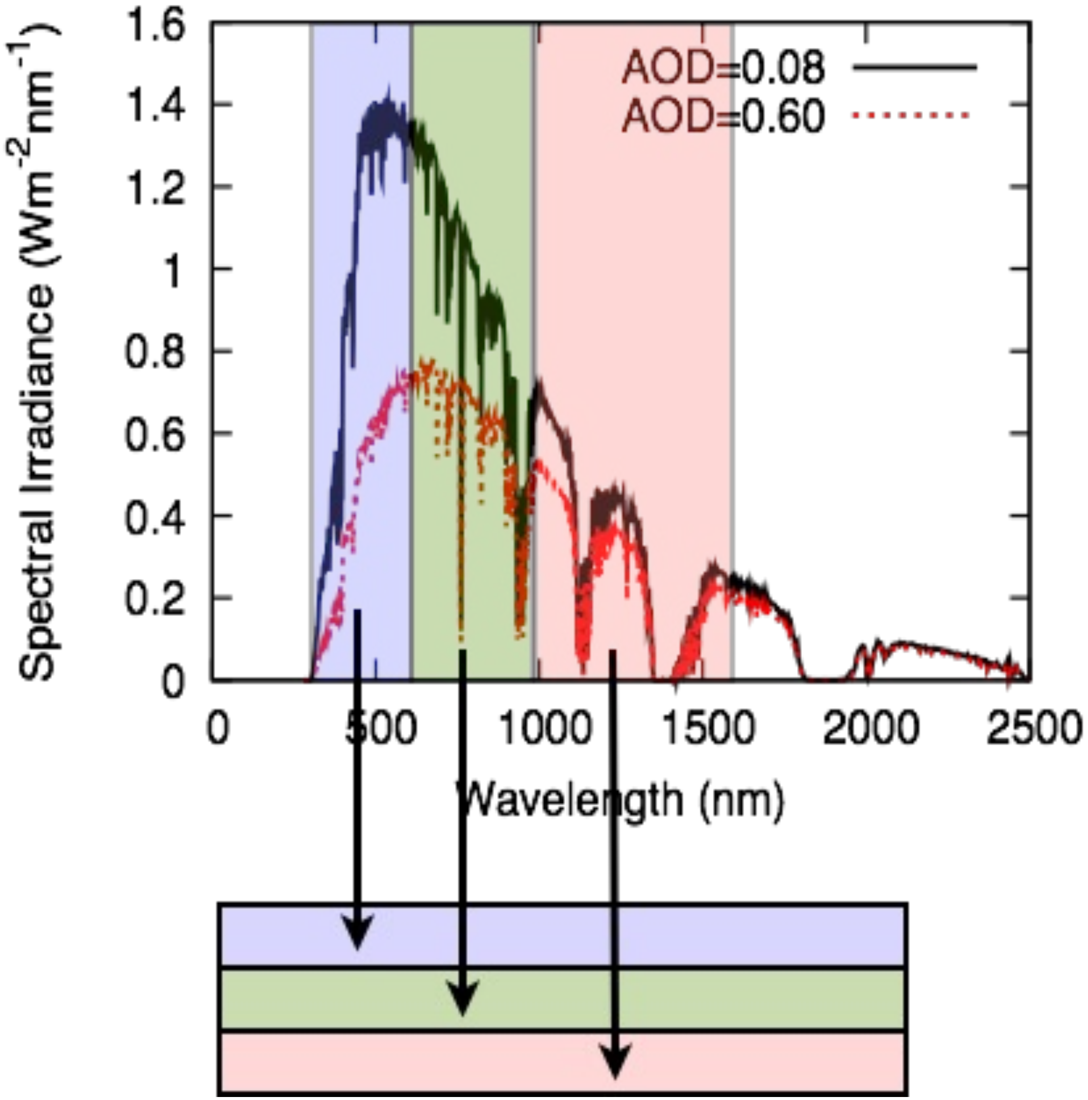
- Air Mass
  - Latitude, Longitude, Time of day
- Aerosol type :
  - Shettle & Fenn models:
    - Rural, Urban, Maritime, Tropospheric
- Aerosol concentration
  - Aerosol optical depth (AOD)
  - Atmospheric turbidity (β)
  - Ångström coefficient (α)
- Precipitable Water column thickness
- Meteorological conditions:
  - Pressure
  - Humidity
  - Ozone

Anders Ångström (1930) On the Atmospheric Transmission of Sun Radiation. II, Geografiska Annaler, 12:2-3, 130-159,

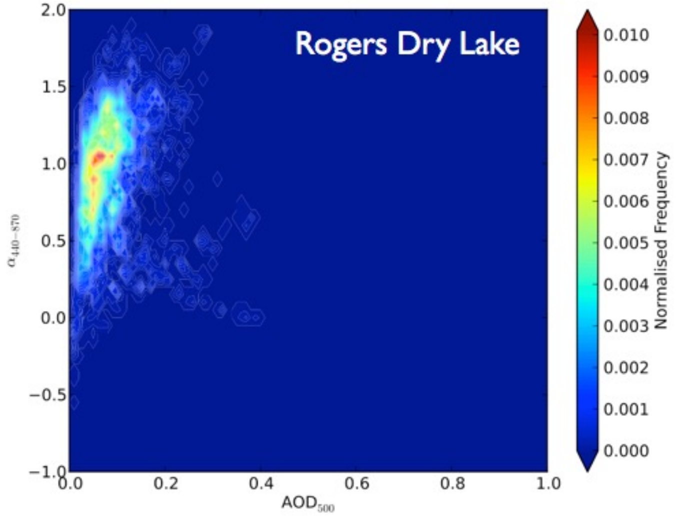
Effect of Aerosol Optical Density on Solar Spectral Irradiance

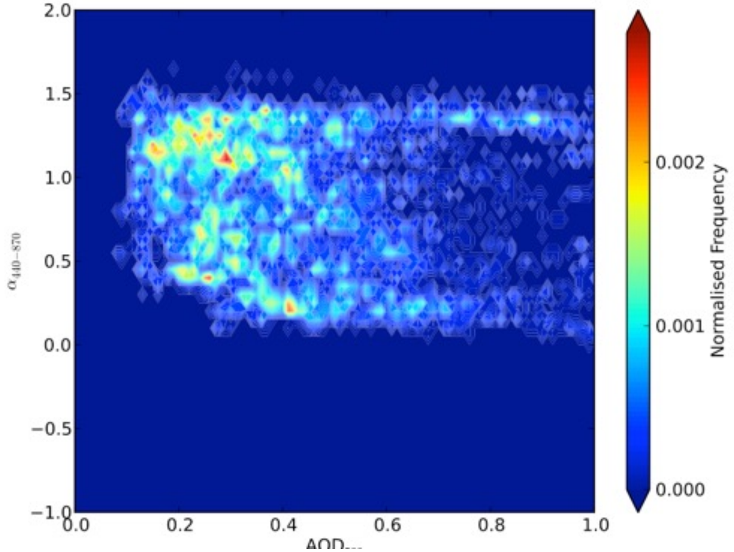
Low AOD

High AOD



Complex atmospheres in India





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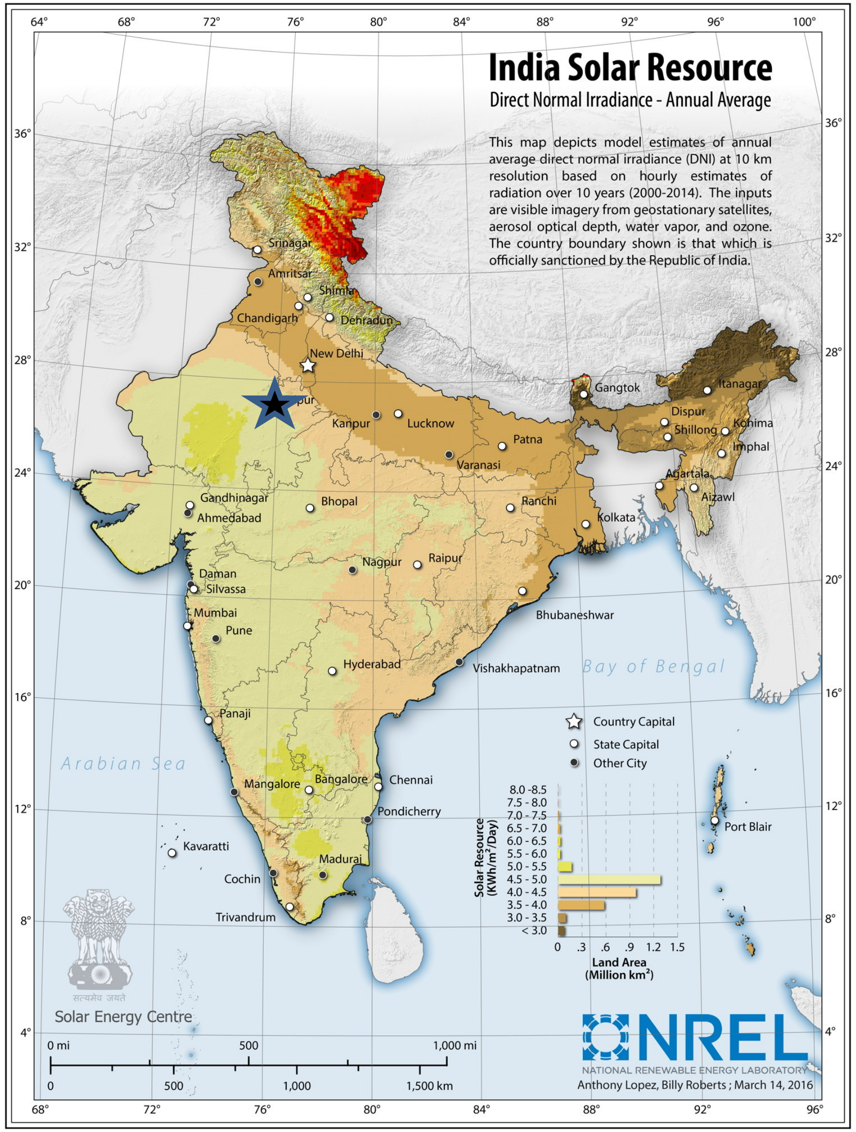

http://www.nrel.gov/international/ra_india.html

N. L. A. Chan, et al., IEEE JPV 4 (5) , pp. 1306–1313, 2014.

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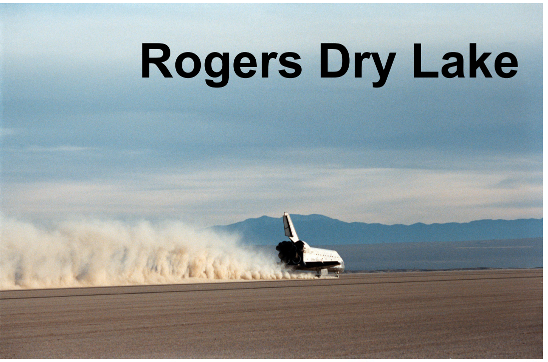
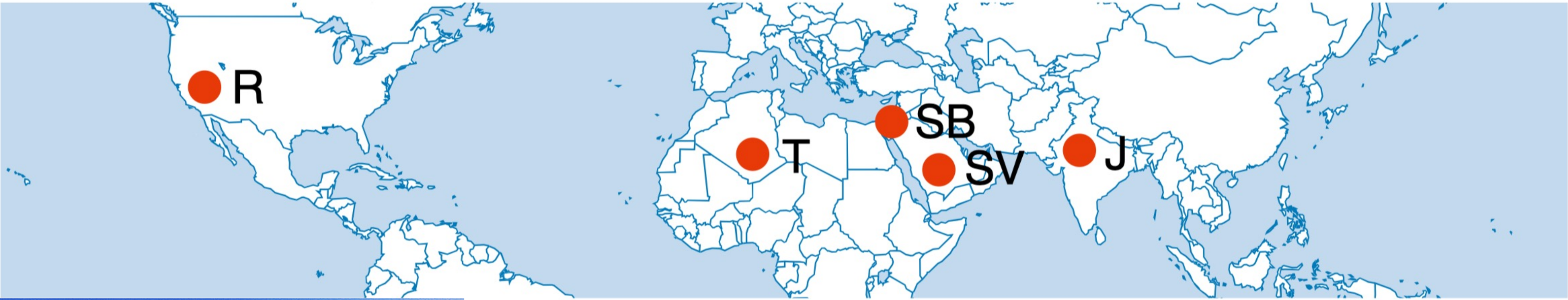
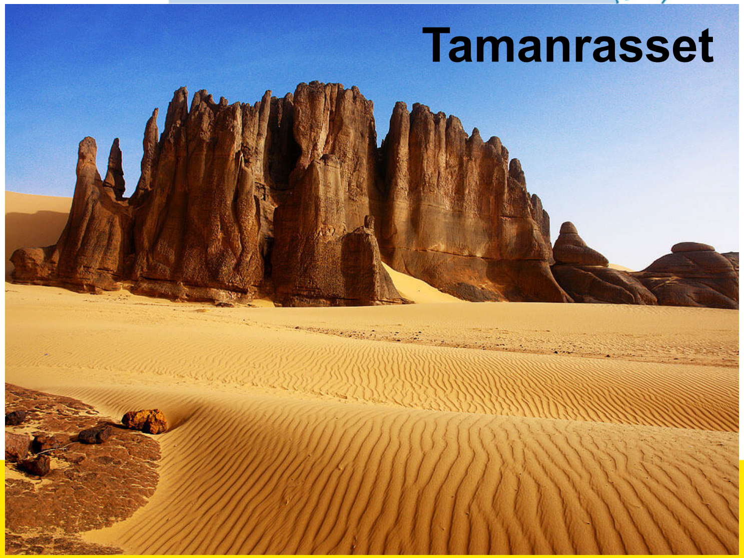
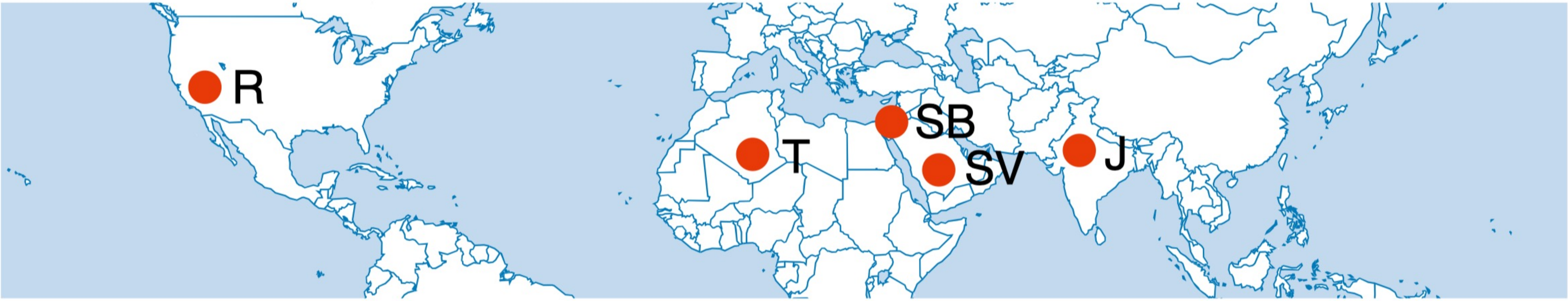
Atmospheric variation worldwide

