Rigorous Coupled Wave Analysis (RCWA) for Optical Simulations of Solar Cells

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Outline

- Motivation behind modeling
- Rigorous Coupled Wave Analysis (RCWA) description
- Results
- Conclusion

Motivation

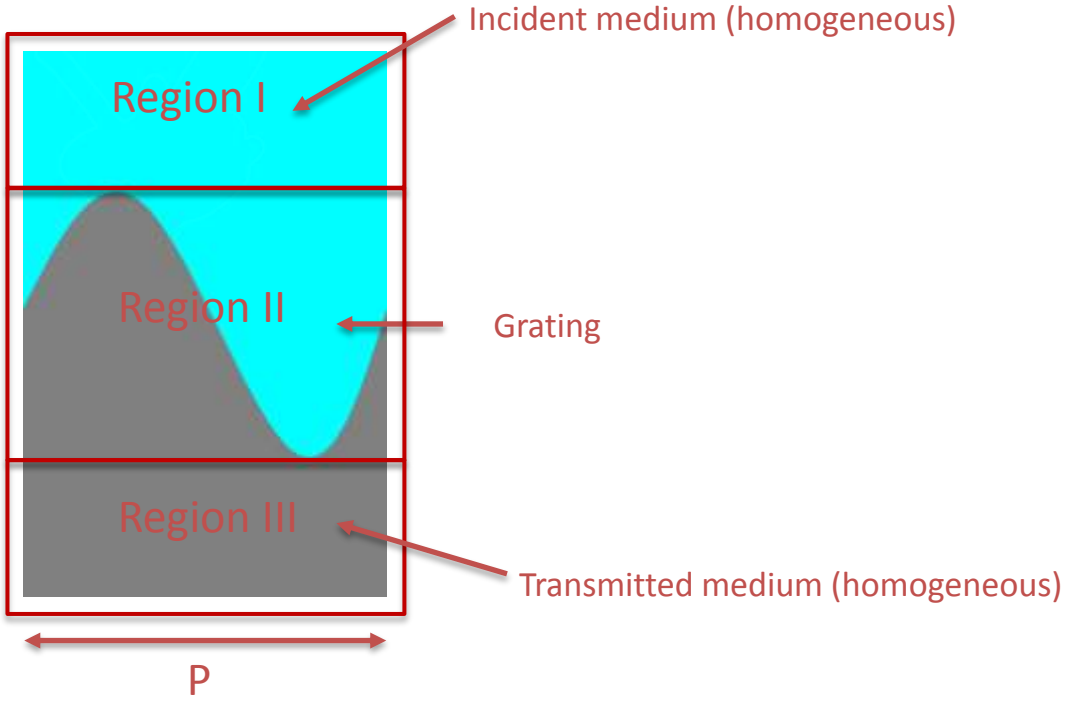
- Optical modeling
  - To design and optimize light management concepts
- Light management
  - To improve absorption → short circuit current → efficiency

Introduction to RCWA

- RCWA is a differential method for solving Maxwell equations.
  - Same category as Modal Method.
  - RCWA is also called Fourier Modal Method (FMM).
- Based on Fourier transform.
- Rigorous method – no approximations for Maxwell equations. But:
  - Limited number of Fourier modes.
  - z-independent dielectric constant ϵ in each layer.

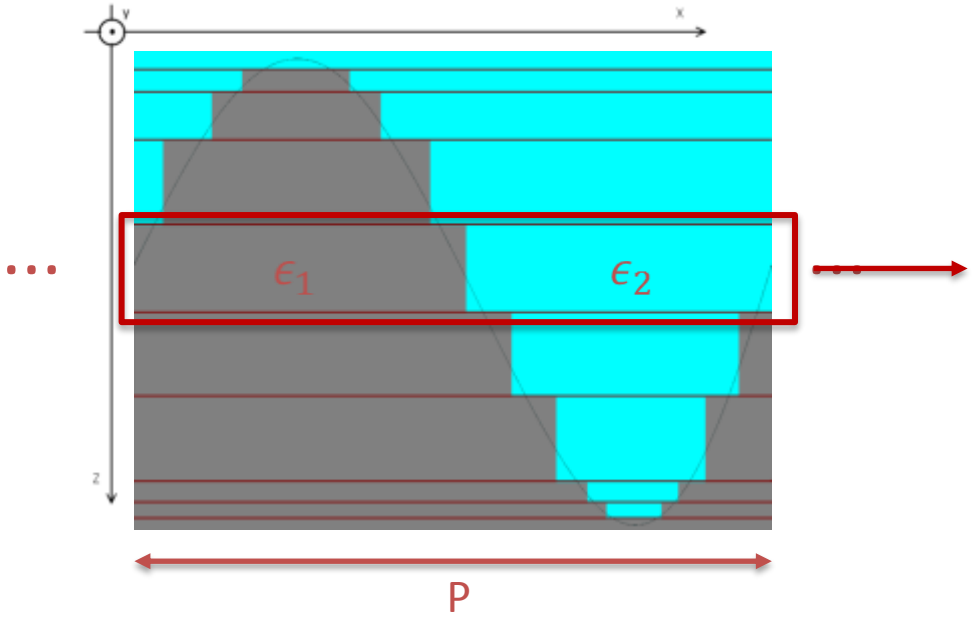
Short description

- Grating structure:
  - Everything that changes is in region II.
  - Region II must have periodic boundary conditions (can be constant).



