COMSOL
CONFERENCE
SEOUL*2013*

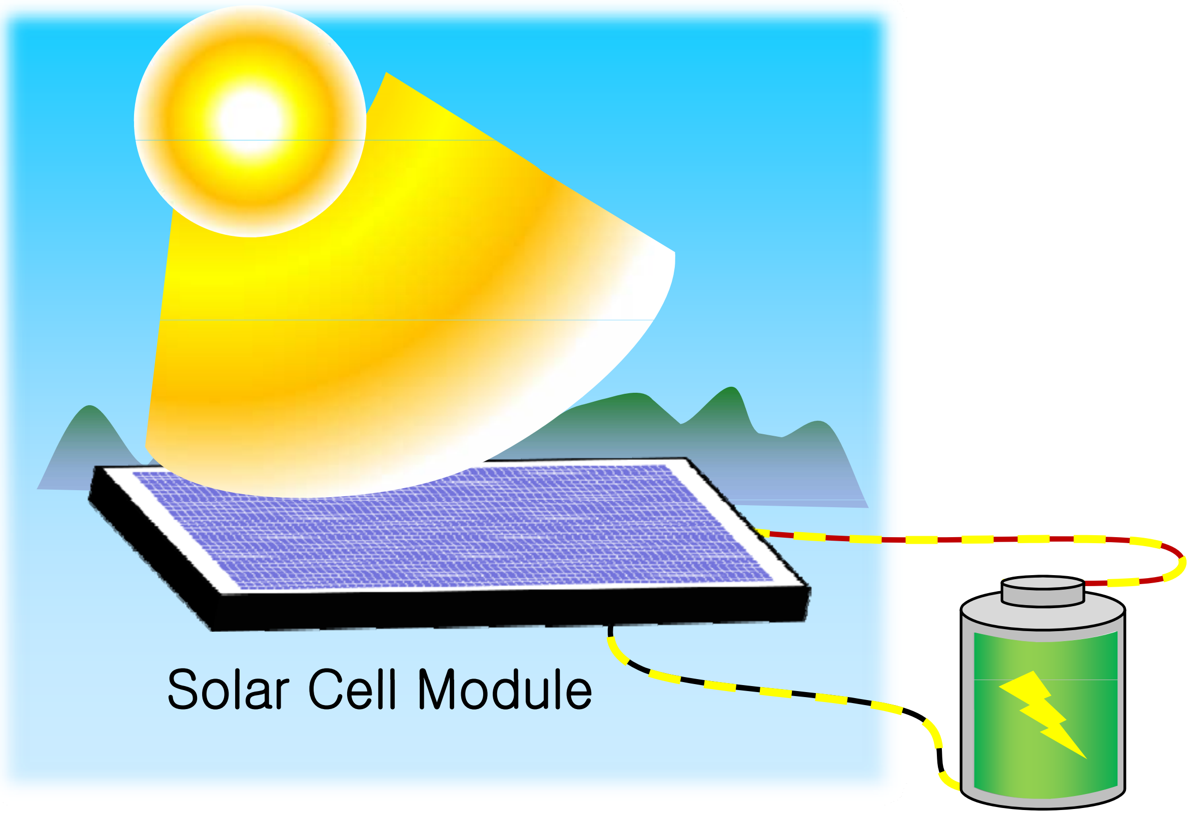
Optical Modeling of Organic Solar Cells Using the COMSOL

Kyung Hee University

Jungho Kim

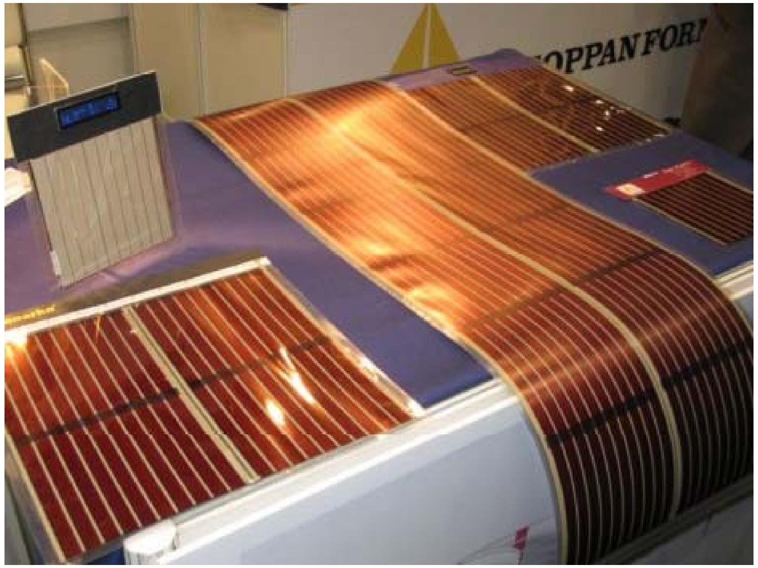
What is a solar cell?