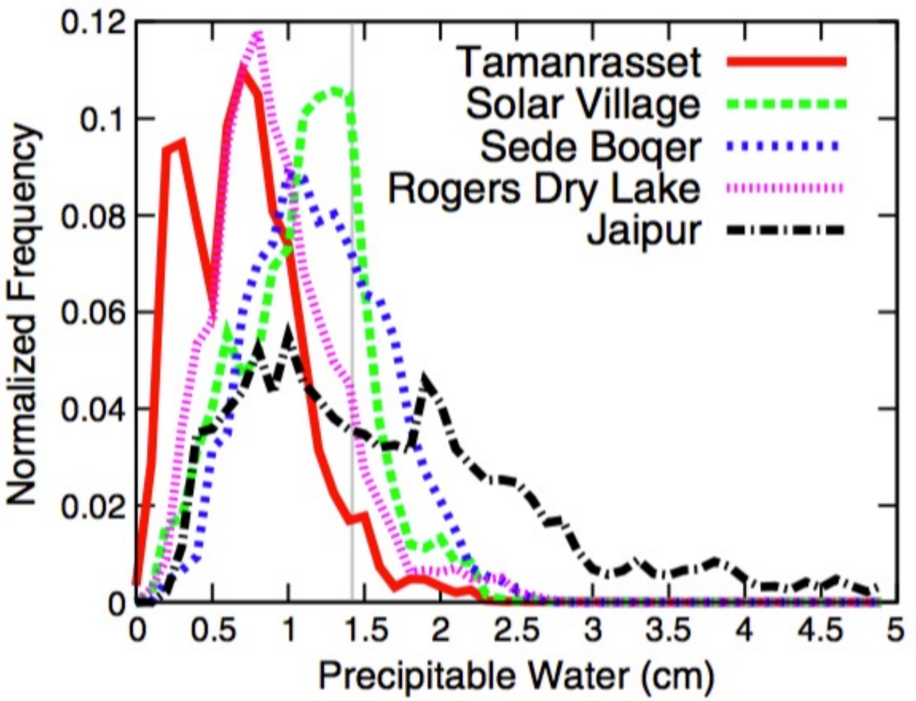






Atmospheric variation worldwide





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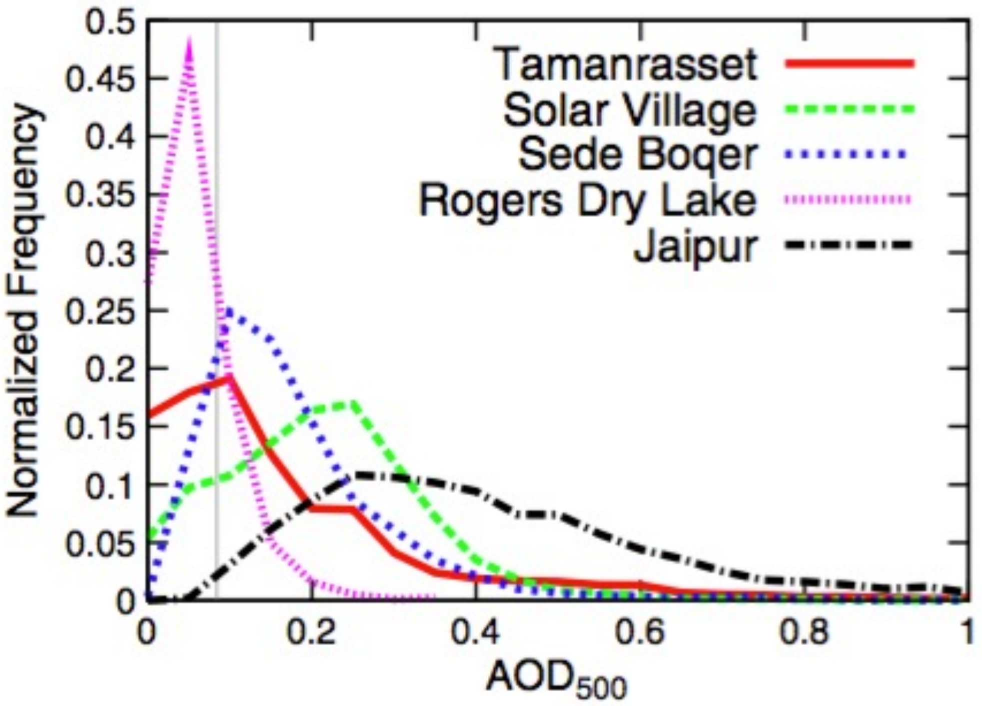


Semiconductor Drift-Diffusion Equations

For electrons:

$$\nabla\left[\underbrace{-D_n\nabla n}_{\text{Diffusion}} + n\mu_n\left(\underbrace{\nabla\Phi}_{\text{Electric field}} + \underbrace{\frac{\nabla\chi}{q}}_{\text{Electron affinity}} + \underbrace{\frac{kT}{q}\nabla\ln N_c}_{\text{Density of states}}\right)\right] = \underbrace{g(x,y,z,\lambda)}_{\text{Generation rate}} - \underbrace{U}_{\text{Recombination rate}}$$

$$U = \underbrace{U_{SRH}}_{\text{Impurity recombination}} + \underbrace{U_{rad}}_{\text{Radiative recombination}} + \underbrace{U_{aug}}_{\text{Auger recombination}}$$

For holes:

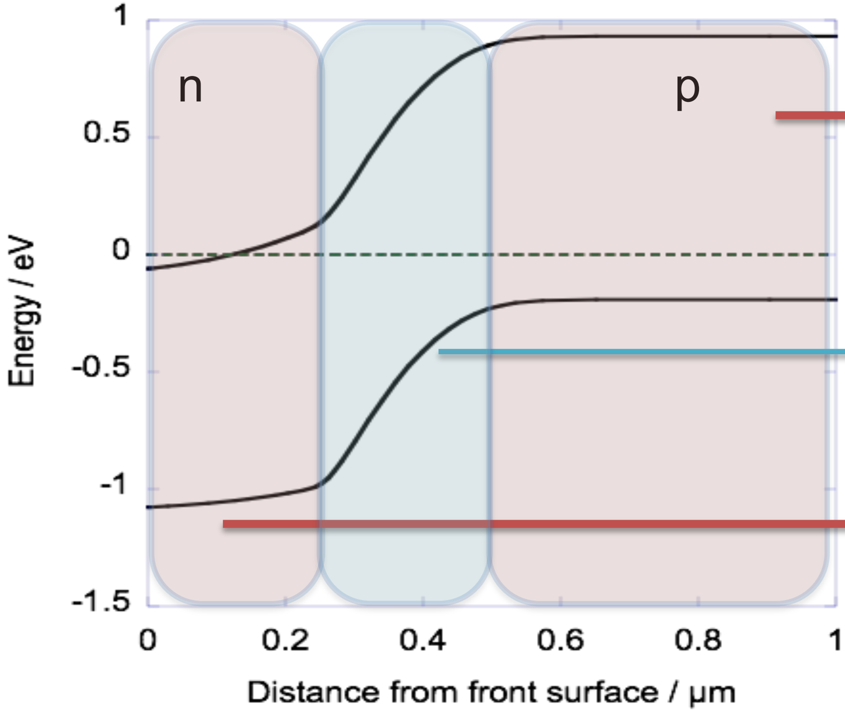
$$\nabla\left[-D_p\nabla p + p\mu_p\left(\nabla\Phi + \frac{\nabla\chi}{q} + \frac{kT}{q}\nabla\ln N_v\right)\right] = g(x,y,z,\lambda) - U$$

Poisson equation: $$\nabla^2\Phi = \frac{q}{\epsilon_0\epsilon_r}(n - p - (N_D - N_A))$$

Numerical solution to D-D eqns for QE: Xiaofeng Li, *Prog. Photovolt: Res. Appl.*, vol. 21, no. 1, pp. 109–120, 2013.

Analytical solution to D-D eqns for QE : Jenny Nelson, The Physics of Solar Cells, Imperial College Press, 2003

Carrier collection probability at short-circuit (V=0)



$-D_n \nabla n$

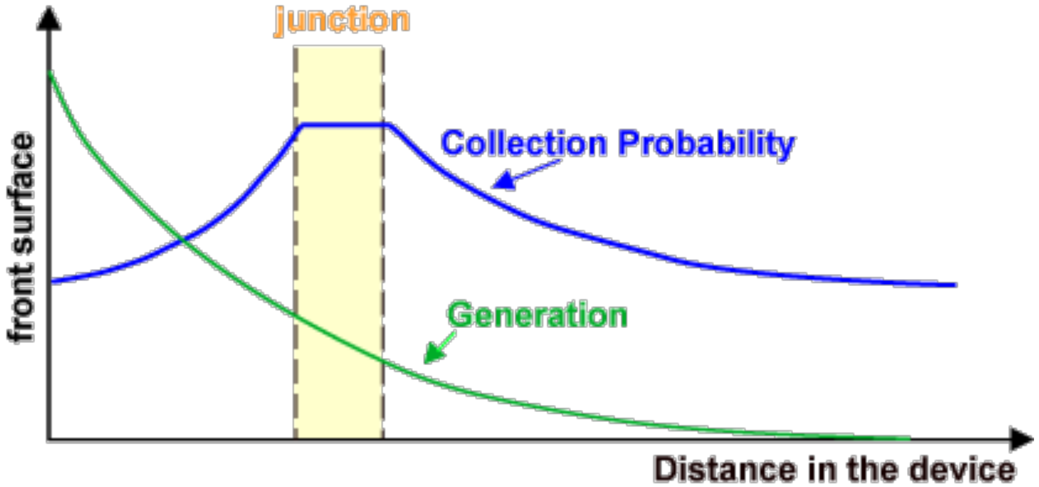
Minority electron diffusion

$n\mu_n \nabla \Phi$ Carrier

$-p\mu_p \nabla \Phi$ Drift

$-D_p \nabla p$

Minority hole diffusion



Beer Lambert Law:

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

Recombination terms:

$$U = U_{SRH} + U_{rad} + U_{aug}$$

Impurity recombination | Radiative recombination | Auger recombination

Shockley-Read-Hall (SRH) recombination

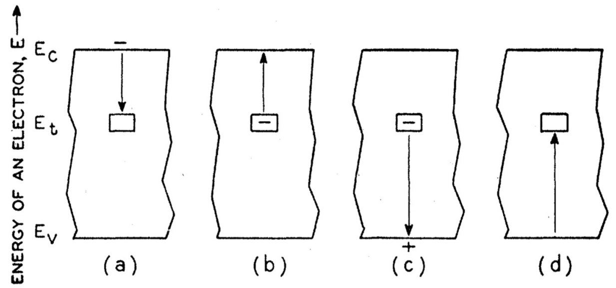
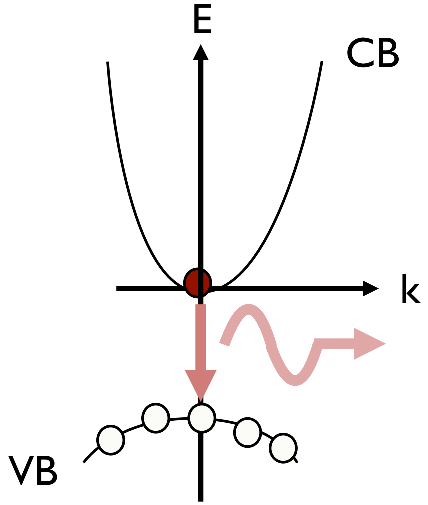


FIG. 1. The basic processes involved in recombination by trapping: (a) electron capture, (b) electron emission, (c) hole capture, (d) hole emission.

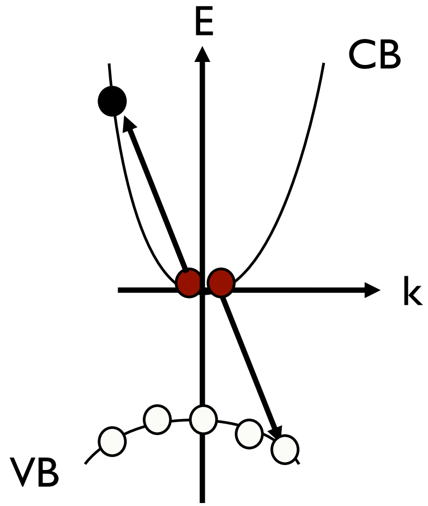
$$U_{\mathrm{SRH}} = \frac{np - n_i^2}{\tau_n(p + p_{\mathrm{t}}) + \tau_p(n + n_{\mathrm{t}})}$$

Radiative recombination



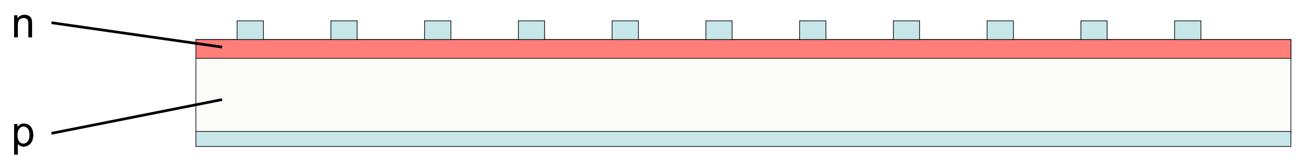
$$U_{\mathrm{rad}} = B_{\mathrm{rad}}\left(np - n_i^2\right)$$