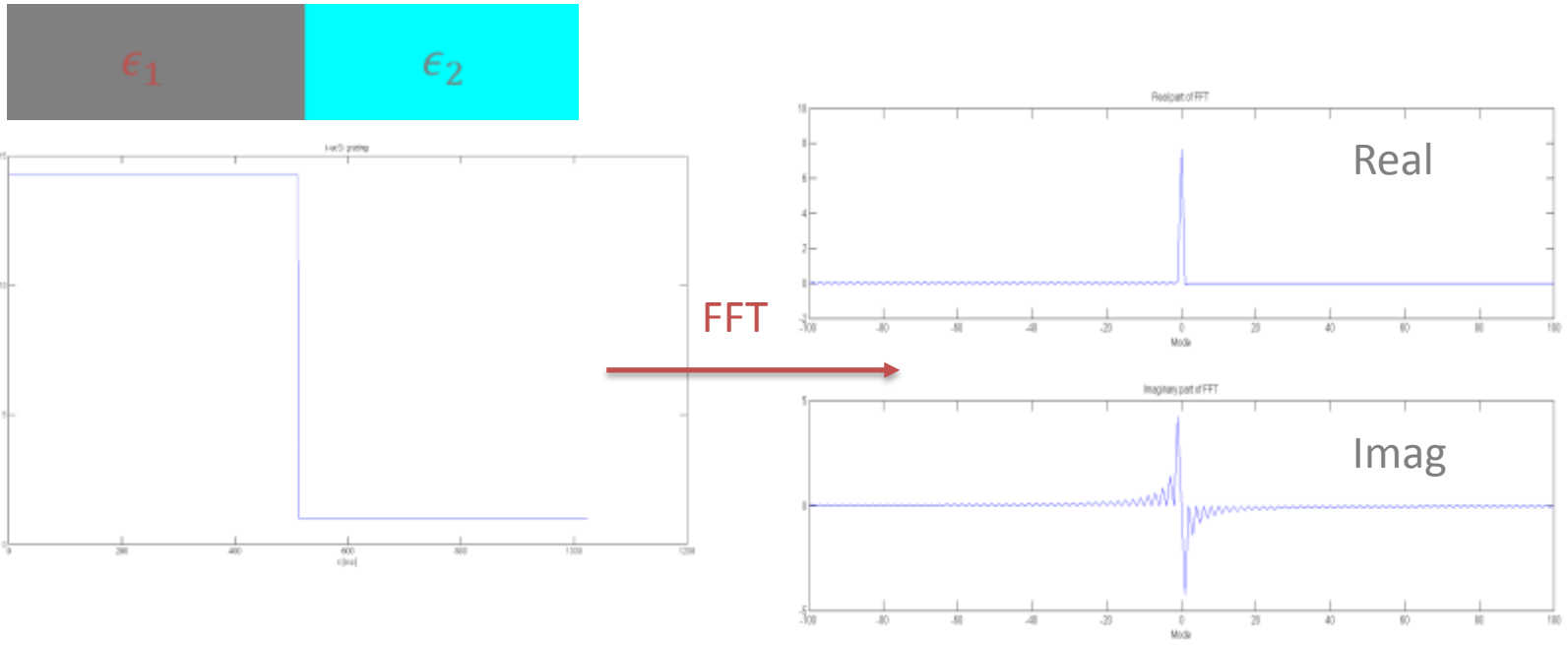
RCWA

- **Grating is sliced to z-independent layers:**
  - This enables Fourier transform of dielectric constant $\epsilon(x)$



RCWA

- Grating is sliced to z-independent layers.
- **FFT of dielectric constant $\epsilon(x)$:**



RCWA

- Grating is sliced to z-independent layers.
- FFT of dielectric constant $\epsilon(x)$.
- **Diffraction modes are calculated:**
  - Floquet function: $\boldsymbol{k}(x+P) = \boldsymbol{k}(x)$
  - Arbitrary number of modes.
    - Recommended to have at least all R and T modes.
    - Improved accuracy with additional modes.