- To generate electrical power converted from the sunlight
- Cost effective and pollution-free solutions to energy shortage problems
- To achieve sufficient power-conversion efficiency



Organic solar cells (OSCs)

- Advantages
  - Low-cost and easy processing
    * Printable OSCs
  - Versatile uses and applications
    * Flexible OSCs

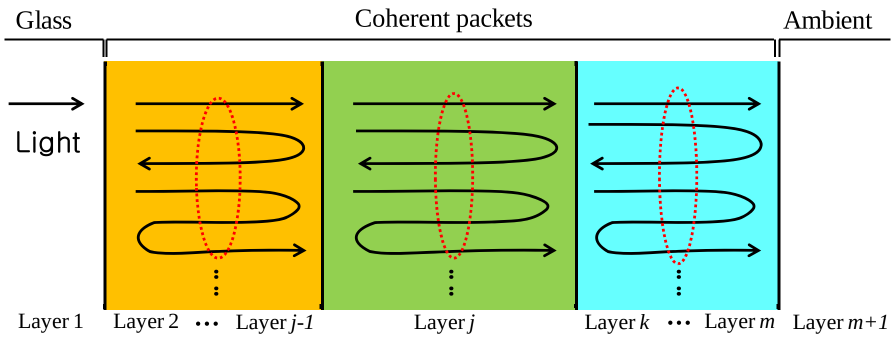


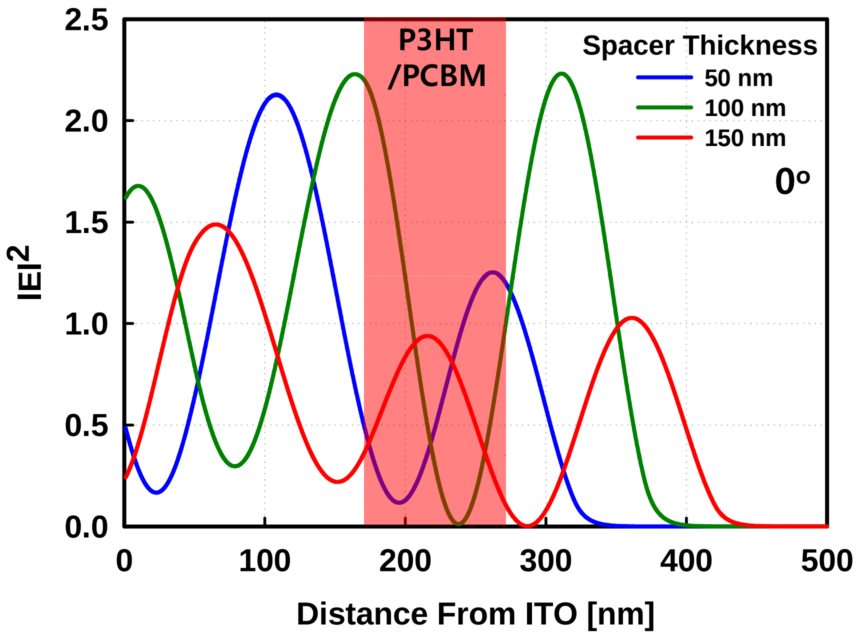
http://cdn.ubergizmo.com/photos/2009/2/ konarka-solar.jpg

- Challenges
  - Low efficiency (10.6%)
  - Short device lifetime

http://evworld.com/press/konarka_solarcanopy.jpg

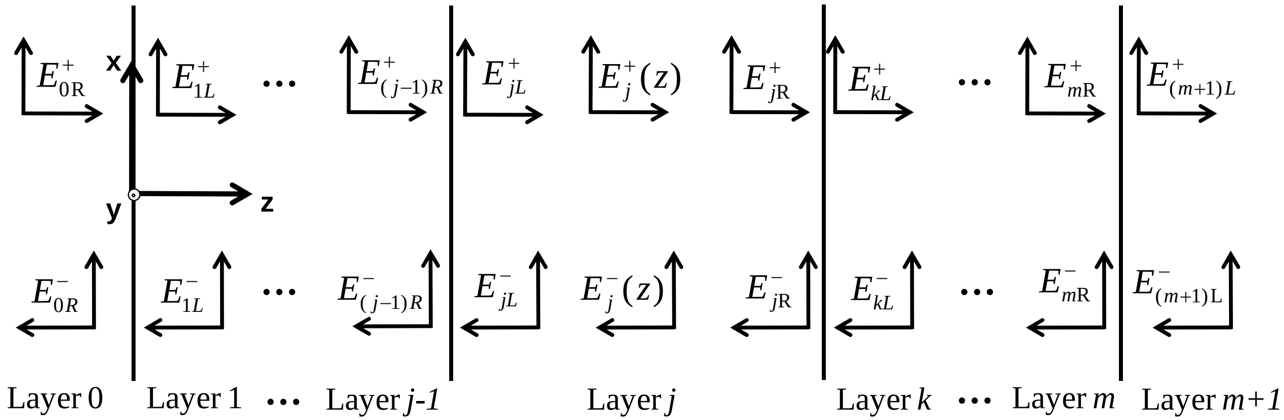
Optical interference effect on thin-film OSCs