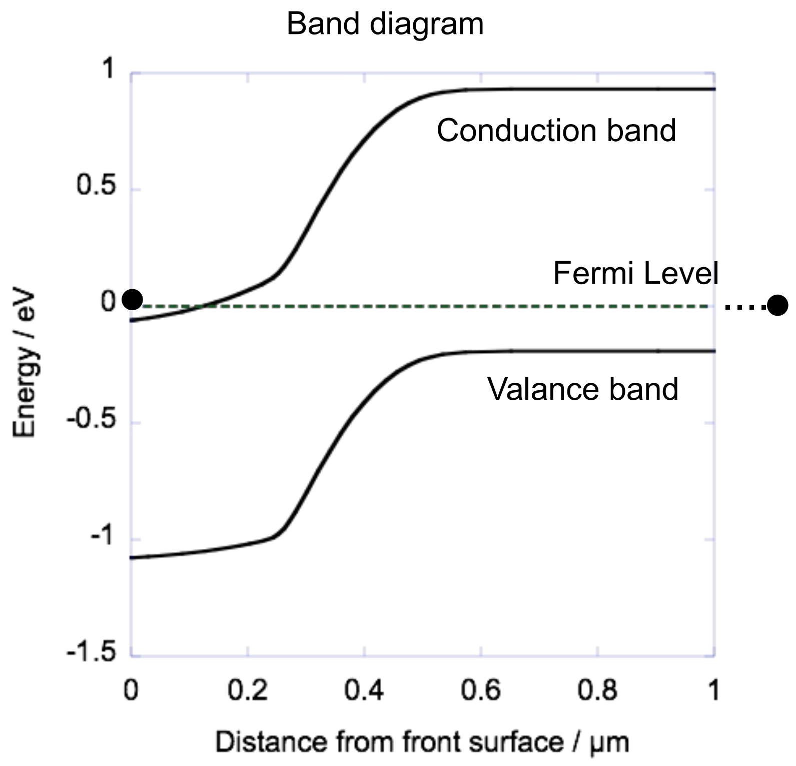
Auger recombination

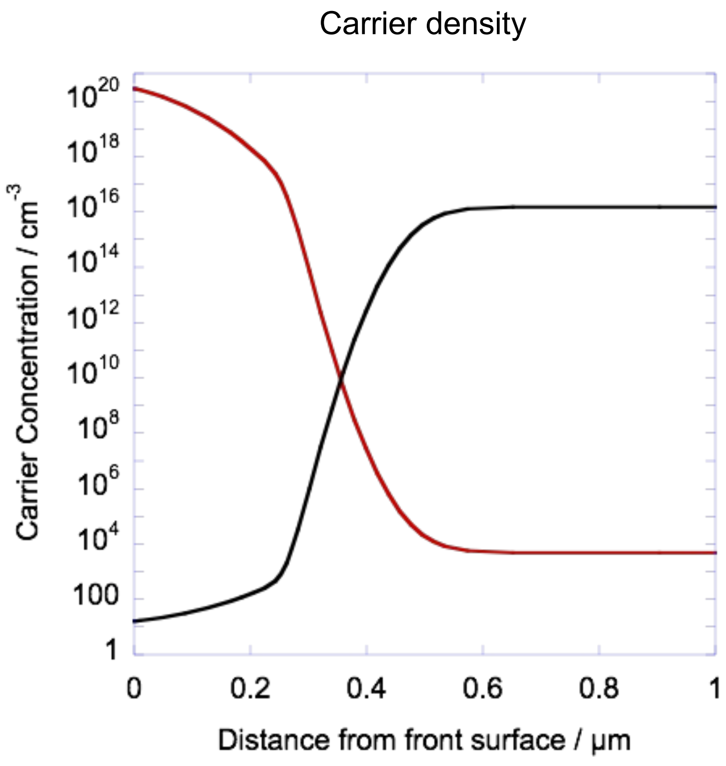


$$U_{\mathrm{aug}} = \left(C_n n + C_p p\right)\left(np - n_i^2\right)$$

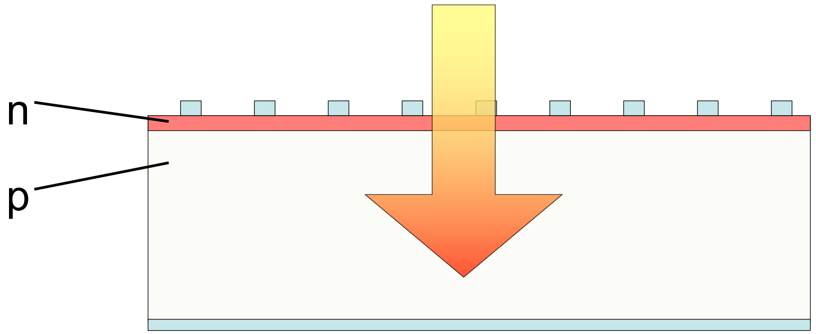
Silicon n/p solar cell : 0V Dark

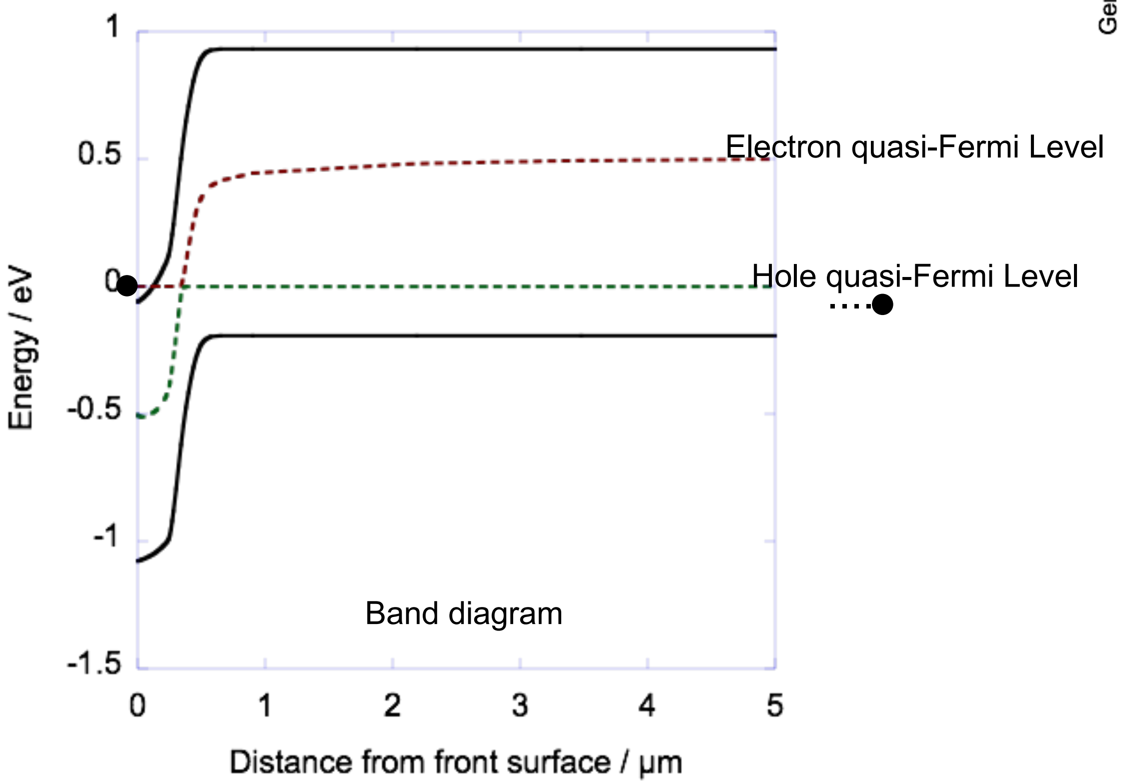


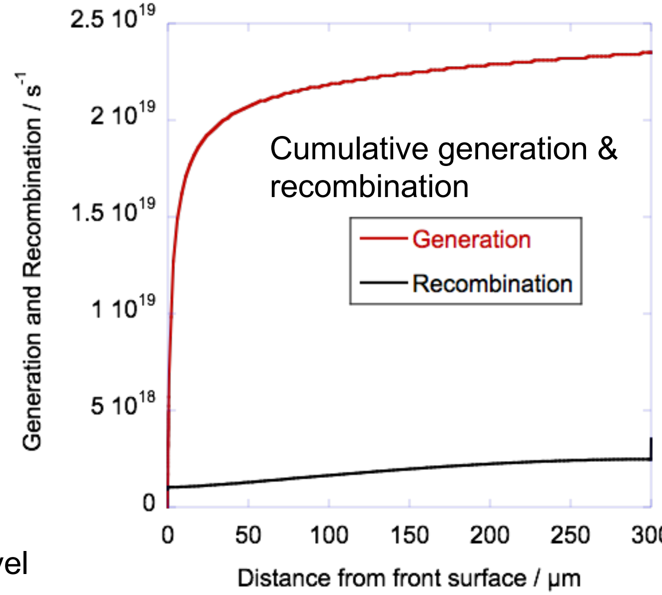


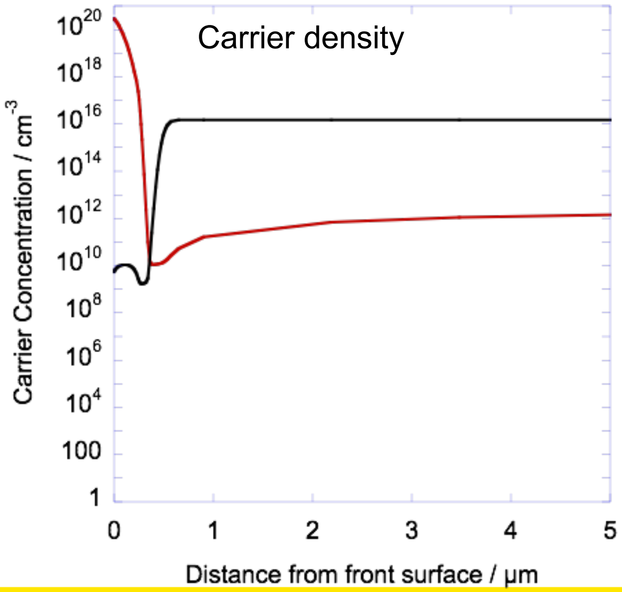


Silicon n/p solar cell : 0V Illuminated - AM1.5G

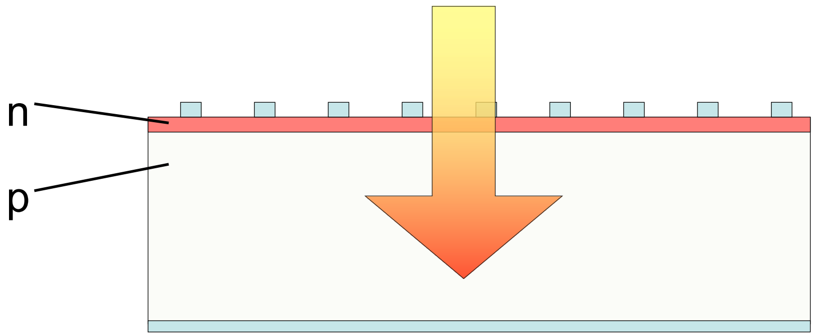


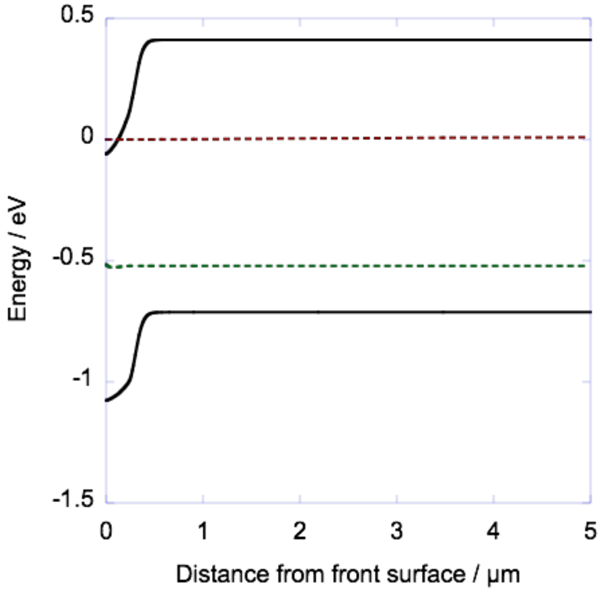


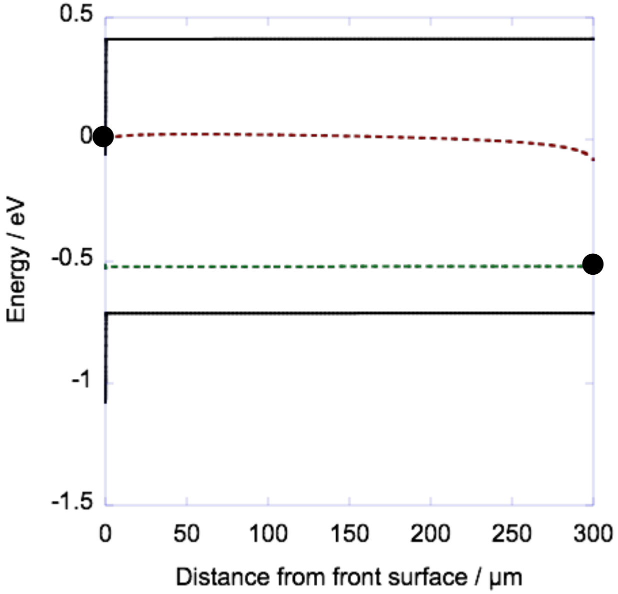


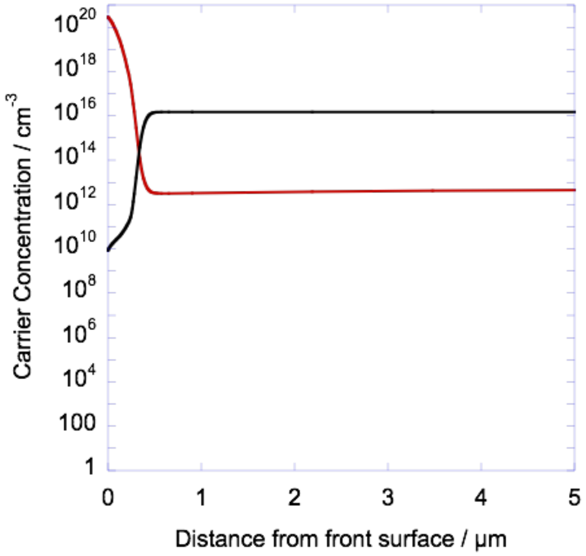


Silicon n/p solar cell : Maximum power point
Vmax Illuminated AM1.5G









p/n Junction : Depletion approximation

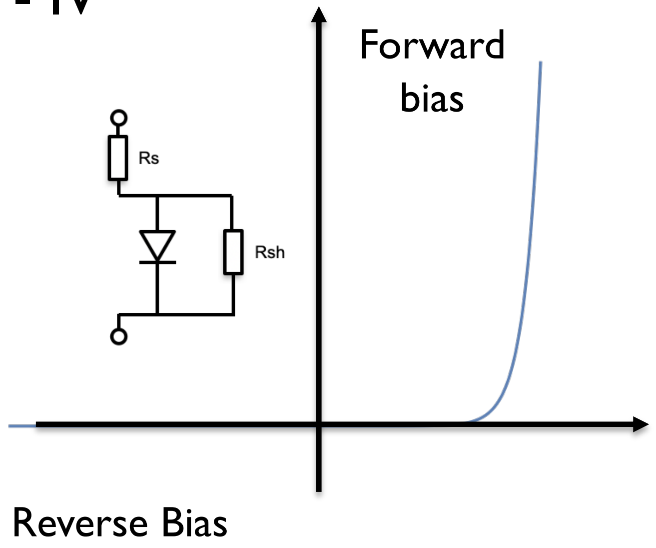
Shockley Diode Equation

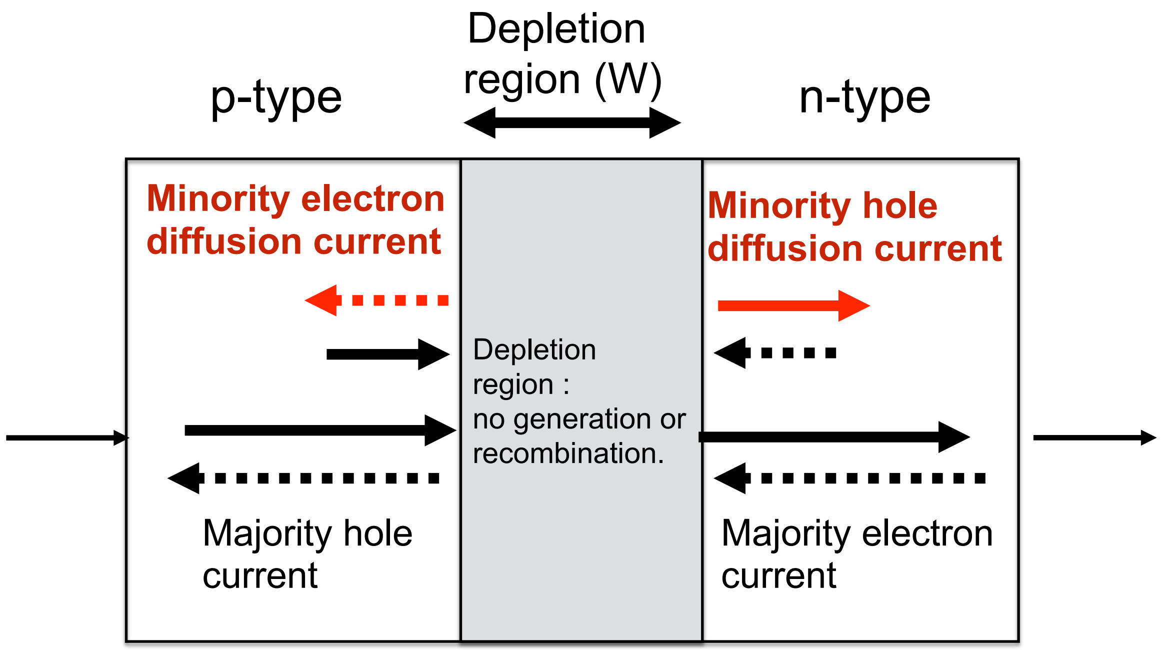
$$J(V) = J_0\left(e^{\frac{qV}{kT}} - 1\right)$$

where $$J_0 = n_i^2\left(\frac{qD_h}{L_hN_d} + \frac{qD_e}{L_eN_a}\right) \qquad D = \mu\frac{kT}{q}$$

Minority carrier diffusion length $$L = \sqrt{D\tau}$$

Dark - IV





Electron flow /
Hole flow

p/n Junction : Depletion approximation

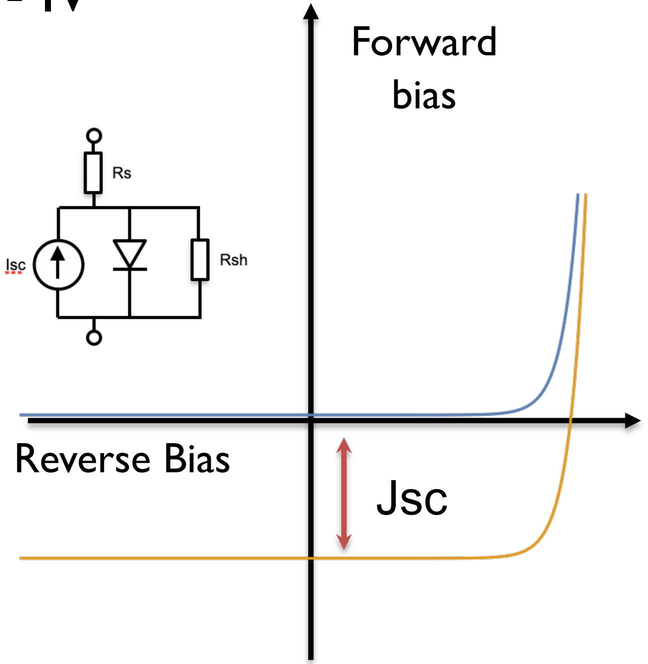
Shockley Diode Equation

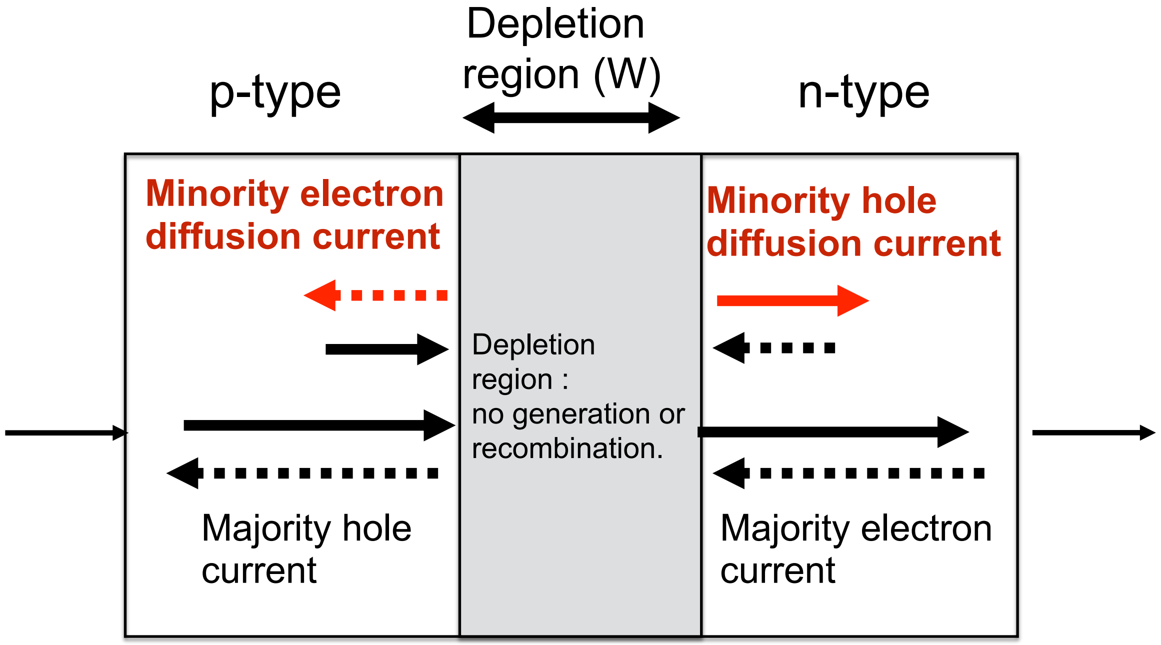
$$J(V) = J_0\left(e^{\frac{qV}{kT}} - 1\right) - \underline{J_{sc}}$$

where $J_0 = n_i^2\left(\frac{qD_h}{L_hN_d} + \frac{qD_e}{L_eN_a}\right)$ $D = \mu\frac{kT}{q}$