$$k_{xi} = k_0\left(n_I \sin(\phi_{inc}) - m\frac{\lambda}{P}\right)$$

$$k_0 = \frac{2\pi}{\lambda}$$

RCWA

- Grating is sliced to z-independent layers.
- FFT of dielectric constant $\epsilon(x)$.
- Diffraction modes are calculated.
- **TE/TM equations are solved:**
  - Equation is $\frac{\partial^2 S}{\partial z^2} = AS$; for each layer.
  - $A = \frac{k_x^2}{k_0^2} - E$; for TE
  - $A = IE^{-1}\left(\frac{k_x}{k_0}E^{-1}\frac{k_x}{k_0} - I\right)$; for TM
  - Eigenvalues and eigenvectors of the matrix A for each layer.

TE => Electric field E_y

TM => Magnetic field H_y

Toeliptz matrix of Fourier transforms of ϵ

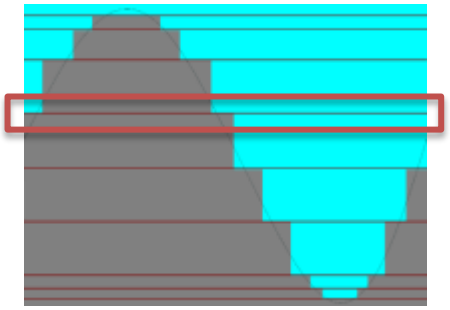
Toeliptz matrix of Fourier transforms of $\frac{1}{\epsilon}$

TM case started with incorrect factorization:

$$A_y = E\left(\frac{k_x}{k_0}IE\frac{k_x}{k_0} - I\right)$$

RCWA

- Grating is sliced to z-independent layers.
- FFT of dielectric constant $\epsilon(x)$.
- Diffraction modes are calculated.
- TE/TM equations are solved.
- **Boundary conditions:**
  - Matching of electric and magnetic fields on layer boundaries.



$$\begin{bmatrix} WX & W \\ VX & -V \end{bmatrix}_{L-1} \begin{bmatrix} c_{L-1}^{+} \\ c_{L-1}^{-} \end{bmatrix} = \begin{bmatrix} W & WX \\ V & -VX \end{bmatrix}_{L} \begin{bmatrix} c_{L}^{+} \\ c_{L}^{-} \end{bmatrix}$$

Similar for incident – first grating layer and last grating layer – outgoing.