- Due to the optical reflection at each interface, optical interference effect occurs between the forward- and backward-propagating waves.
- The spatial distribution of the electromagnetic field depends on the optical interference effect.
- Optical modeling is important to improve the absorption efficiency of thin-film OSCs due to optical interference effect.

Analytical model: the transfer matrix method



$$\mathbf{I}^{j/k} = \frac{1}{t_{j,k}} \begin{bmatrix} 1 & r_{j,k} \\ r_{j,k} & 1 \end{bmatrix}$$

$$\mathbf{L}^{j}(d_j) = \begin{bmatrix} e^{-i\beta_j d_j} & 0 \\ 0 & e^{i\beta_j d_j} \end{bmatrix}$$

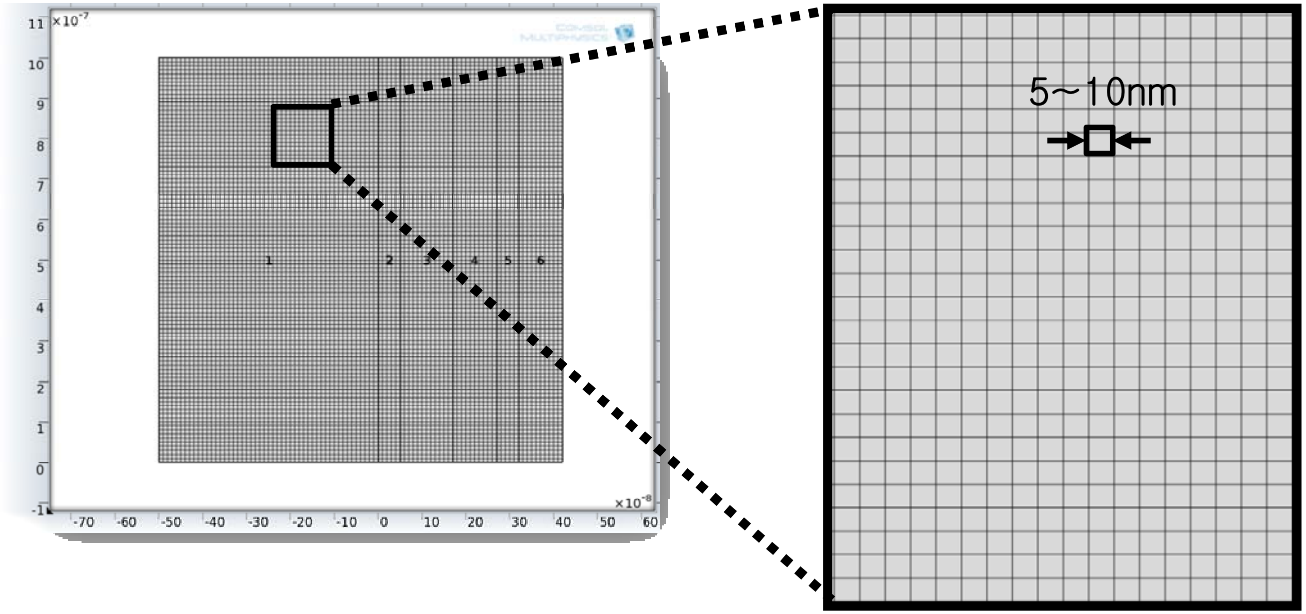
$$\begin{bmatrix} E_{0R}^{+} \\ E_{0R}^{-} \end{bmatrix} = \mathbf{S}^{1/(m+1)} \begin{bmatrix} E_{(m+1)L}^{+} \\ E_{(m+1)L}^{-} \end{bmatrix} = \begin{bmatrix} S_{11}^{1/(m+1)} & S_{12}^{1/(m+1)} \\ S_{21}^{1/(m+1)} & S_{22}^{1/(m+1)} \end{bmatrix} \begin{bmatrix} E_{(m+1)L}^{+} \\ E_{(m+1)L}^{-} \end{bmatrix} = \mathbf{I}^{1/2}\mathbf{L}^{2}\mathbf{I}^{2/3}\cdots\mathbf{L}^{m}\mathbf{I}^{m(m+1)} \begin{bmatrix} E_{(m+1)L}^{+} \\ E_{(m+1)L}^{-} \end{bmatrix}$$

- The light propagation within thin films can be described by means of the interface matrix (*I*) and the layer matrix (*L*).
- The optical electric field at any position in the j-th layer can be calculated based on the combination of the matrix.