Minority carrier diffusion length $L = \sqrt{D\tau}$

Dark - IV

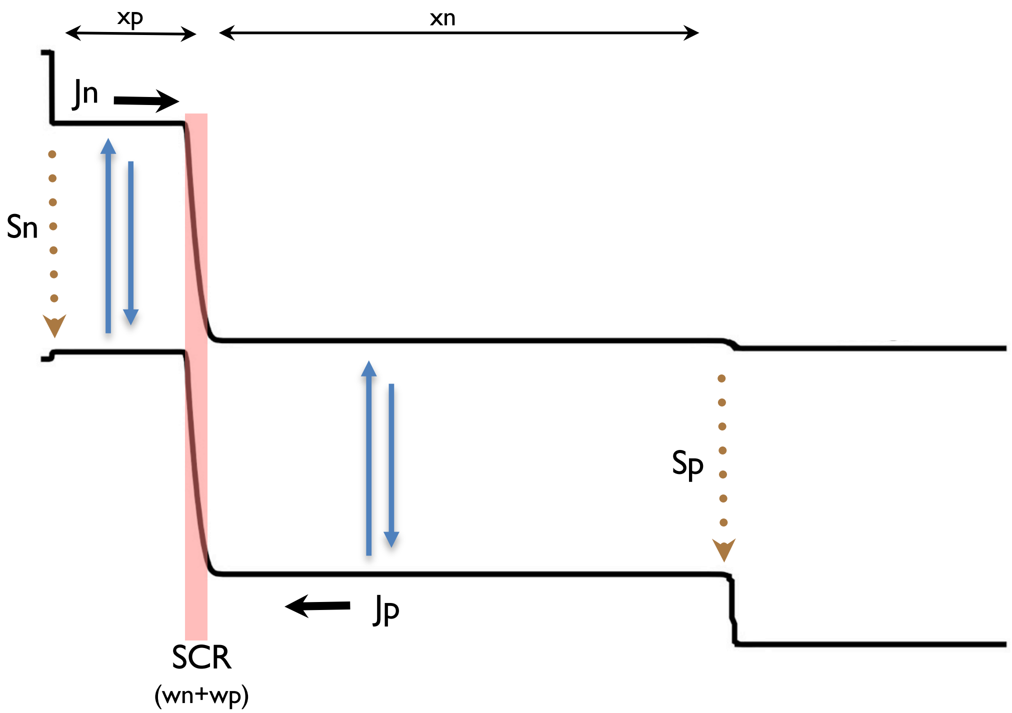




Electron flow /
Hole flow

Depletion approximation model for QE

Jn / Jp	Minority electron/hole current density
R	Surface reflection
α	Absorption coefficient
Ln / Lp	Minority electron, hole diffusion length
xp / xn	width of p / n regions
Dn / Dp	Carrier diffusivity for electrons and holes
wn / wp	Depletion widths on n/p side of the junction
n0/p0	Equilibrium electron/hole carrier density
Sn/Sp	Front / Rear surface recombination velocity
τn/τp	Electron / hole minority carrier lifetime
ni	Intrinsic carrier concentration
T	Junction temperature
V	External junction bias



$$J_n(E, w_p) = \left(\frac{qb_s(1-R)\alpha L_n}{\alpha^2 L_n^2 - 1}\right) \left(\frac{\left(\frac{S_n L_n}{D_n} + \alpha L_n\right) - e^{-\alpha(x_p - w_p)}\left(\frac{S_n L_n}{D_n}\cosh\frac{x_p - w_p}{L_n} + \sinh\frac{x_p - w_p}{L_n}\right)}{\frac{S_n L_n}{D_n}\sinh\frac{x_p - w_p}{L_n} + \cosh\frac{x_p - w_p}{L_n}} - \alpha L_n e^{-\alpha(x_p - w_p)}\right)$$

$$J_{scr}(E, w_n, w_p) = qb_s(1-R)e^{-\alpha(x_p - w_p)}(1 - e^{-\alpha(w_p + w_n)})$$

$$J_p(E, w_n) = \left(\frac{qb_s(1-R)\alpha L_p}{\alpha^2 L_p^2 - 1}\right) e^{-\alpha(x_p + w_n)} \left(\alpha L_p - \frac{\frac{S_p L_p}{D_p}\cosh\frac{x_n - w_n}{L_p} - e^{-\alpha(x_n - w_n)} + \sinh\frac{x_n - w_n}{L_p}) + \alpha L_p e^{-\alpha(x_n - w_n)}}{\frac{S_p L_p}{D_p}\sinh\frac{x_n - w_n}{L_p} + \cosh\frac{x_n - w_n}{L_p}}\right)$$

J.Nelson, Physics of Solar Cells, Imperial College Press 2003

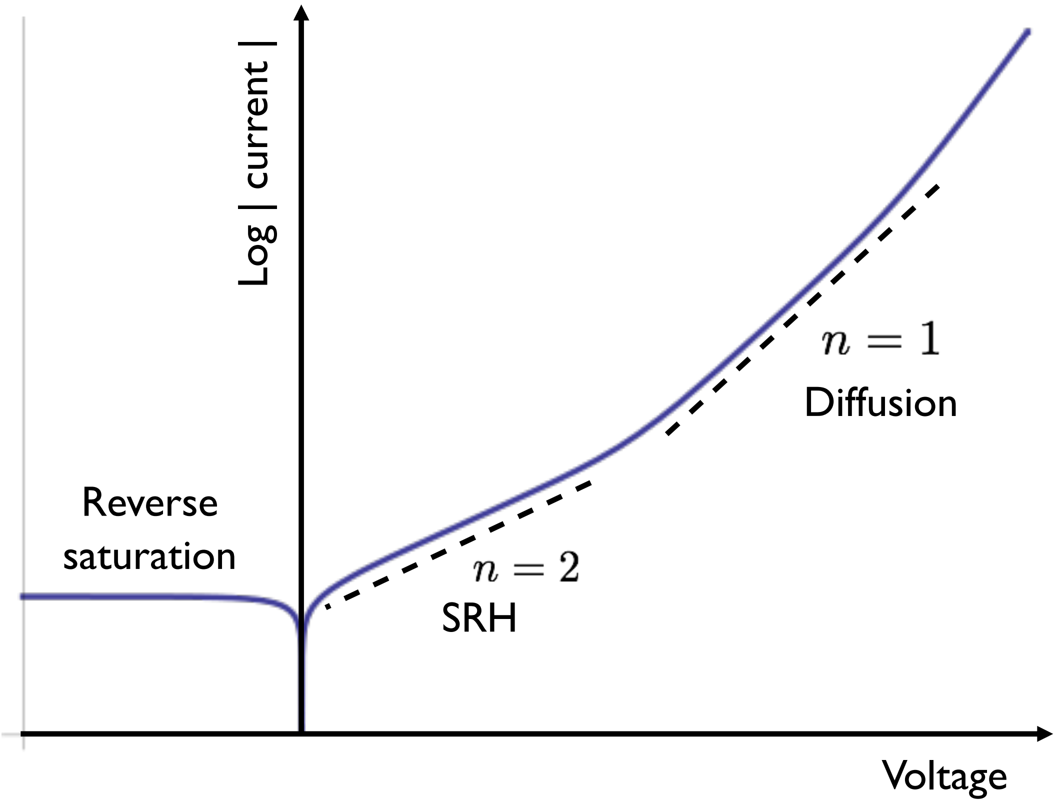
p/n Junction Diode : Dark-IV

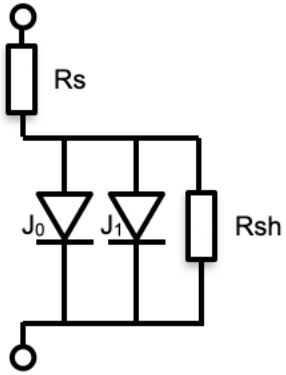
Diode Equation

$$J(V) \approx J_0(e^{\frac{qV}{kT}} - 1) \quad \leftarrow \text{Diffusion (radiative \& non-radiative)}$$
$$+ \; J_1(e^{\frac{qV}{2kT}} - 1) \quad \leftarrow \text{Impurity (SRH)}$$

Diode Equation with ideality factor

$$J_F(V) \approx J_s e^{\frac{qV}{nkT}}$$

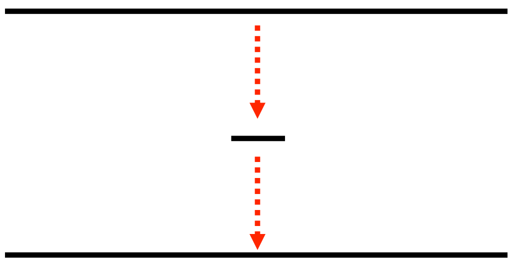




Shockley Read Hall Recombination

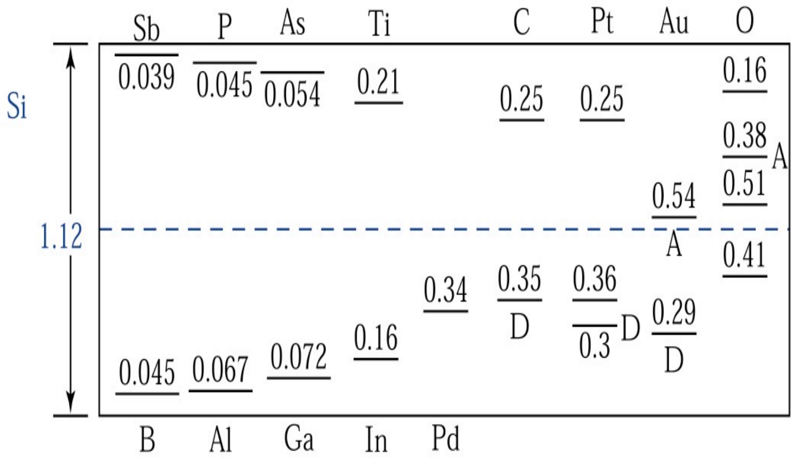
$J(V)$	$\approx$	$J_0(e^{\frac{qV}{kT}} - 1)$	←Diffusion
	$+$	$J_1(e^{\frac{qV}{2kT}} - 1)$	←Impurity

Shockley Read Hall (SRH) recombination



- Non-radiative process
- Releases phonons

Deep & shallow levels



•Shallow levels are ionized at room temperature and can donate or accept electrons

•<u>Deep levels trap carriers</u>

capture cross-section

thermal velocity

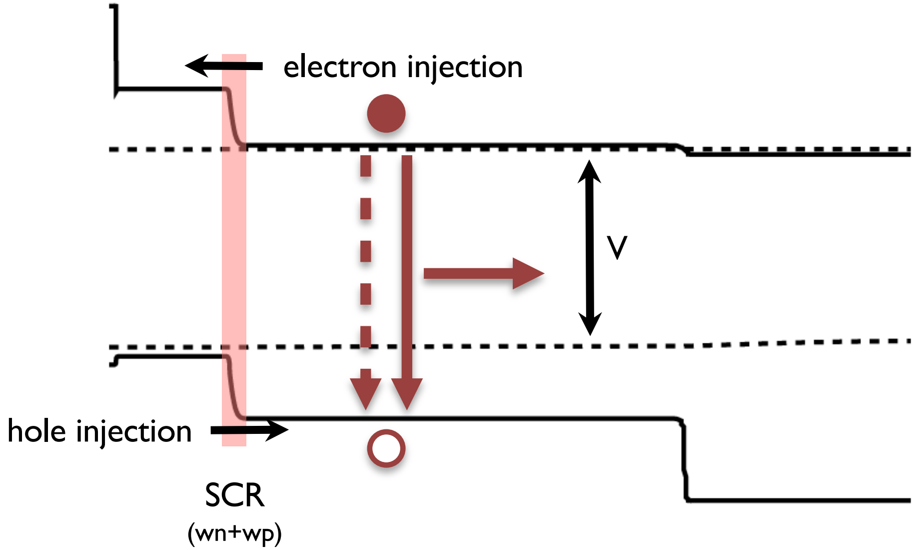
depletion width

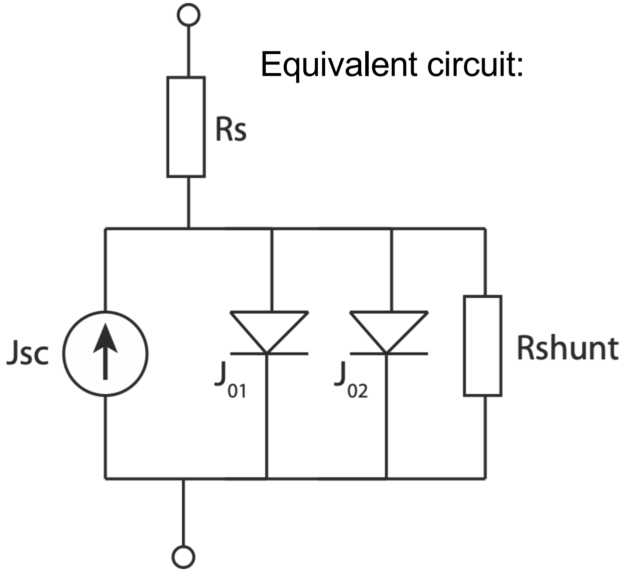
$$J_1 = \sigma v_{th} N_t n_i \frac{qW}{2}$$

trap concentration

C.-T. Sah, R. Noyce, and W. Shockley, Proceedings of the IRE **45**, 1228–1243 (1957).

Shockley diode models for J_0





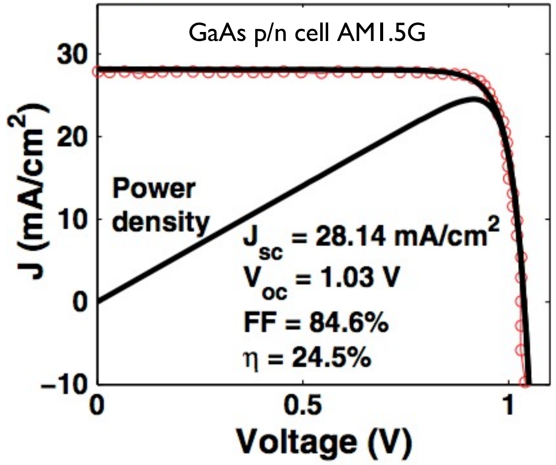
$$J_{\text{Total}} = J_{\text{SC}} - J_{01}(e^{qV/kT} - 1) - J_{02}(e^{qV/2kT} - 1)$$

Shockley diffusion current (Radiative & non-radiative):

$$J_{01} = \left(\frac{qD_n n_i^2}{L_n N_A} \cdot \frac{\cosh\left(\frac{W_P}{L_n}\right) + \frac{D_n}{S_n L_n}\sinh\left(\frac{W_P}{L_n}\right)}{\frac{D_n}{S_n L_n}\cosh\left(\frac{W_P}{L_n}\right) + \sinh\left(\frac{W_P}{L_n}\right)} + \frac{qD_p n_i^2}{L_p N_D} \cdot \frac{\cosh\left(\frac{W_N}{L_p}\right) + \frac{D_p}{S_p L_p}\sinh\left(\frac{W_N}{L_n}\right)}{\frac{D_p}{S_p L_p}\cosh\left(\frac{W_N}{L_p}\right) + \sinh\left(\frac{W_N}{L_p}\right)} \right)$$

Shockley-Read-Hall current: (non-radiative)

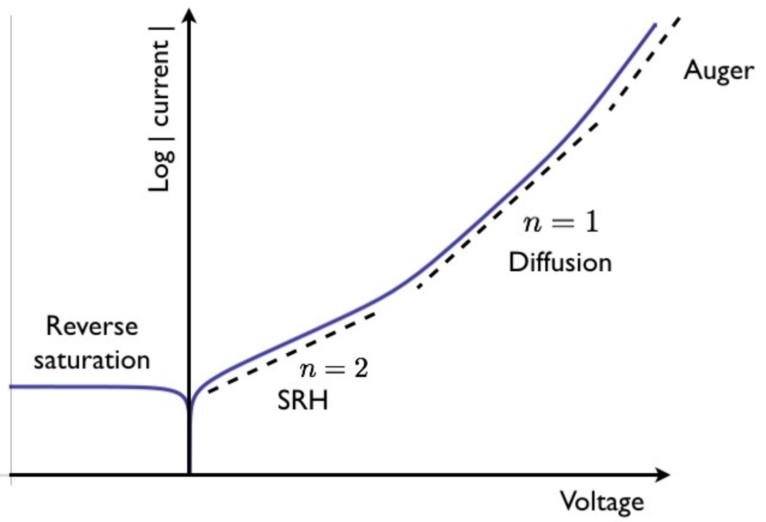
$$J_{02} = \frac{qn_i(W_n + W_p)}{\sqrt{\tau_n \tau_p}}$$