Results

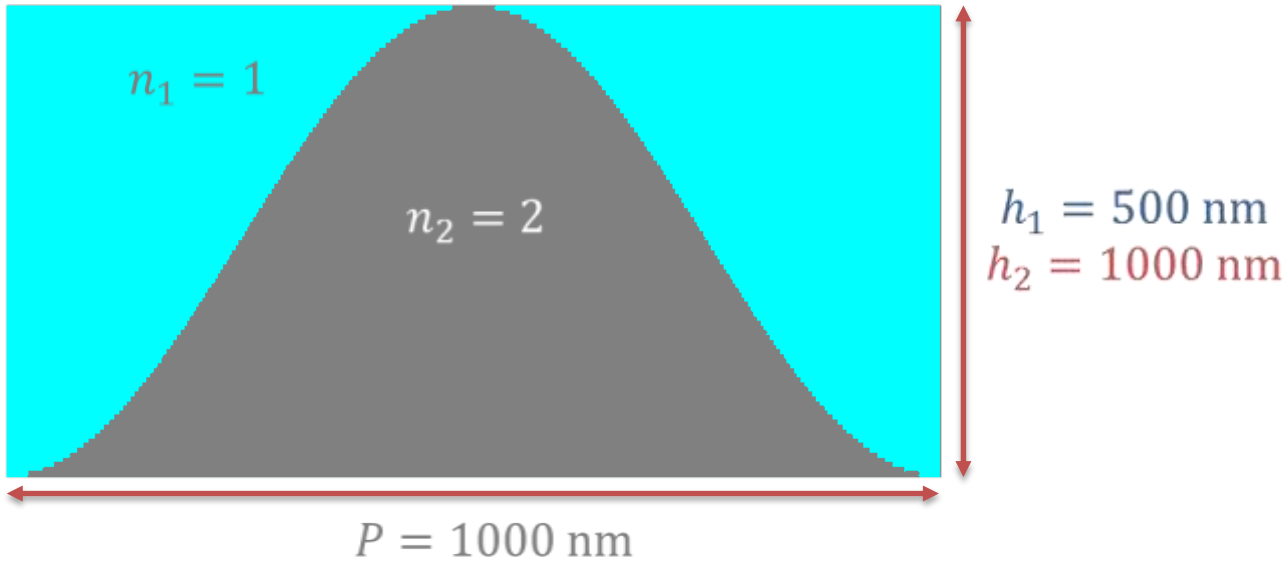
Sinusoidal grating

Comparison with FEM

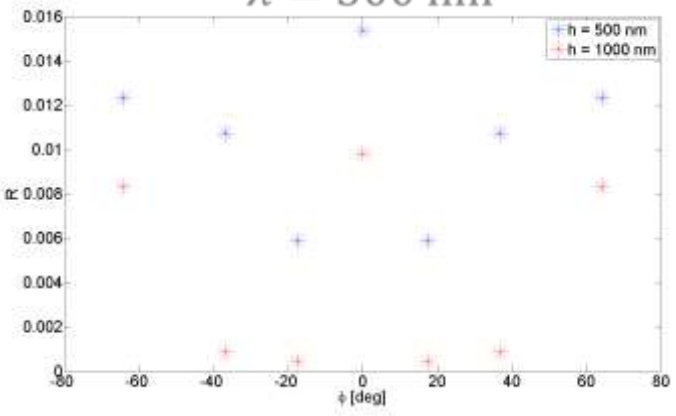
Simulation speed

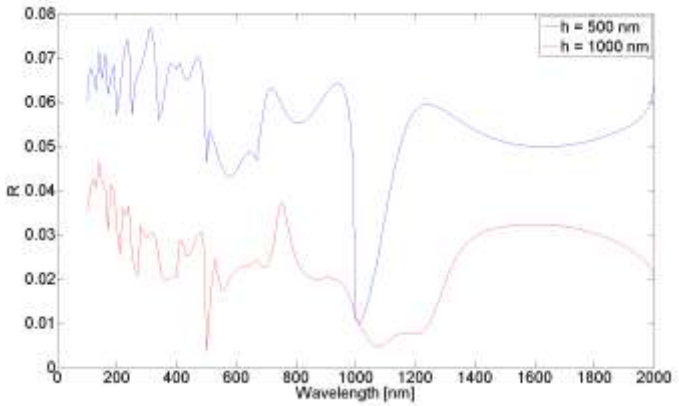
Sinusoidal grating

- 100 layers
- 50 modes



$\lambda = 300$ nm

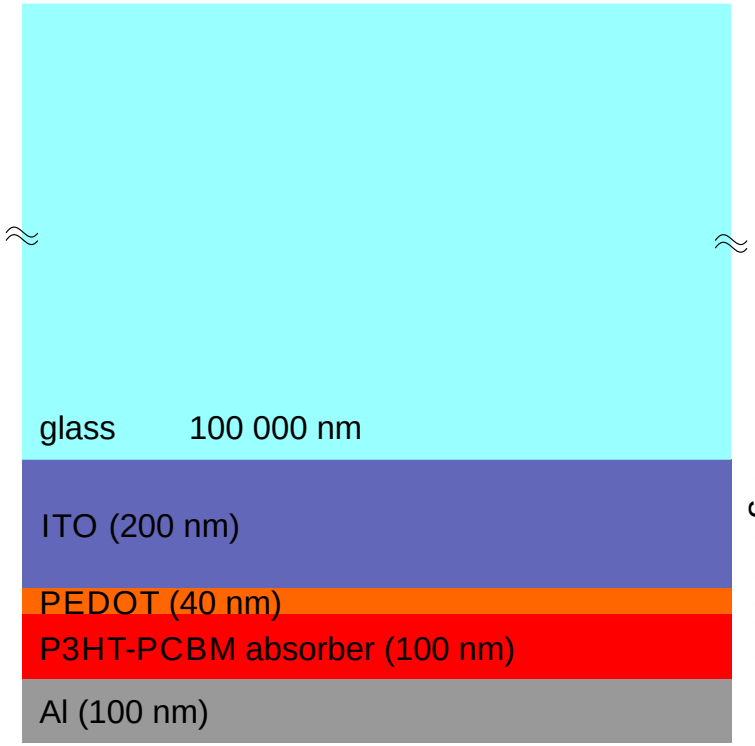


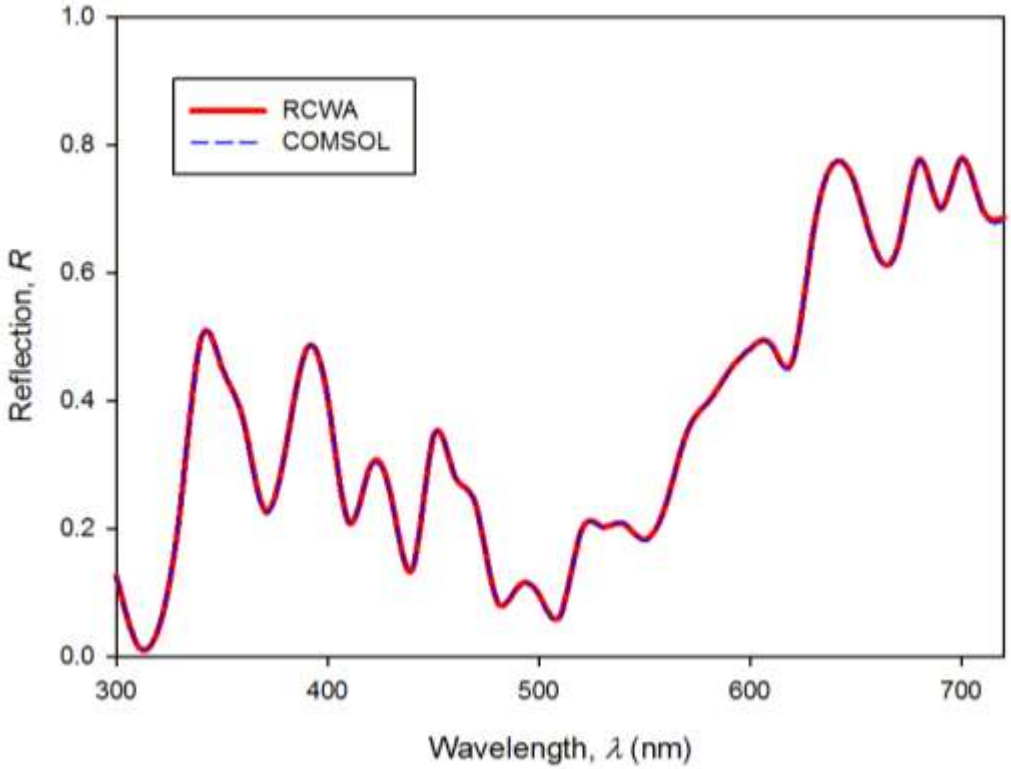


Comparison with FEM

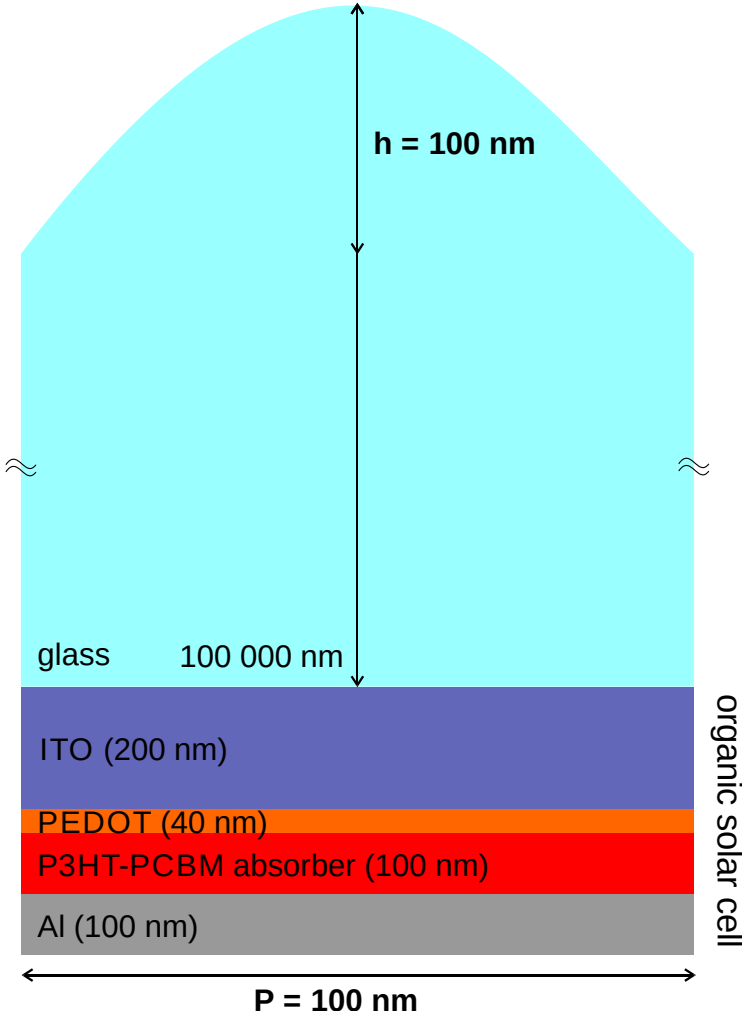
- COMSOL (commercial; FEM – finite elements method)
  - Rigorous
  - Applicable for small gratings – large take a lot of time and memory.
- Comparison done on an organic solar cell.
  - Glass thickness reduced to $0.1\ \mathrm{mm}$ instead of $1.1\ \mathrm{mm}$ because of COMSOL limitations
  - R instead of absorption, as my code for absorption of each layer does not work properly.
  - Varying texture on the top of the grating.
    - Flat, parabolic and triangular
    - Different P and h