L. A. A. Pettersson, L. S. Roman, and O. Inganäs, J. Appl. Phys. **86,** 487 (1999).

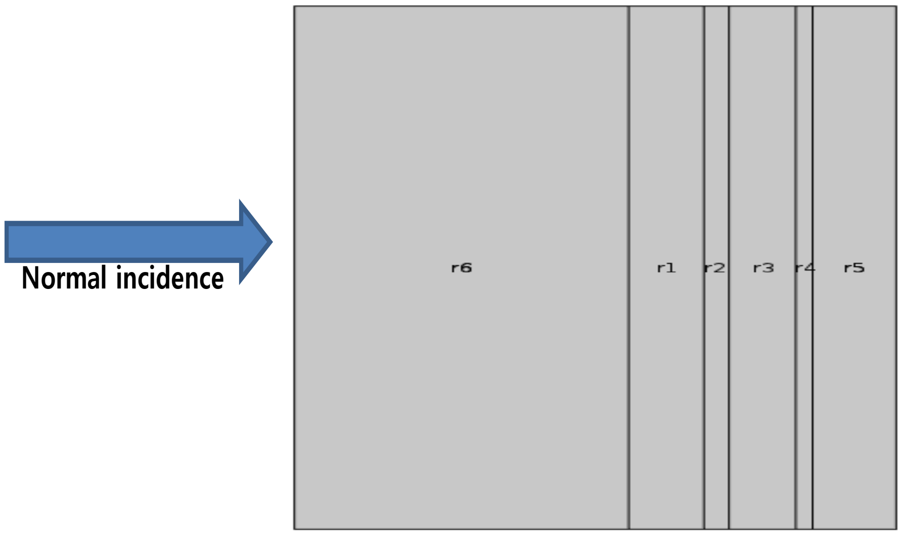
Numerical model: the finite element method

$$\nabla^2 \vec{E} + k^2 \vec{E} = 0$$



- Finite element method (FEM) directly solves the Maxwell's equations.
- The system is divided into meshes of 5~10 nm boundary length.
- The commercial product COMSOL™ is used for simulation.

OSC device structure for optical modeling

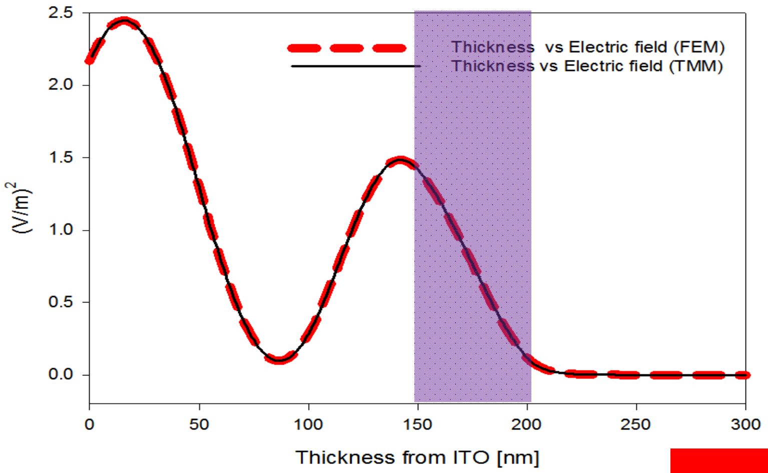


Material	Thickness
Glass	400 nm
ITO	50 nm
PEDOT:PSS	50 nm
P3HT:PCBM	50 nm
Spacer	50 nm
Al	100 nm

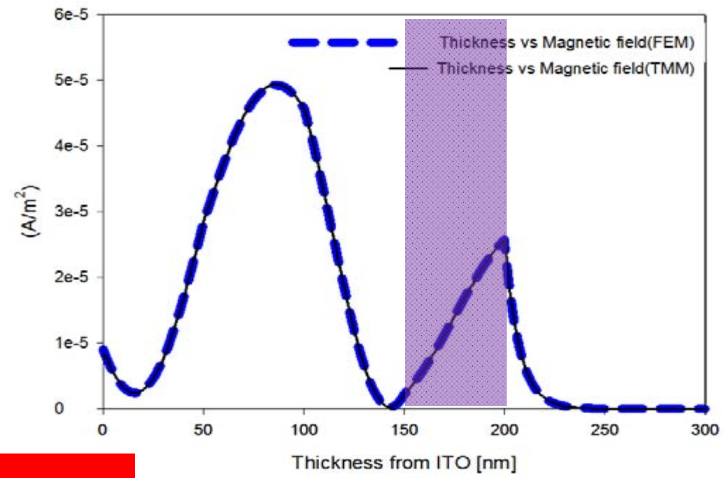
- Thin multi-layered structure leads to the optical interference effect in each layer.
- The optical spacer layer, having very high electrical conductivity and no optical absorption coefficient, adjusts the optical field distribution in the OSC.