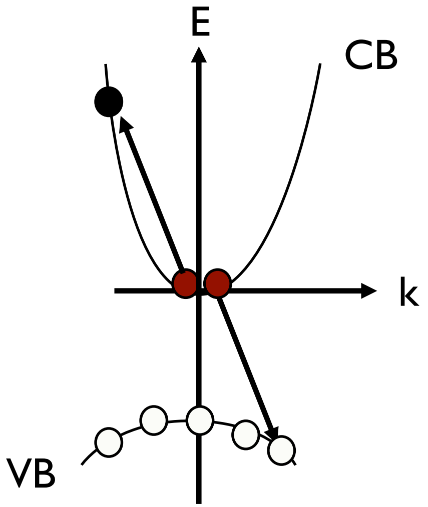


X. Li, et al. Prog. Photovolt: Res. Appl. 21, 109 (2013).

Auger Recombination

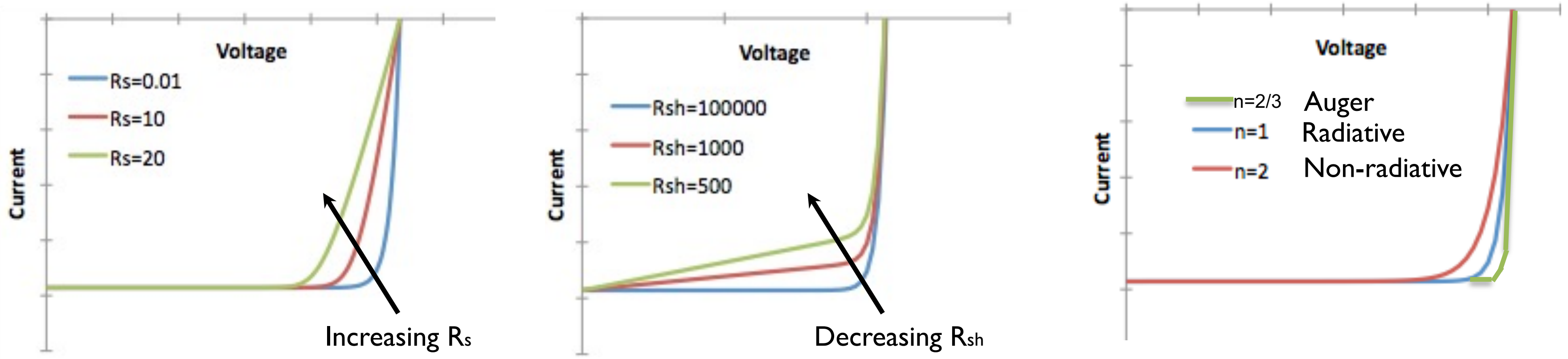
$$
\begin{aligned}
J(V) &\approx J_0(e^{\frac{qV}{kT}}-1) \leftarrow \text{Diffusion}\\
&+ J_1(e^{\frac{qV}{2kT}}-1) \leftarrow \text{Impurity}\\
&+ J_2(e^{\frac{3qV}{2kT}}-1) \leftarrow \text{Auger}
\end{aligned}
$$



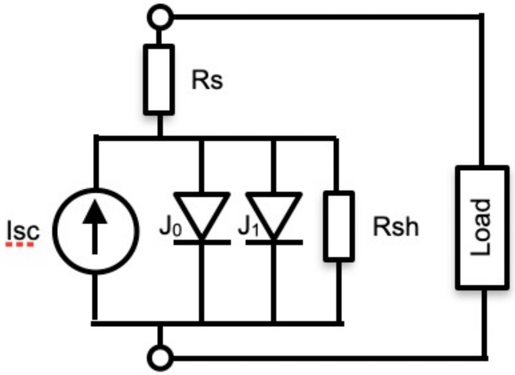


- Three particle process
  - e.g. two electrons one hole shown
- Momentum must be conserved
- Favoured at high carrier density
- Somewhat material dependent (m*)

Fill Factor

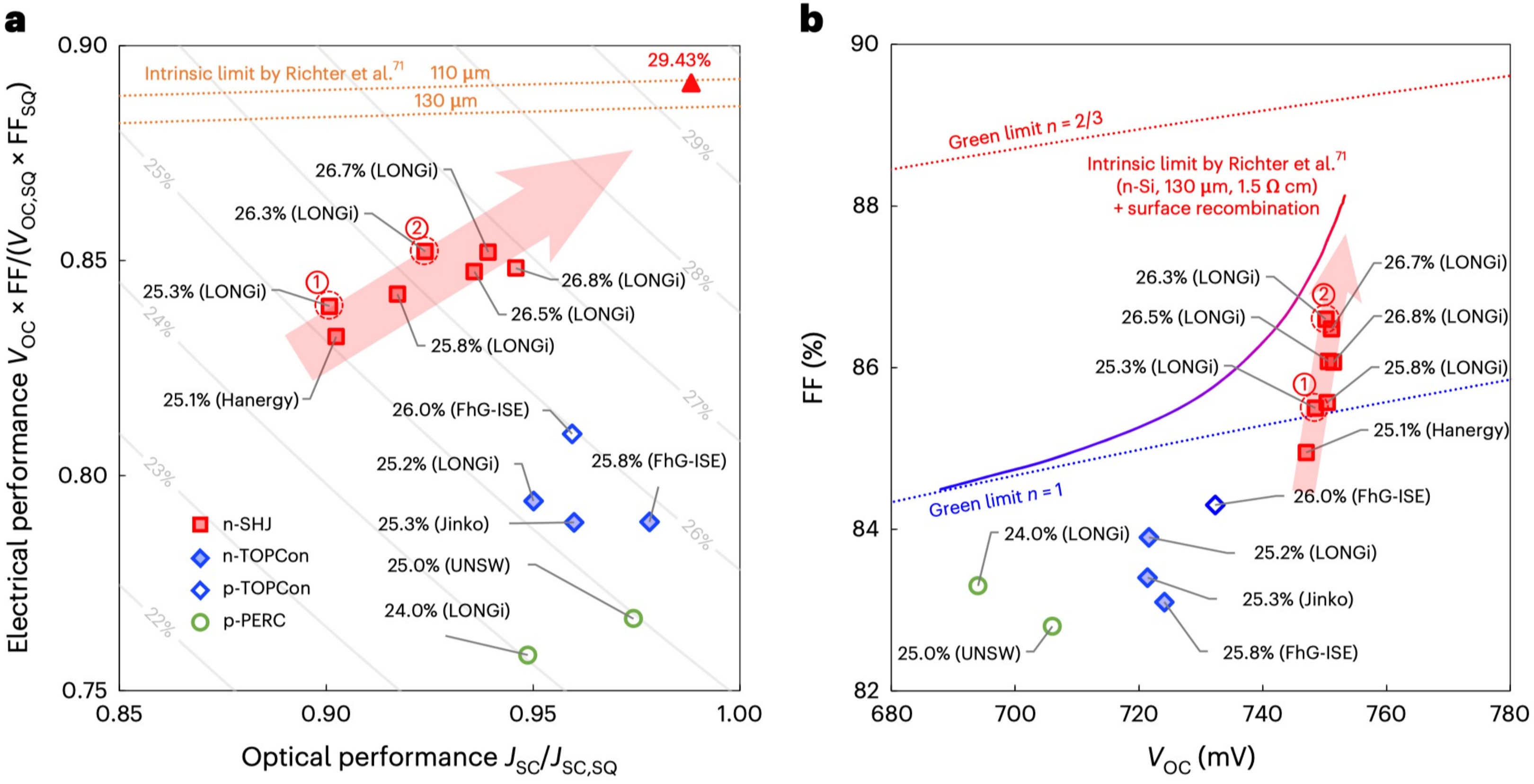


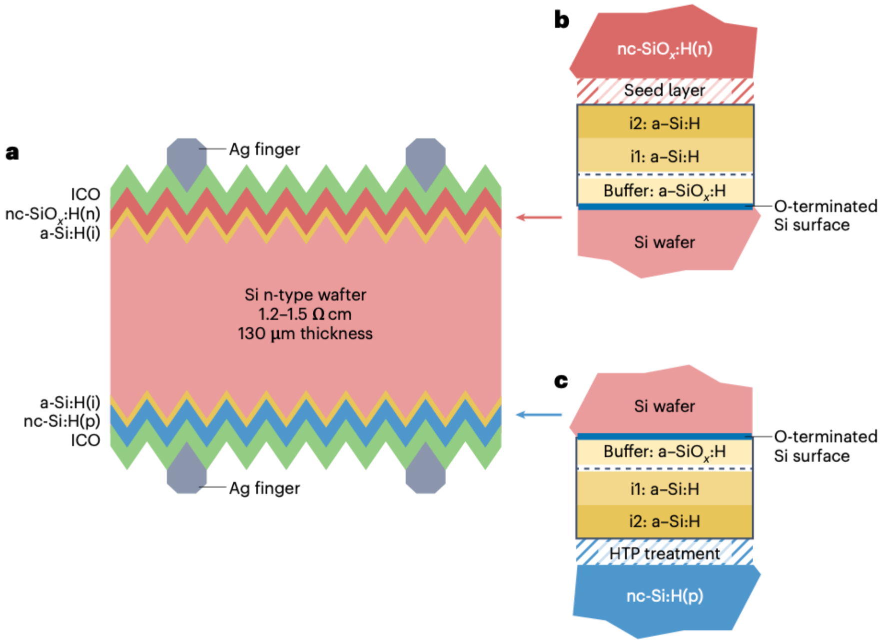
Voltage
Current
Rs=0.01
Rs=10
Rs=20
Increasing Rs
Voltage
Current
Rsh=100000
Rsh=1000
Rsh=500
Decreasing Rsh
Voltage
Current
n=2/3 Auger
n=1 Radiative
n=2 Non-radiative



Rs
Isc
J0
J1
Rsh
Load

Silicon solar cells are approaching the Auger limit





Lin, Hao, et al., *Nature Energy*, (2023)
doi:10.1038/s41560-023-01255-2

Green, M.A. *Nature Energy*, (2023)
doi:10.1038/s41560-023-01296-7

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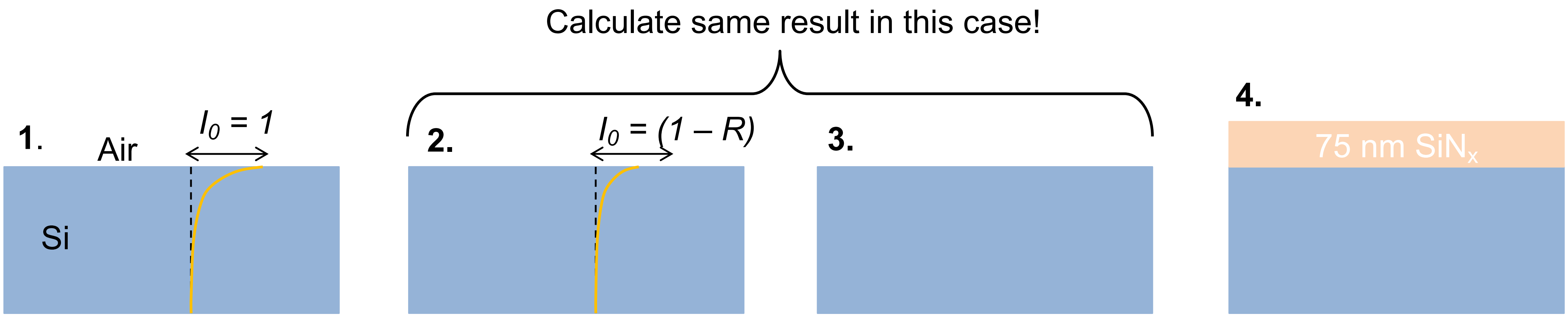
Session 5: Simple Si and GaAs cells using the depletion approximation

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)



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)

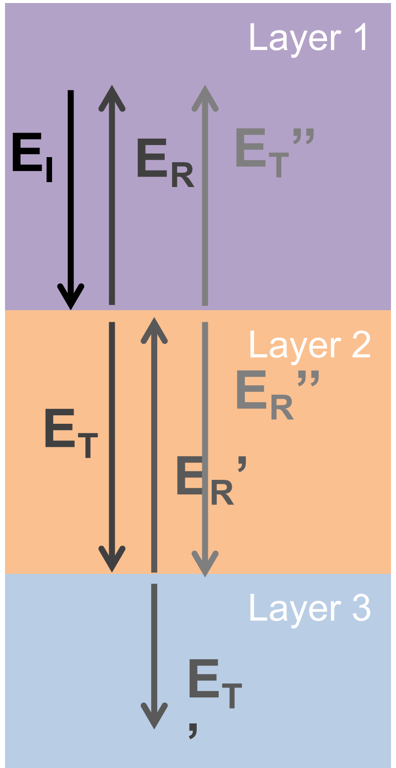
Efficiently handles **planar multilayer** stacks (including thin film interference effects)

$M_{\text{Layer 1}}$

$M_{\text{Layer 2}}$

Relates waves entering and exiting layer 2 (both directions)

$M_{\text{Layer 3}}$



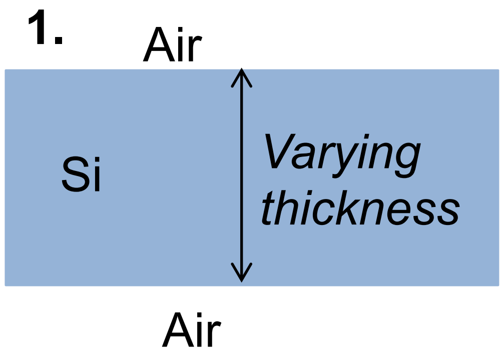
R, A, T of stack

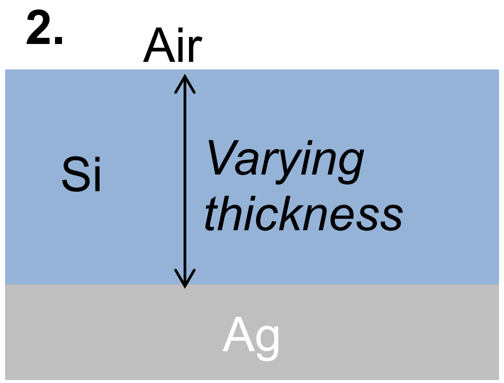
$$M_{\text{stack}} = M_{01} \times M_{\text{Layer 1}} \times M_{\text{Layer 2}} \times M_{\text{Layer 3}} \times \ldots$$

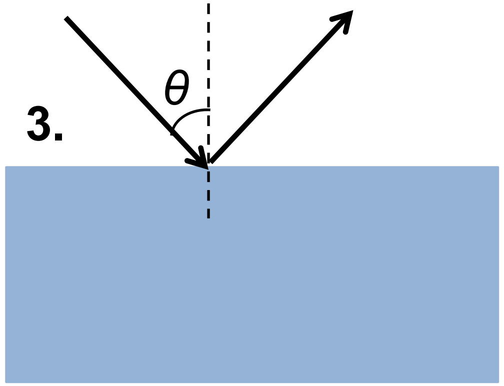
Solcore integrates & streamlines the **tmm** Python package

Example 6a: More exploration of TMM

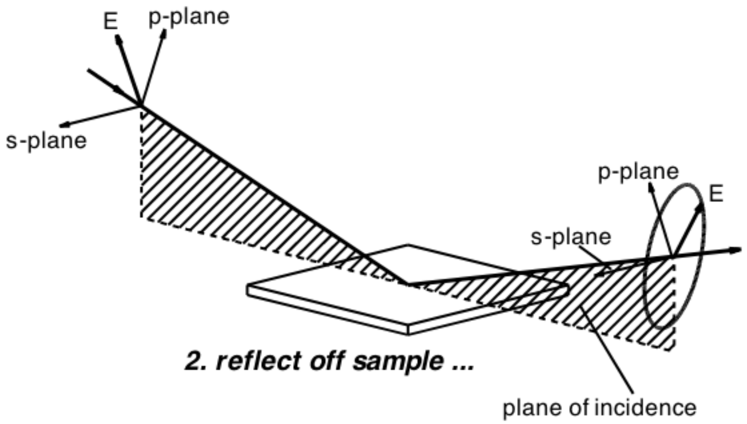
No longer ignore back-surface reflection. Explore effect of different assumptions about coherency, the incidence angle, and the polarization of the incident light







Varying angle of incidence and polarization

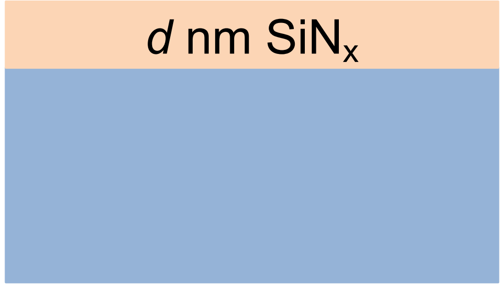


Treating a layer **incoherently** means **discarding the phase information** inside that layer; no **Fabry-Perot/thin-film interference**. The absorption profile is assumed to follow the Beer-Lambert law.