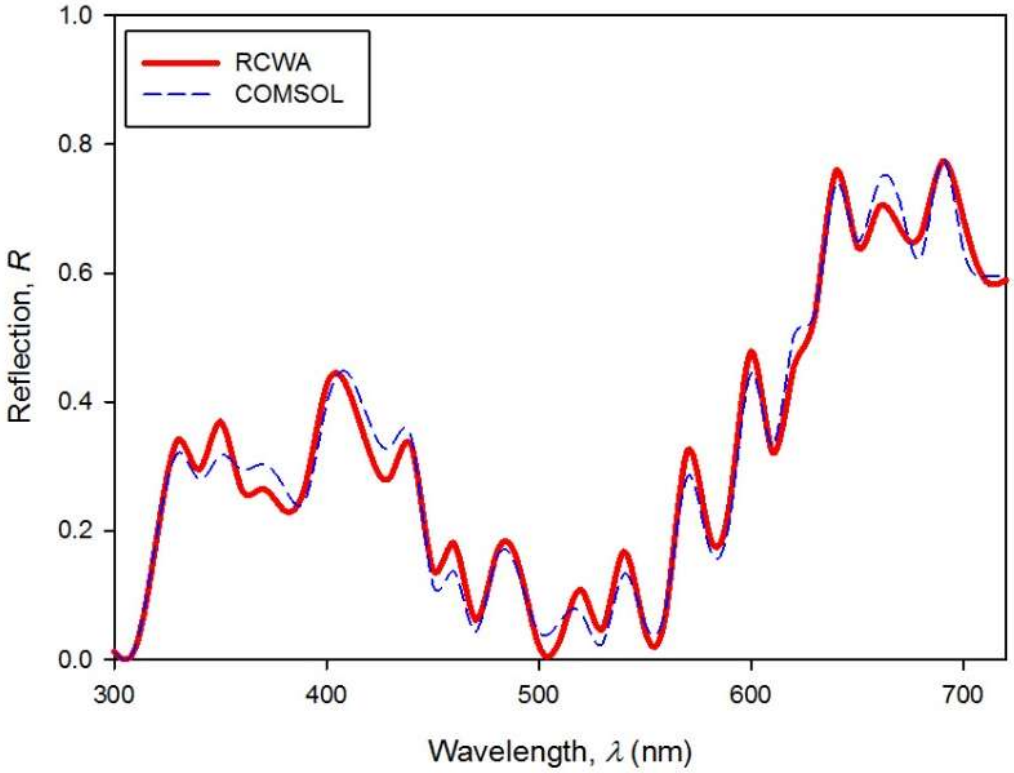
flat


glass 100 000 nm
ITO (200 nm)
PEDOT (40 nm)
P3HT-PCBM absorber (100 nm)
Al (100 nm)
organic solar cell