Comparison of the calculated results between the TMM and the FEM

Electric field distribution

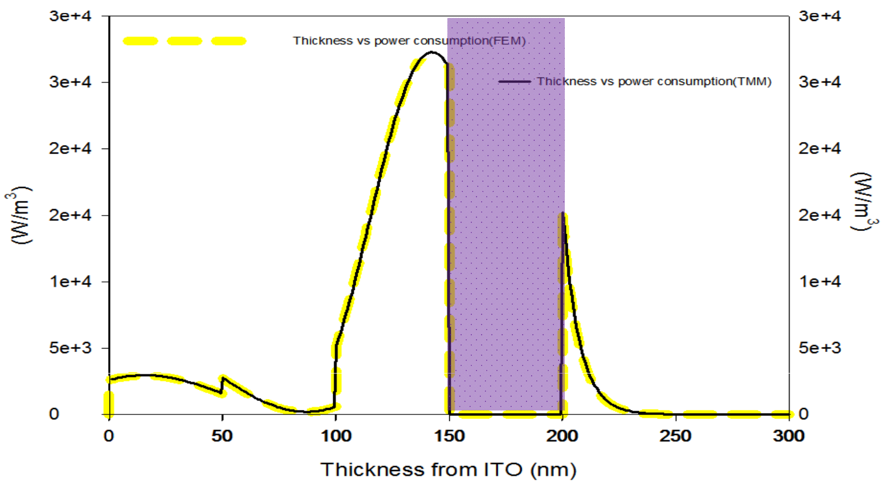


Magnetic field Distribution

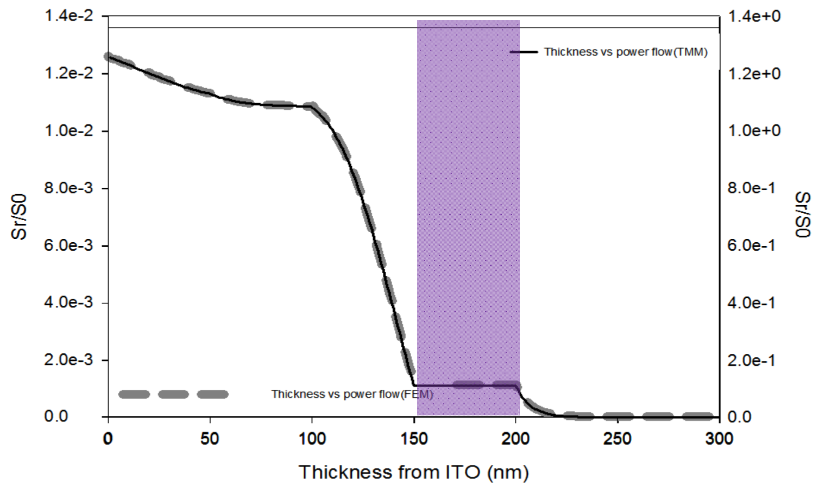


Matched!