Example 6b: Simple ARC optimization

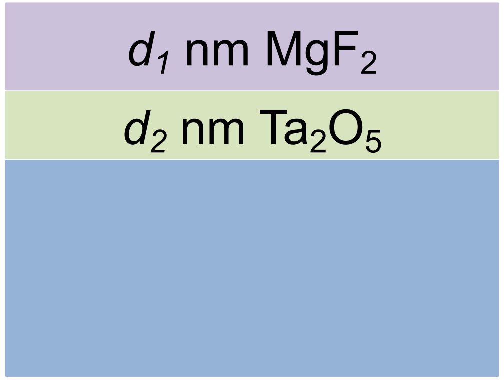
Find ARC layer thicknesses which minimize reflectance

1.



Vary d

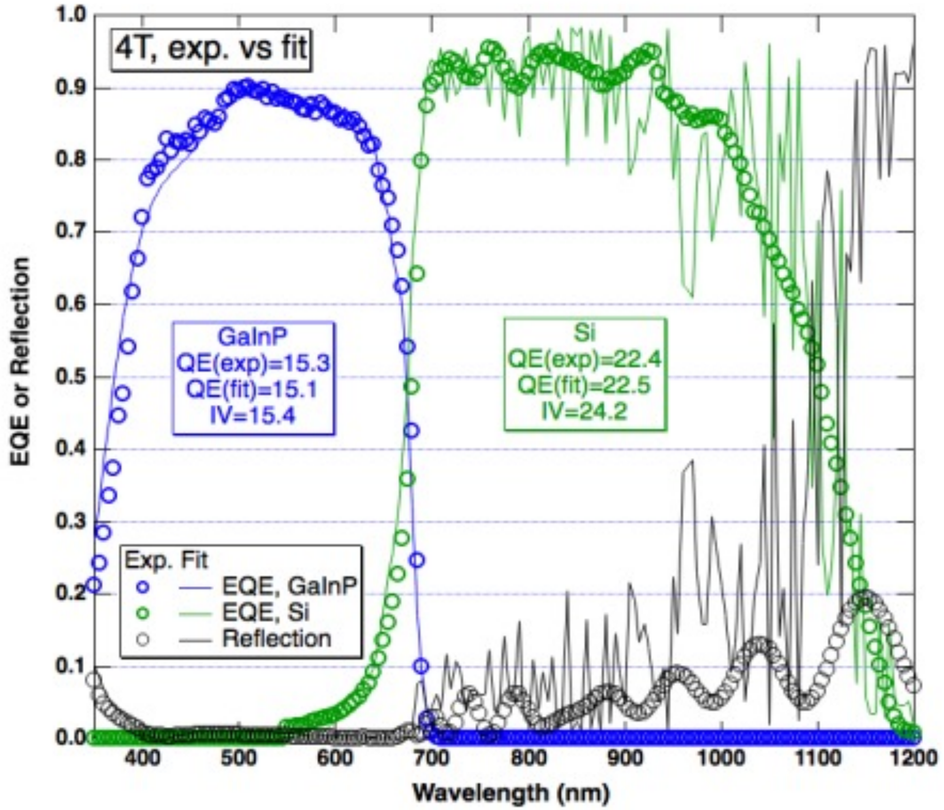
2.



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

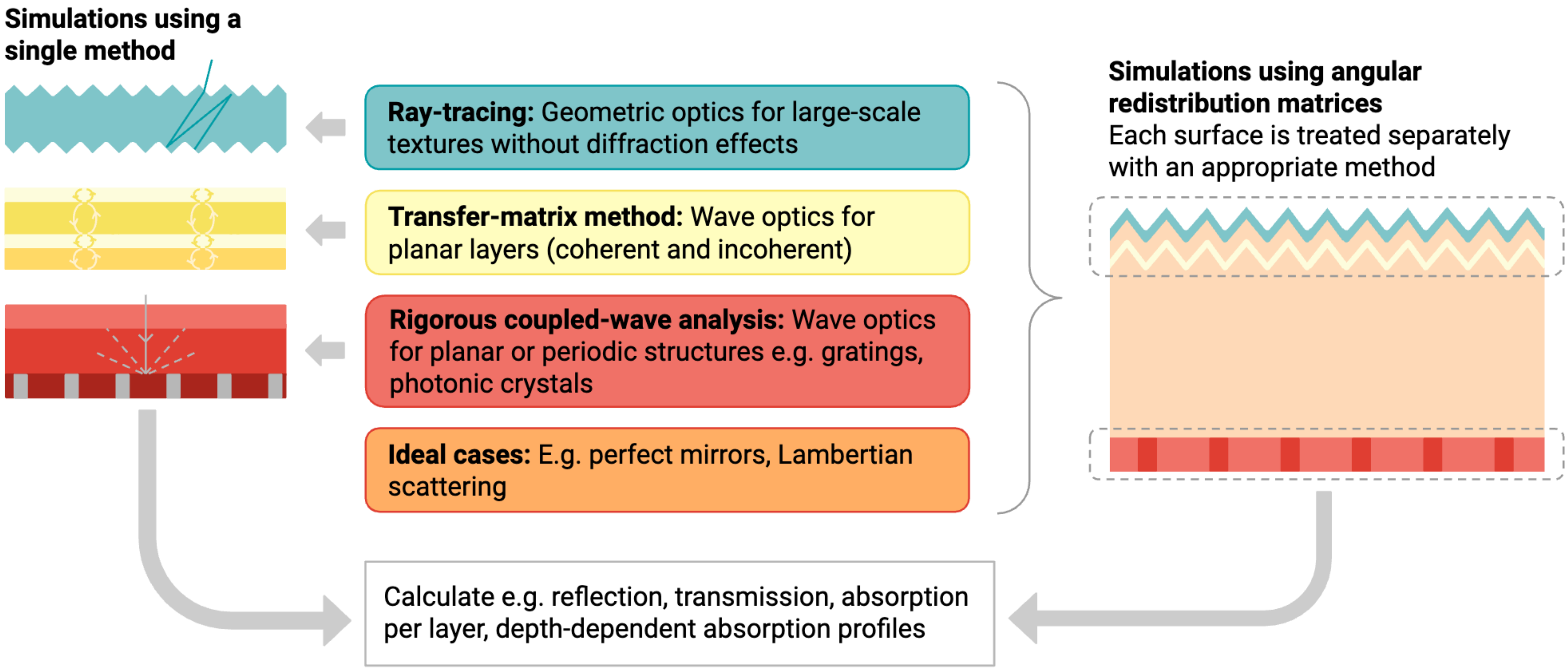
3rd August 2023

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!)
- More instructions for running Linux inside Windows: http://docs.solcore.solar/en/latest/Installation/Solcore_on_Windows.html

RayFlare capabilities



Documentation: https://rayflare.readthedocs.io

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.

Transfer-matrix method (TMM)

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
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Modelling optics

Transfer-matrix method (TMM)

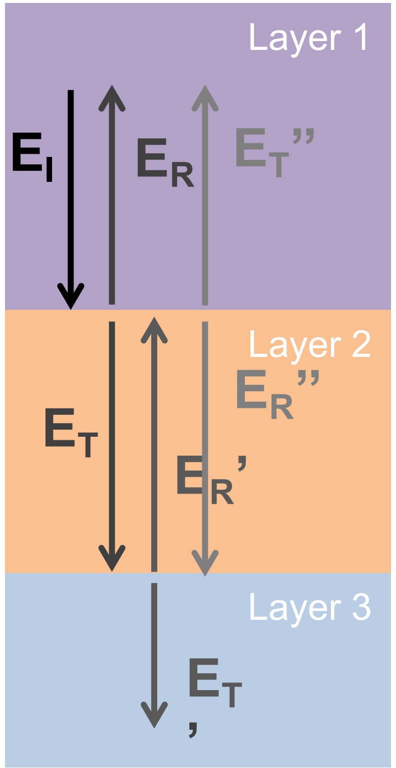
Efficiently handles **planar multilayer** stacks (including thin film interference effects)

$\mathbf{M}$ Layer 1

$\mathbf{M}$ Layer 2

Relates waves entering and exiting layer 2 (both directions)

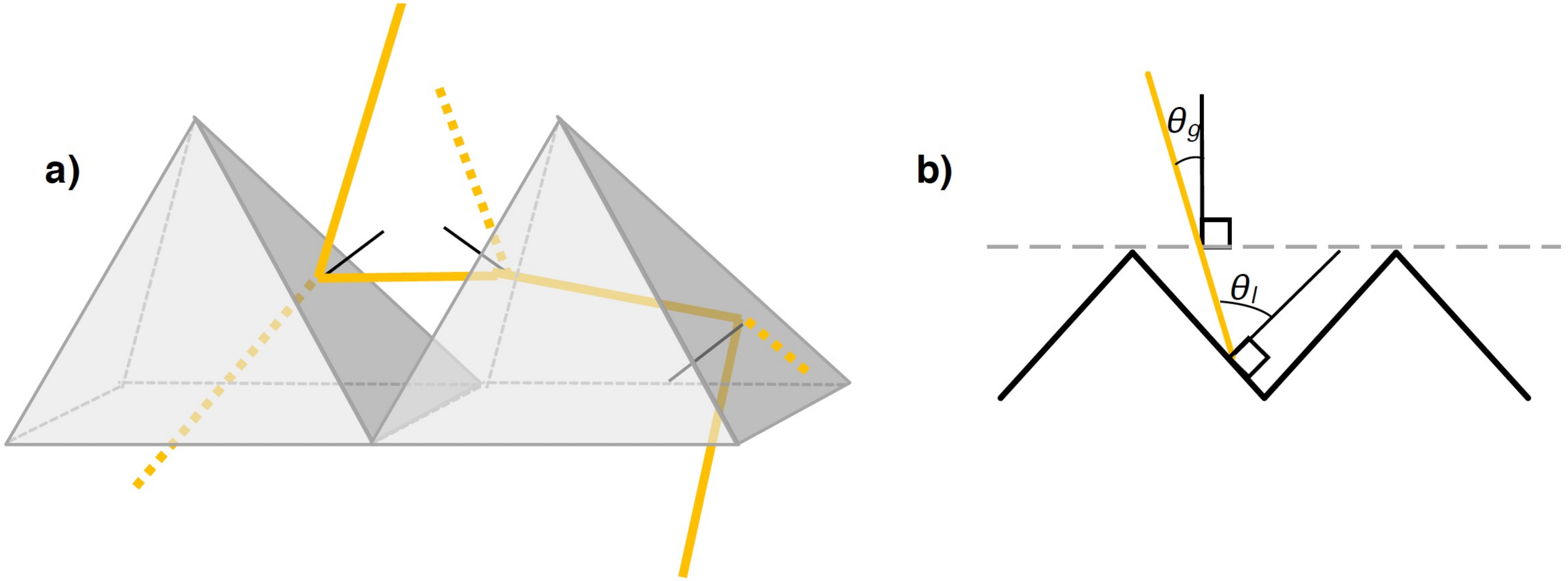
$\mathbf{M}$ Layer 3



R, A, T of stack

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

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)

Further reading: https://doi.org/10.25560/88448 (P. Pearce PhD thesis)

Rigorous coupled-wave analysis (RCWA)

(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

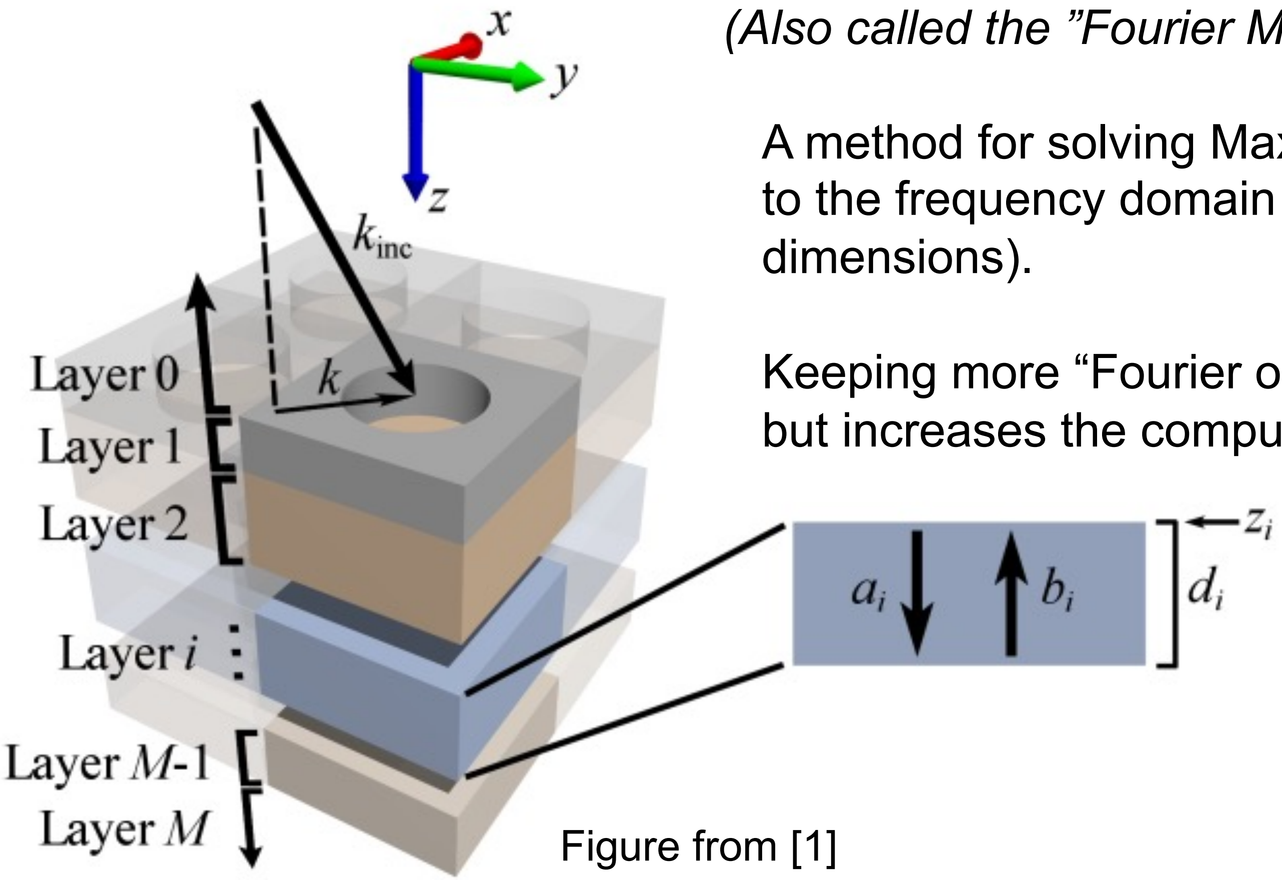


Figure from [1]