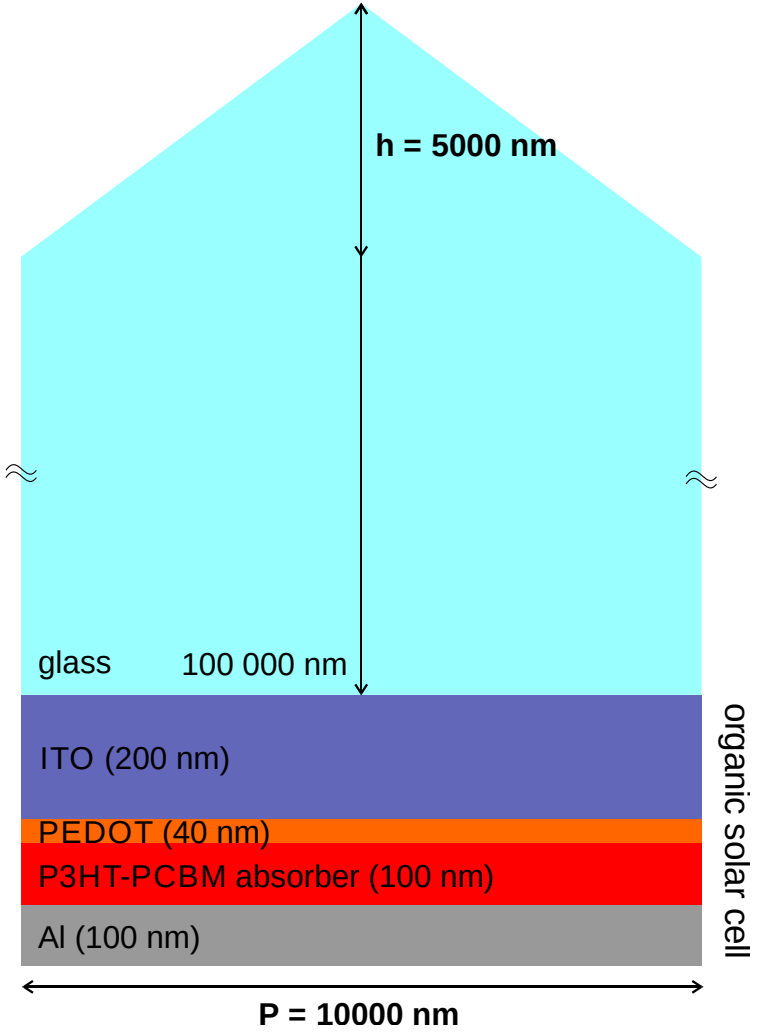

RCWA
COMSOL
Reflection, R
Wavelength, λ (nm)
1.0
0.8
0.6
0.4
0.2
0.0
300
400
500
600
700