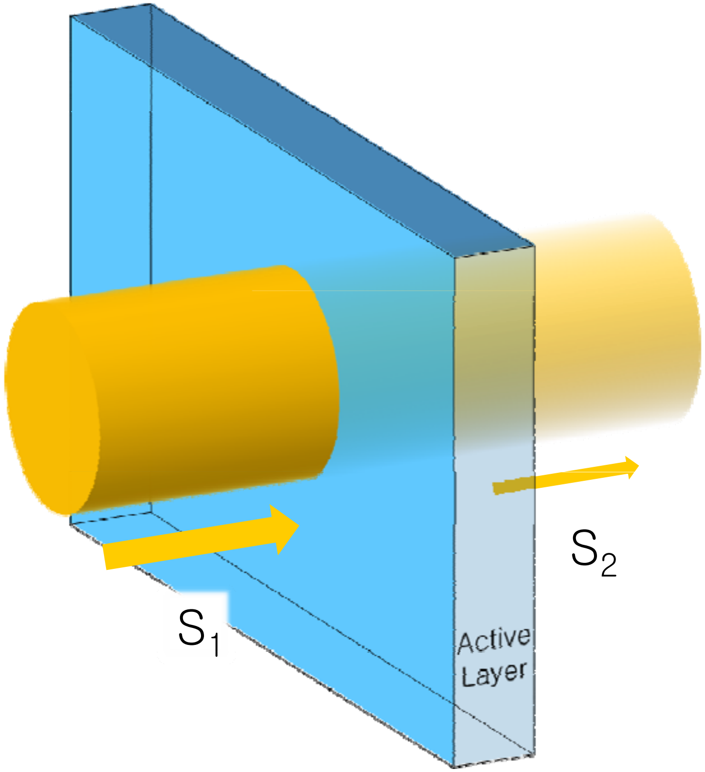
Power consumption



Power flow



Key parameters related with absorptivity



- Time-average Poynting vector

$$\bar{\mathbf{S}} = \frac{1}{2}\mathrm{Re}\left(\mathbf{E}\times\mathbf{H}^*\right)$$ - power flow

- Power dissipation

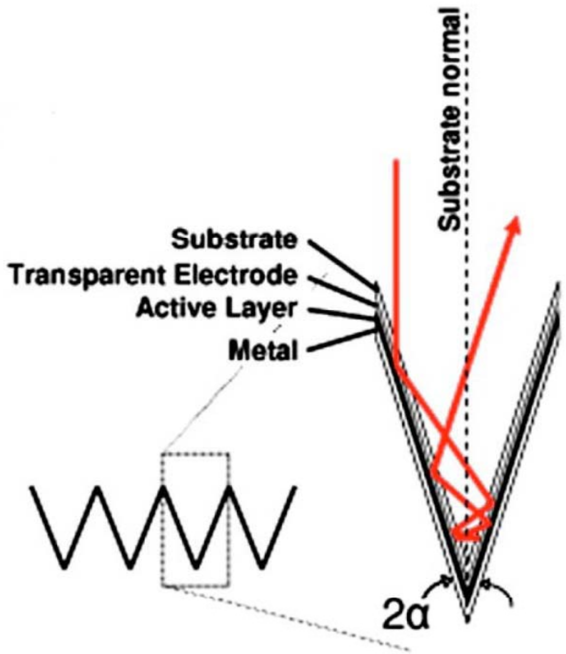
$$Q_z = -\frac{dS_z}{dz} = \frac{1}{2}c\varepsilon_0 n_j \alpha_j \left|E_y\right|^2$$

- optical power absorbed by the material

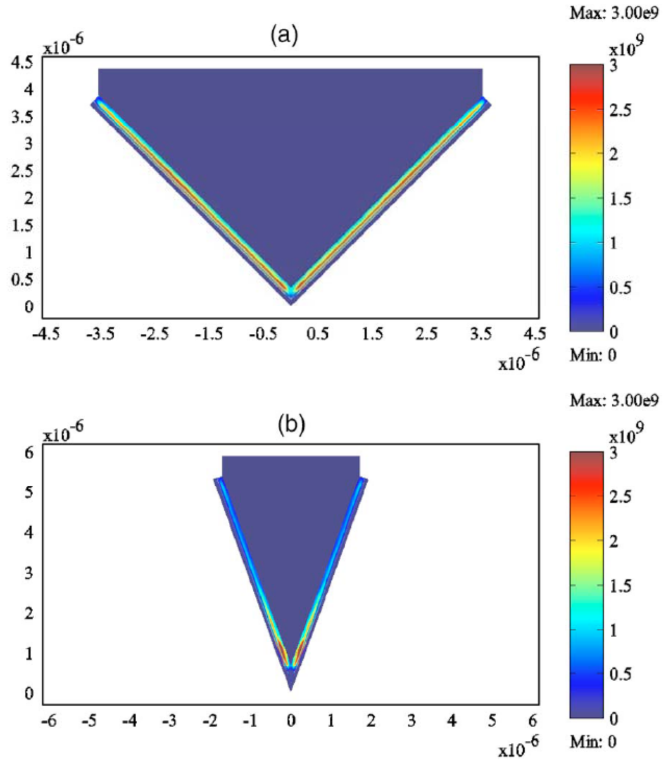
- Absorptivity at the active layer

$$A_z = \int_{z_1}^{z_2} Q_z dz = \frac{\bar{\mathbf{S}}_1 - \bar{\mathbf{S}}_2}{\bar{\mathbf{S}}_{input}}$$

Shaped-substrate OSCs for light trapping



S.-B. Rim *et al*., Appl. Phys. Lett. **91**, 243501 (2007).