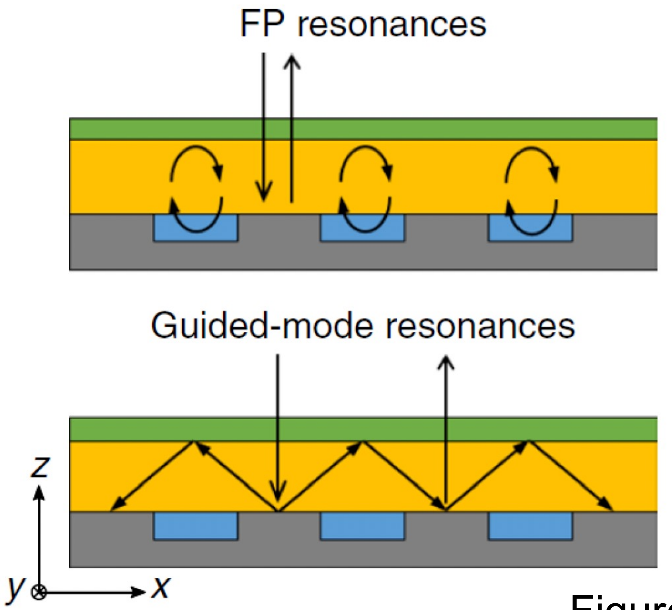
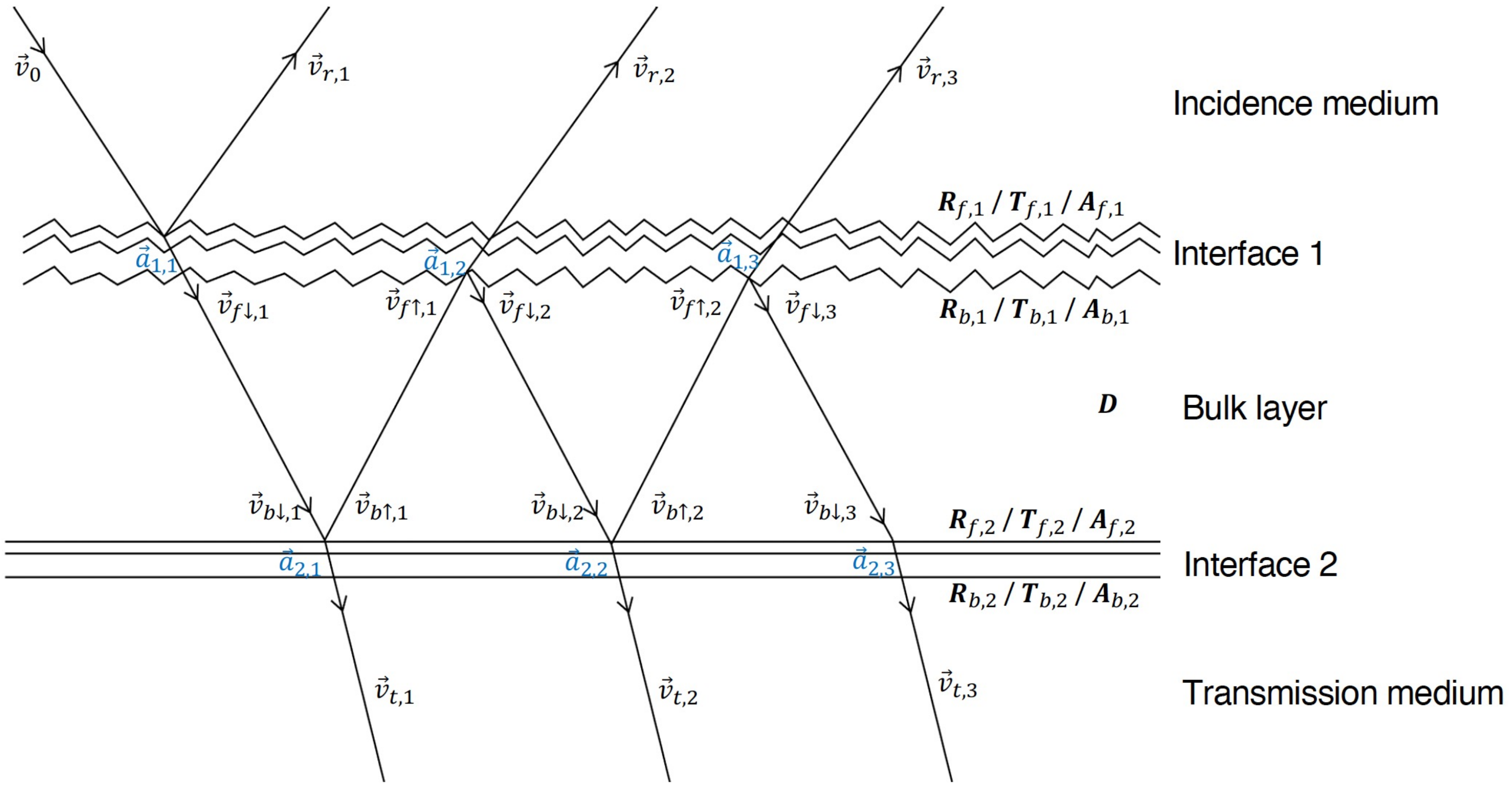


Figure from [2]

[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



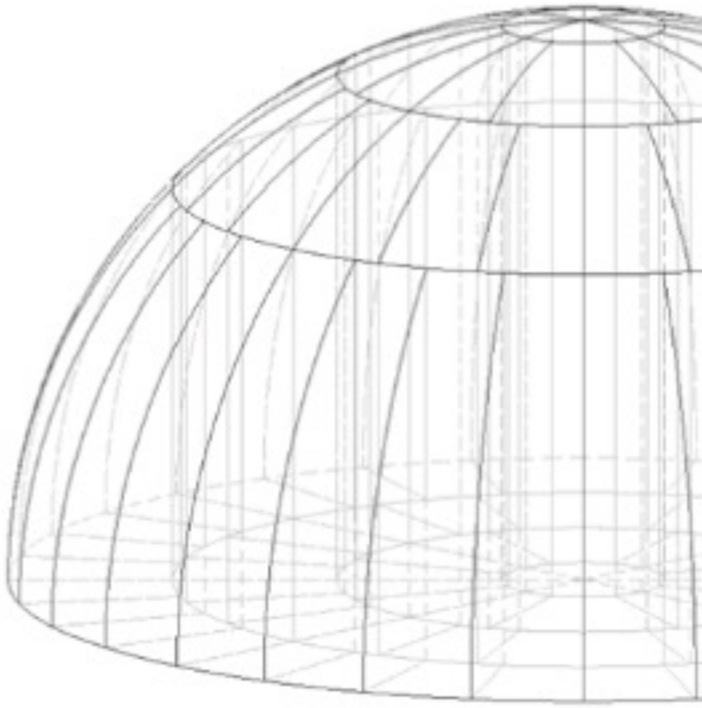


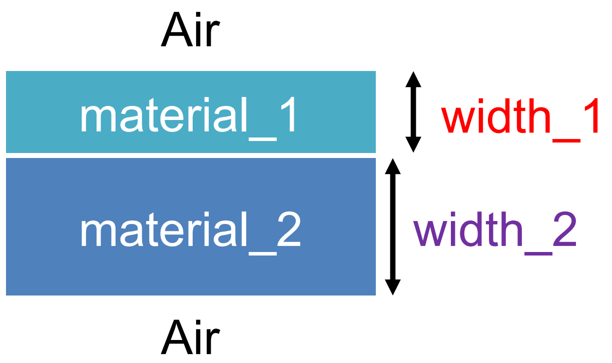
Image from [1]

[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

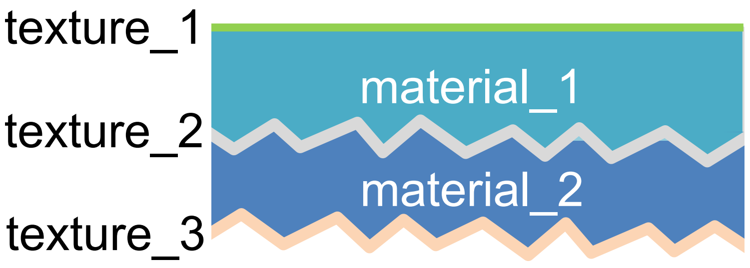
Using a single method: what does it look like in the code?

TMM




```
from rayflare.transfer_matrix_method import tmm_structure

TMM_stack = tmm_structure(
    layer_stack=[Layer(width_1, material_1), Layer(width_2, material_2)],
    incidence=Air,
    transmission=Air)
```

Ray-tracing (RT)

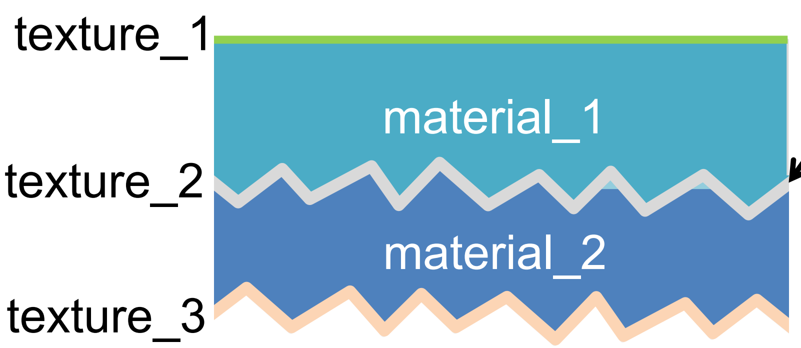



```
from rayflare.ray_tracing import rt_structure

RT_stack = rt_structure(
        textures=[texture_1, texture_2, texture_3],
        materials=[material_1, material_2],
        widths=[width_1, width_2],
        incidence=Air, transmission=Air)
```

RCWA

```
from rayflare.rigorous_coupled_wave_analysis import rcwa_structure

RCWA_stack = rcwa_structure(
        structure=[Layer(width_1, material_1), Layer(width_2, material_2)],
        size=((100, 0), (0, 100)), # in nm
        options=user_options,
        incidence=Air,transmission=Air)
```

Some more detail about ray-tracing structures: `rt_structure`



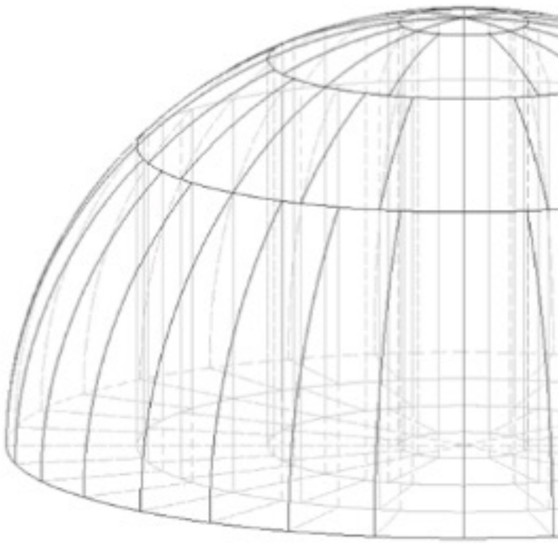

```
texture_2 = regular_pyramids(
        elevation_angle=50,
        upright=True,
        interface_layers = [Layer(width_a, material_a),
                            …, …]
        )
```

In `rt_structure`, It is assumed that the **bulk layers** (material_1, material_2 in the diagram) are thick enough (or absorbing enough) that we can **ignore thin-film interference.**

However, the **interface textures themselves can be modified with additional thin-film layers**! If there are interface layers, RayFlare will first calculate reflection/absorption/reflection probabilities using TMM, and then use these probabilities during the ray-tracing calculation:

→ **Fully integrated ray-tracing + TMM, inside** `rt_structure`**!**

But what if we want to combine other methods?



- Previous slide: integrated ray-tracing + TMM
- But what if we want to integrate e.g.:
  - TMM and RCWA
  - Ray-tracing and RCWA
  - Other methods we define ourselves (or maybe real measured data!)

→ **Use the <u>angular redistribution matrix method</u>** (ARMM), also called the “OPTOS method”

- Calculate angular redistribution matrices for each surface: how light incident from any angle is scattered by the surface (or absorbed). Use an appropriate method for each surface.

$$\mathbf{R},\mathbf{T} = \begin{pmatrix} p(\{\theta_1,\phi_1\} \to \{\theta_1,\phi_1\}) & p(\{\theta_1,\phi_2\} \to \{\theta_1,\phi_1\}) & \dots & p(\{\theta_n,\phi_m\} \to \{\theta_1,\phi_1\}) \\ p(\{\theta_1,\phi_1\} \to \{\theta_1,\phi_2\}) & p(\{\theta_1,\phi_2\} \to \{\theta_1,\phi_2\}) & \dots & p(\{\theta_n,\phi_m\} \to \{\theta_1,\phi_2\}) \\ \vdots & \ddots & & \vdots \\ p(\{\theta_1,\phi_1\} \to \{\theta_n,\phi_m\}) & p(\{\theta_1,\phi_2\} \to \{\theta_n,\phi_m\}) & \dots & p(\{\theta_n,\phi_m\} \to \{\theta_n,\phi_m\}) \end{pmatrix}$$

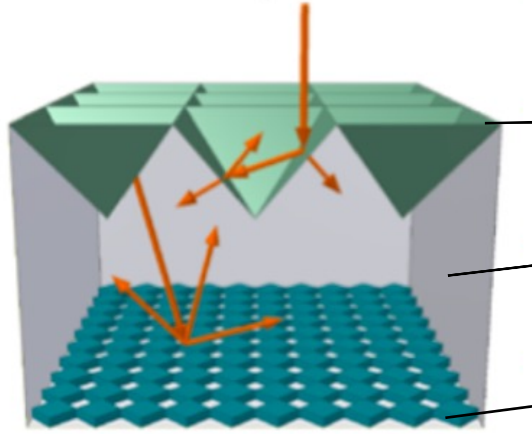
<u>Figure from: https://doi.org/10.1364/OE.23.0A1720</u>

ARMM (continued)

- Assume Beer-Lambert-like absorption in bulk medium which connects the two surfaces:

$$D = \begin{bmatrix} e^{-\alpha d/|\cos\theta_1|} & 0 & \dots & 0 \\ 0 & \ddots & & 0 \\ 0 & \vdots & \vdots & 0 \\ 0 & \dots & 0 & e^{-\alpha d/|\cos\theta_m|} \end{bmatrix}$$

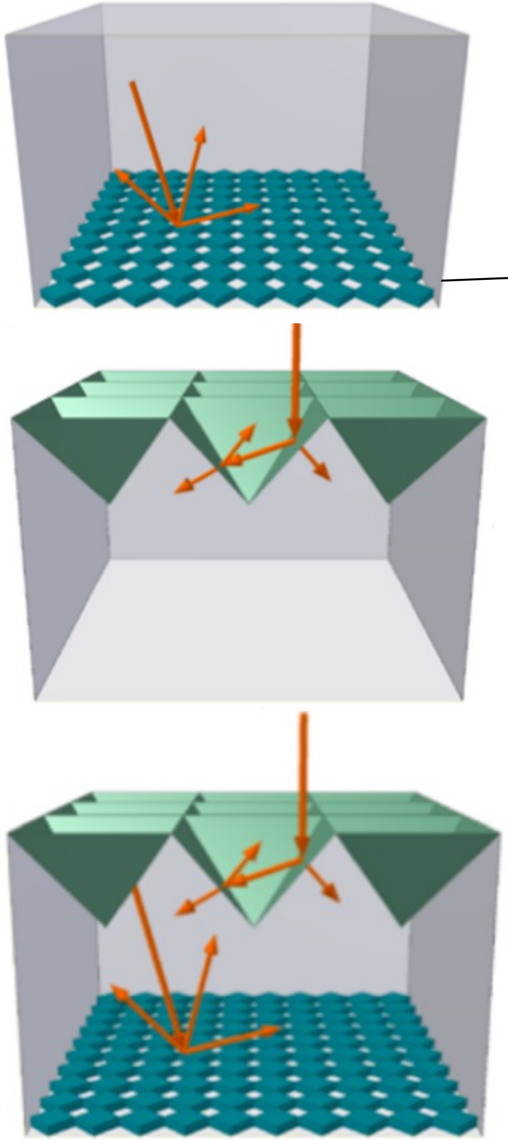
- Now, we have turned the complex optics problem into **matrix multiplication**
- In the code:

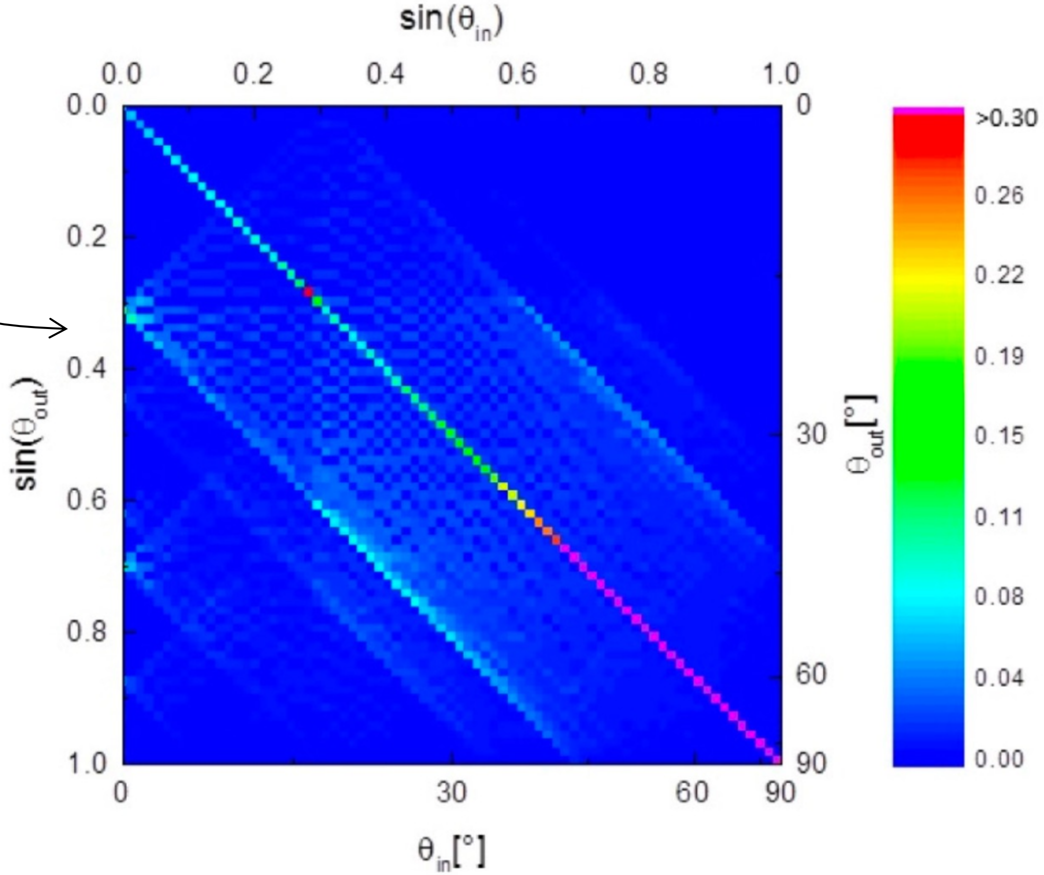


```
from rayflare.structure import Interface, BulkLayer, Structure
front_surf = Interface(method="RT_TMM", …)

bulk_mat = BulkLayer(width=200e-6, material=material_1)

back_surf = Interface(method=”RCWA", …)

whole_stack = Structure([front_surf, bulk_mat, back_surf], incidence=Air, transmission=Air)
```