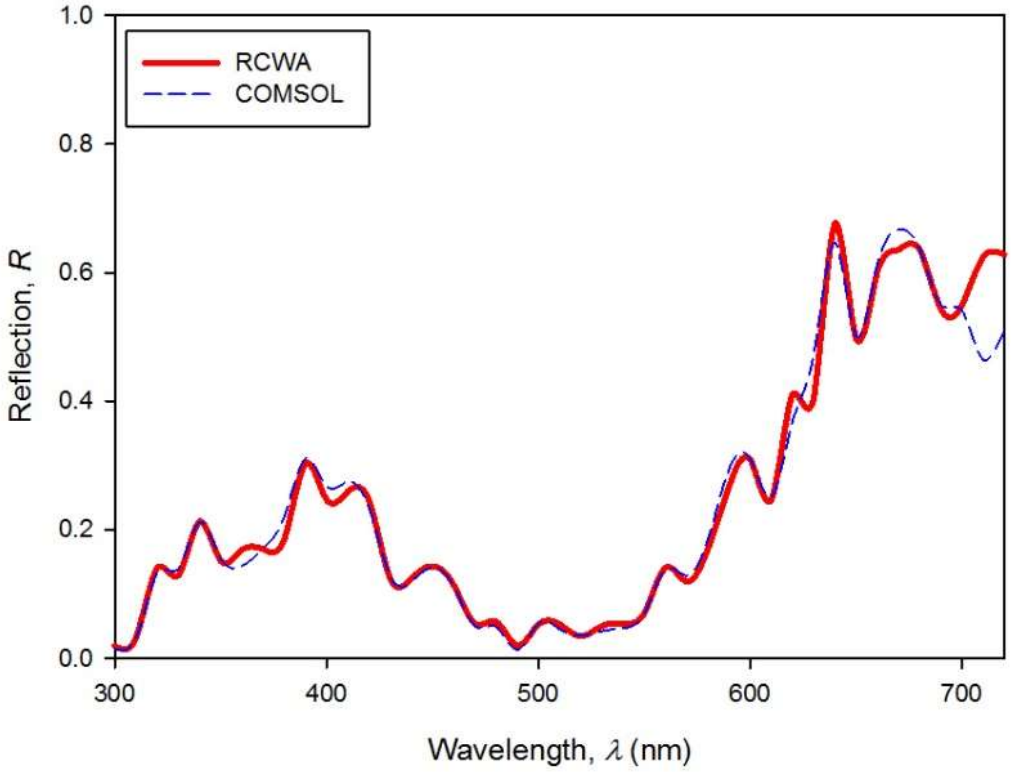
nm period, parabolic texture



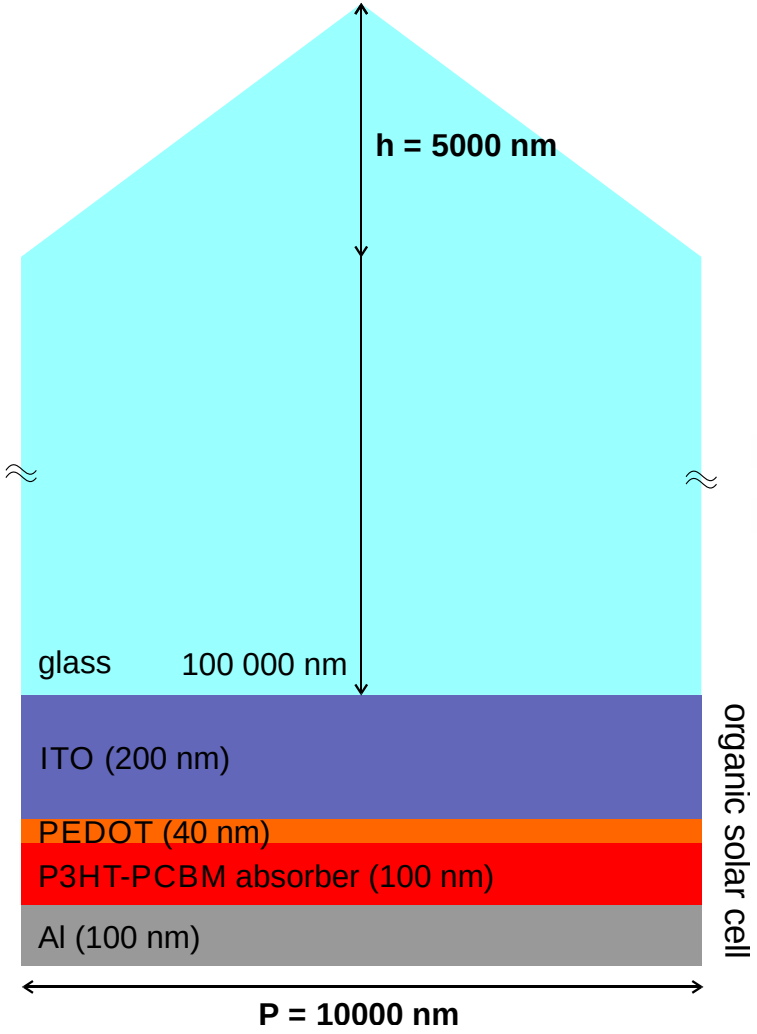


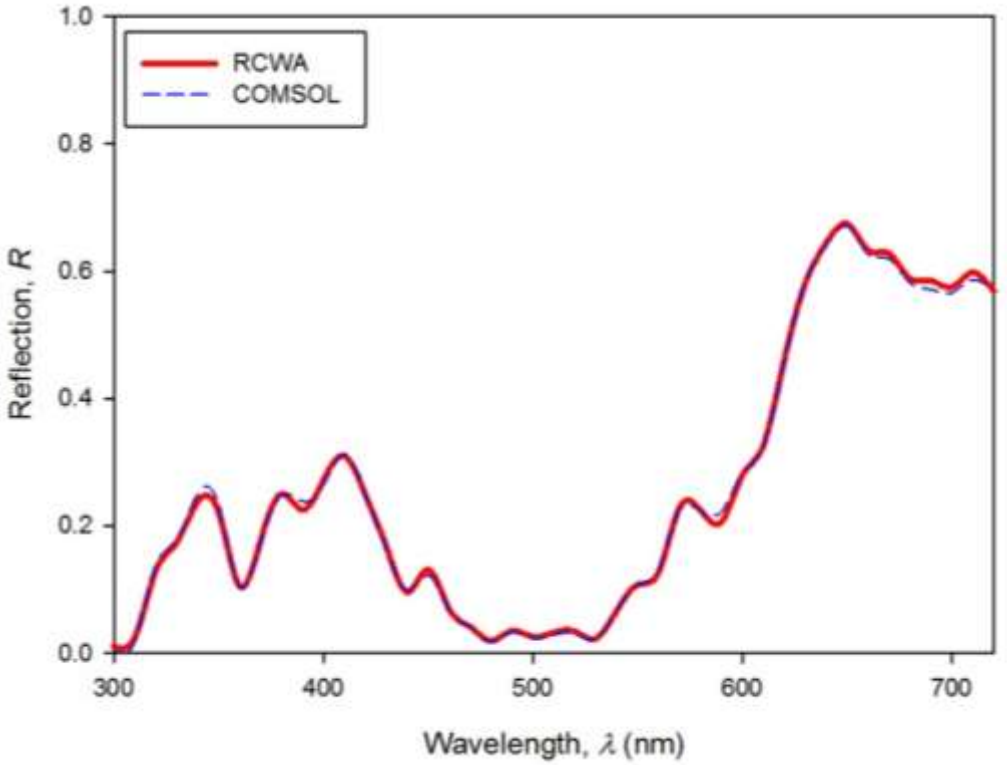
μm period, triangular texture





μm period, triangular texture, TM





Simulation speed

- RCWA
  - 50 modes (except flat)
  - 100 texture layers (except flat)

	RCWA	COMSOL
Flat	10 s	6 min
$P = 100$ nm	5 min	30 min
$P = 1$ μm	5 min	1 h
$P = 10$ μm	5 min	10 h

Conclusion

- RCWA shows good matching with FEM.
  - Differences disappear with denser FEM mesh and more RCWA modes.
- RCWA advantages:
  - Speed (for similar precision).
  - Works with all scales.
- RCWA disadvantages
  - Unstable matrix calculation in some cases.
  - Poor for deep and overhanging metallic gratings.