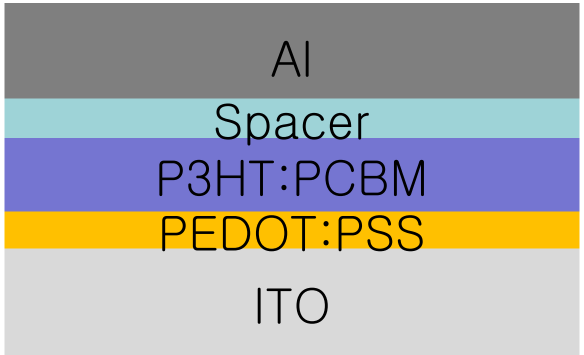


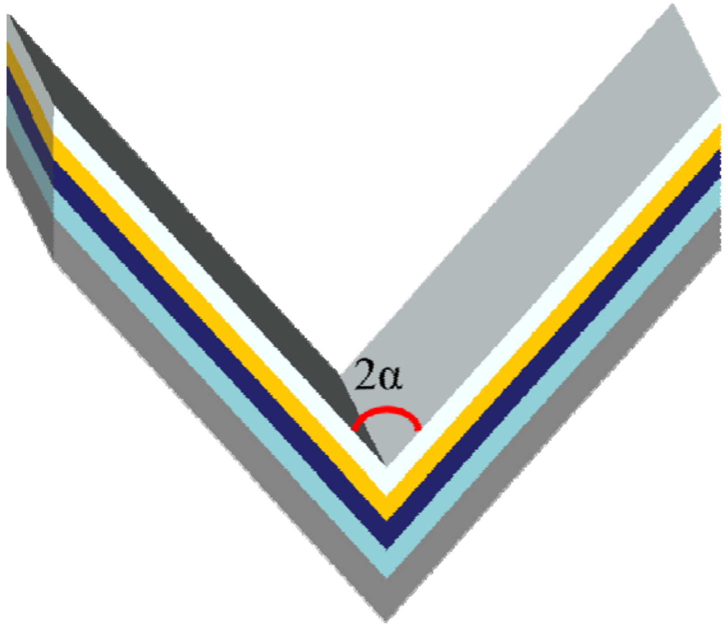
V. Andersson *et al*., J. Appl. Phys. **103**, 094520 (2008).

- Folded OSCs can increase light trapping and the external quantum efficiency.
- This analysis is very important for developing flexible or wearable OSCs.

Device structure for V-shaped OSCs

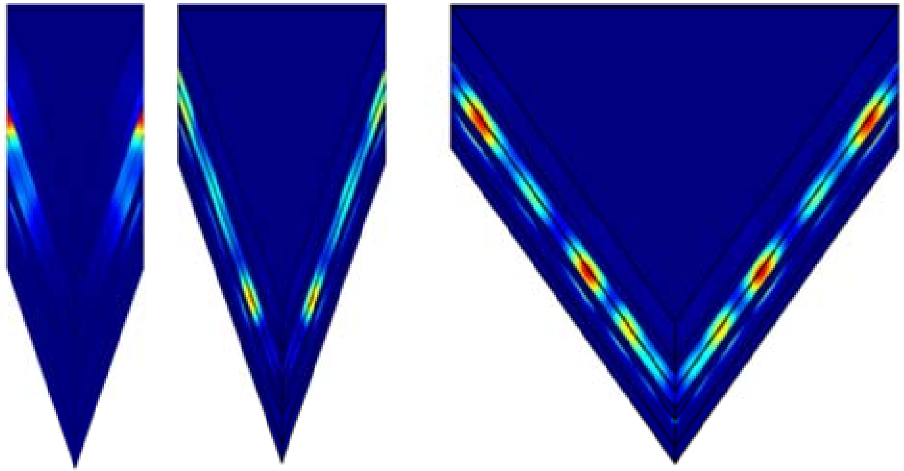
Device structure



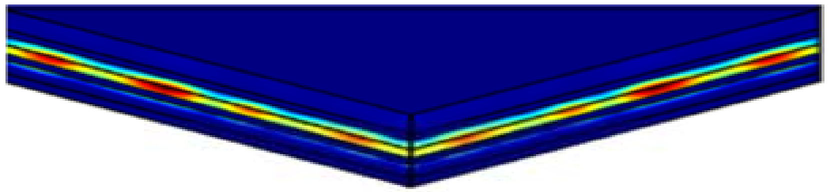


- Device structure: ITO (90nm)/PEDOT:PSS (30nm)/ P3HT:PCBM (80nm)/spacer (x nm)/Al (100nm)
- Effect of thickness of the active and spacer layers on the light trapping effect is investigated.