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

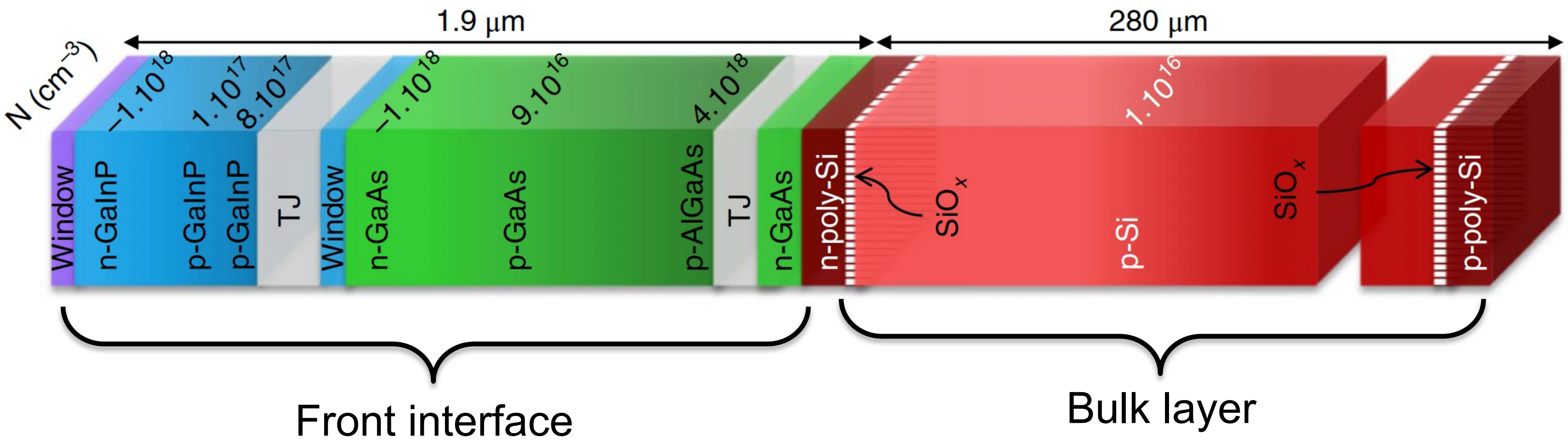
8. Textured Si: pyramids/grating



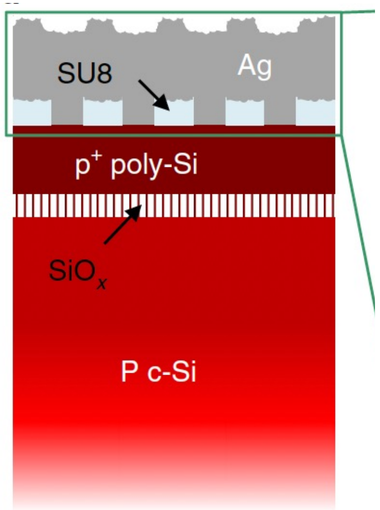


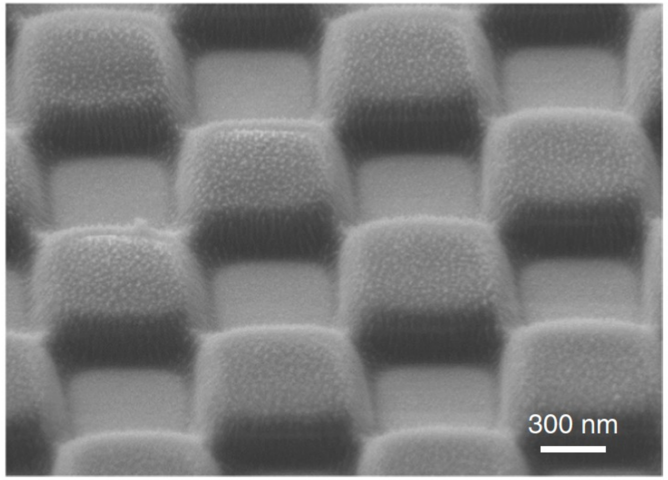
Figures from: https://doi.org/10.1364/OE.23.0A1720

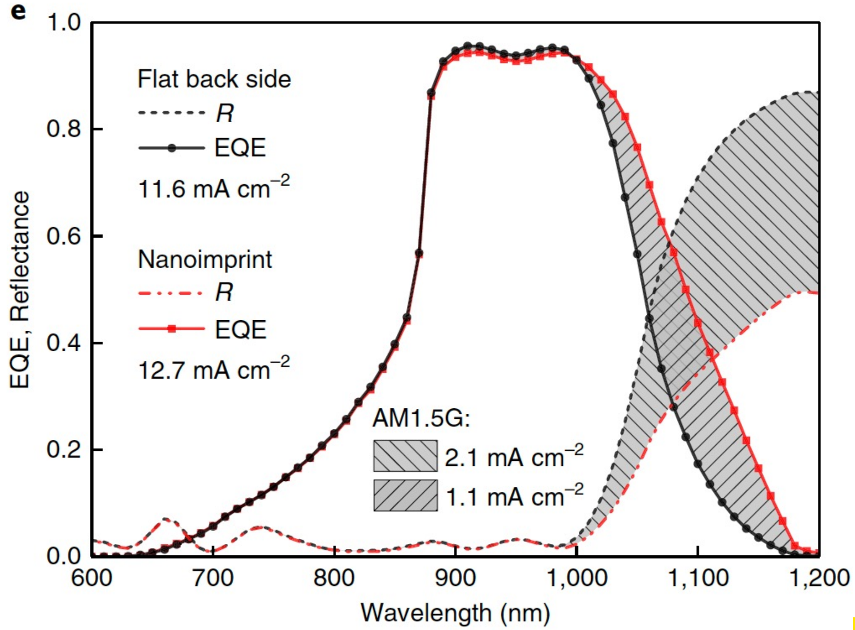
9a. III-V on Si, planar vs. rear grating, using ARMM



Rear interface = grating



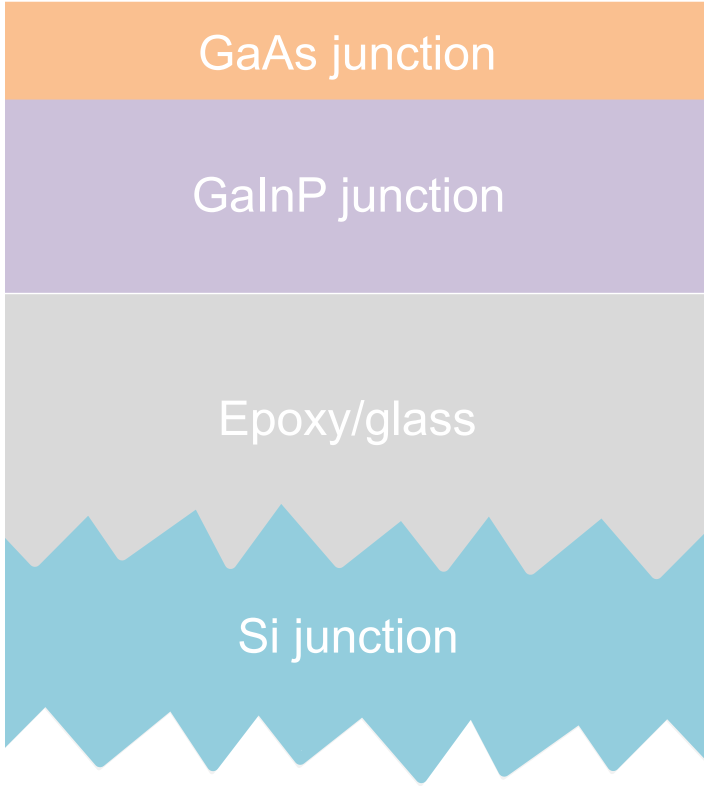




9b. III-V on Si, planar vs. pyramidal Si texture

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.

Use `rt_structure` to define stack



Layers on front surface ("texture" of the front surface is just planar)

Interface 1: thin layers on top of epoxy (planar)

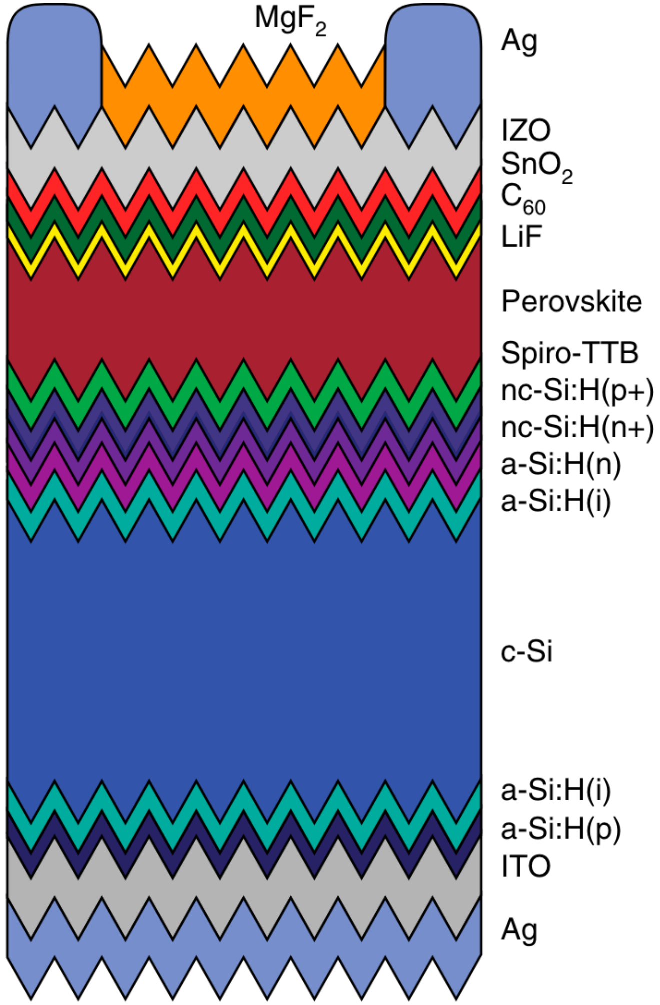
Bulk material 1 (epoxy/glass)

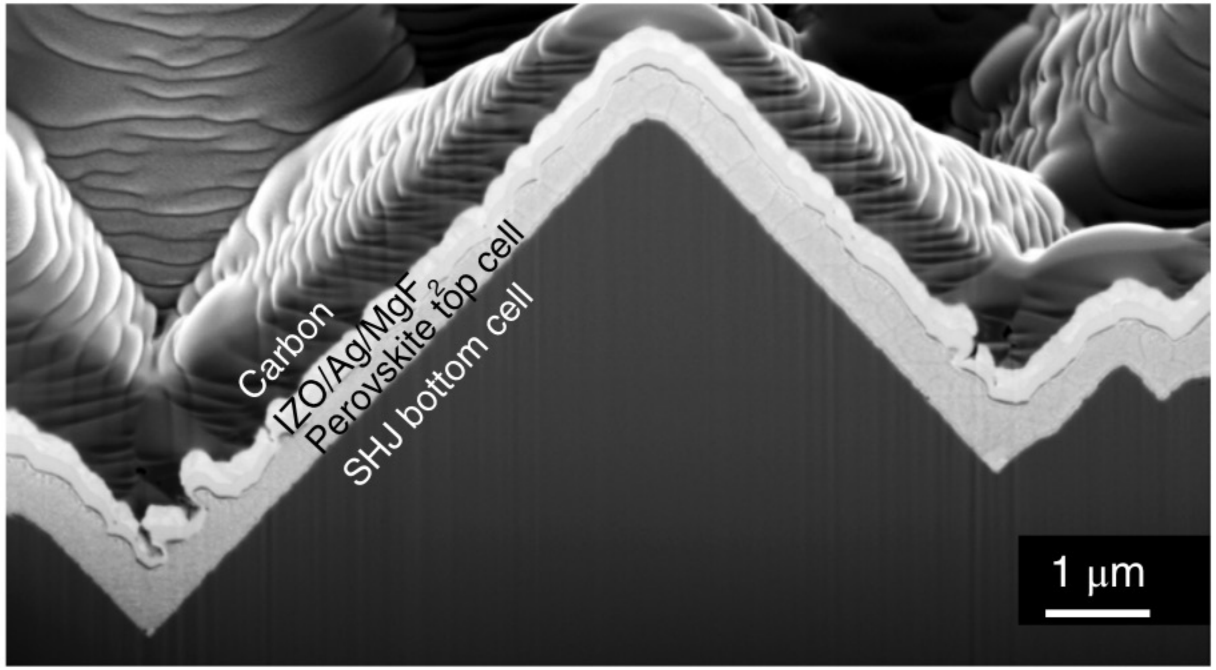
Interface 2: between epoxy and Si cell (pyramids)

Interface 3: textured back of Si cell (pyramids)

Extremely not to scale! Epoxy/glass is orders of magnitude thicker than GaAs/GaInP!

10. Conformal perovskite on pyramidal Si texture

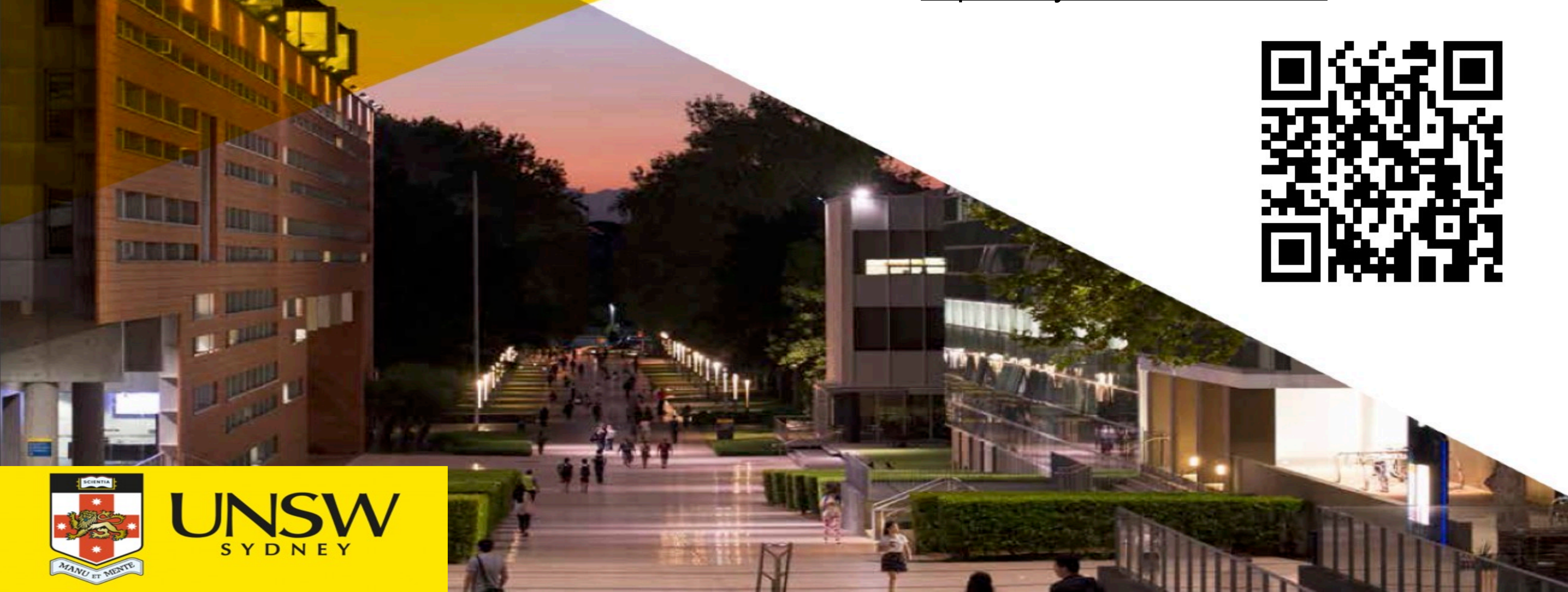




Thank you!

We would really appreciate your feedback:

https://tinyurl.com/bdu29k3x



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