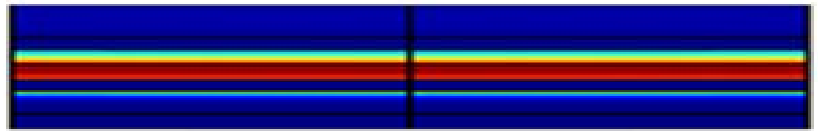
Calculated power dissipation vs. folding angle



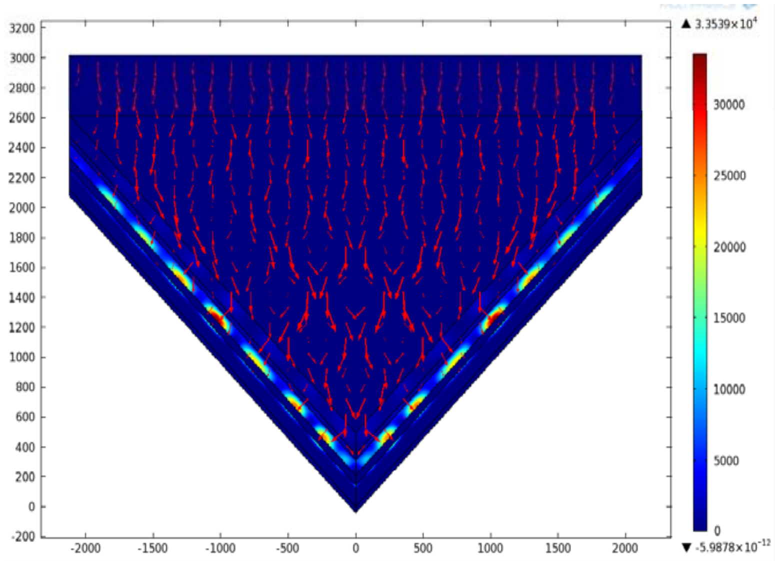
α = 10° α = 30° α = 50°



α = 70°

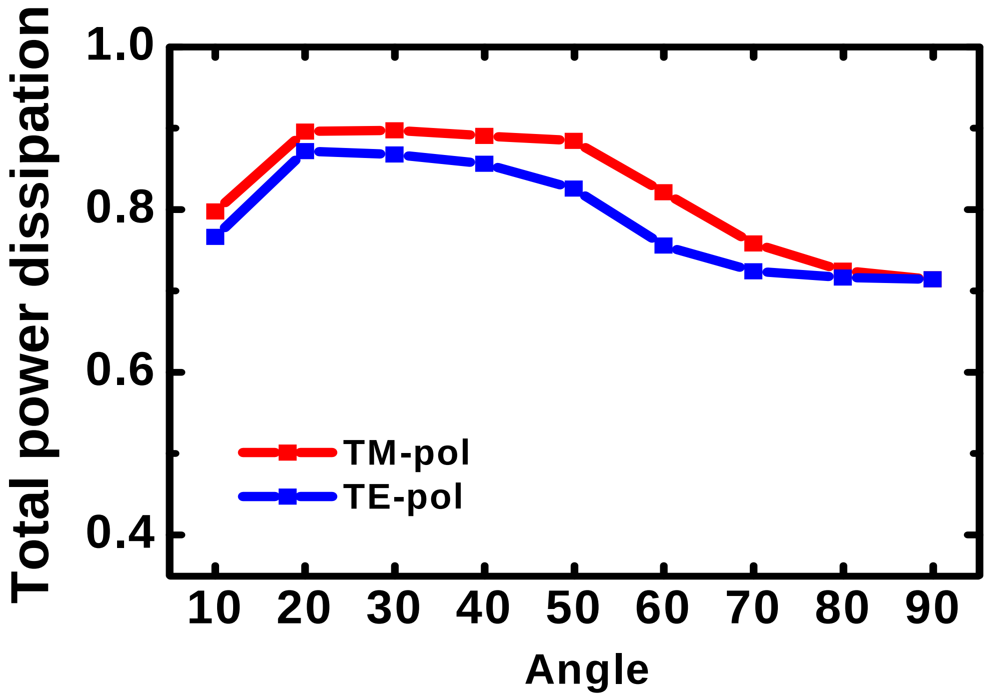


α = 90°



- High power dissipation near the tip of the V-shaped OSC results in the enlarged light trapping at that position.

Calculated power dissipation vs. polarization



- The power dissipation at the small folding angles (α=20°~50°) is higher than that of the planar cell (α=90°).
- TM-polarized light shows the better performance improvement in the V-shaped OSC than TE-polarized light.

Summary

- Optical modeling of OSCs is very important due to the optical interference effect in thin-film multilayers.

- The validity of the calculated results based on the FEM (COMSOL) is demonstrated in OSCs comparison with those obtained by the TMM.

- The optical absorption property of the V-shaped OSC is calculated and analyzed based on the FEM (COMSOL) in terms of the polarization dependency.