How to Simulate and Optimize Solar Cells

Lumerical Solutions, Inc.
Outline

- Introduction
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- Simulation methodology
- Examples
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  - Plasmonic solar cells
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- Demonstration
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- Simulation tips
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Introduction

Solar cells and efficiency trends

How much electrical energy can be extracted from optical energy?

\[ P_m = J_m V_m \]

\[ \eta = \frac{J_m V_m}{I_m} \]

Lawrence Kazmerski, National Renewable Energy Laboratory (NREL)
Complicated sub-wavelength patterning is used to enhance the efficiencies.

Simulations are essential to predict the performance of such devices because we cannot obtain accurate results using analytic methods.

Simulations give the opportunity to cheaply and quickly test ideas, optimize designs and solve problems:

- Expensive and time-consuming to build prototypes
- Design optimization is challenging and results are not always intuitive
Combined optical and electrical simulation

Optical Efficiency
FDTD Solutions

Electrical Efficiency
DEVICE

Quantum efficiency and power conversion efficiency
Introduction

What do we want to simulate?

- Quantum efficiency
  - **Optical Efficiency (OE)**: The fraction of photons absorbed in the solar cells
  - **Electrical Efficiency (EE)**: The fraction of electrons that reach the electrode
  - **Quantum Efficiency (QE) = OE*EE**

- We can then calculate the power conversion efficiency
  - We can determine the maximum power point
  - Note that not all the energy in all photons can be collected in a single cell
    - Photons below the bandgap are not collected at all
    - High energy photons are converted to electrons but much of the energy is lost
    - A quantum efficiency of 100% does not mean a power conversion efficiency of 100%!
Introduction

Optical simulation to solve Maxwell’s equations

- Electric and magnetic fields
  \[ \bar{E}(\vec{r}, \lambda), \bar{H}(\vec{r}, \lambda) \]

- Loss/absorption per unit volume at each wavelength
  \[ L(\vec{r}, \lambda) = -\frac{1}{2} \alpha \left| \bar{E}(\vec{r}, \lambda) \right|^2 \text{Im}[\varepsilon(\vec{r}, \lambda)] \]

- Absorption rate per unit volume under solar illumination
  \[ G(\vec{r}) = \int_{AM1.5} N_p(\lambda) \frac{L(\vec{r}, \lambda)}{\frac{1}{2} \text{Re}(\bar{E}^i(\lambda) \times \bar{H}^i(\lambda))} d\lambda \]
  \( N_p \); Incident photon flux density
  \( E^i (H^i) \); Incident electric (magnetic) field

- Optical efficiency
  \[ OE = \frac{\text{Number of absorbed photon}}{\text{Number of incident photon}} = \frac{\int_{V} G(\vec{r}) dV}{\int_{AM1.5} N_p(\lambda) d\lambda \times S} \]
Introduction

Electrical simulation to solve Poisson and Continuity Equation

- Absorption rate per unit volume from the optical simulation is included in the Continuity Equation
  \[ G(\vec{r}) \]
- Solve for the potential, electron and hole density
  \[ \psi(\vec{r}), p(\vec{r}), n(\vec{r}) \]
- Calculate the electrical efficiency
  \[ EE = \frac{\text{Number of electron reaching electrode}}{\text{Number of absorbed photon}} \]
- Calculate the quantum efficiency and J-V curve
  \[ QE = OE \times EE \]
Introduction

Simulation Challenges

- Complicated simulation methodology
  - Complex device geometry with many small wavelength-scale features
  - Broadband
  - Material dispersion
  - Source modeling
  - Optical and electrical simulations
- Large simulations, long simulation times
Introduction

FDTD

- Finite Difference Time Domain (FDTD) is a state-of-the-art method for solving Maxwell’s equations in complex geometries
  - Few inherent approximations = accurate
  - A very general technique that can deal with many types of problems
  - Arbitrarily complex geometries
  - One simulation gives broadband results

- Can be used to study the effects of micro and nanoscale patterning and its impact on the absorption efficiency of the solar cells.
Plasmonic solar cells

Simulaion example of solar cell using FDTD

Moth-eye anti reflection

Methodology for the Optical Simulation
Simulation methodology

- Design parameterization
- Material properties
  - Multi-coefficient model
- Simulation region
  - Boundary condition
- Source modeling
  - Unpolarized light
- Result analysis
  - Optical absorption calculation
Design parameterization

- Parameterize the Solar cells design
  - Create properties appropriate for your device
  - Use the scripted parameterization
Design parameterization

- Parameterization can include position of sources and monitors
- Any group can set properties of the children
Design parameterization

- Essential for
  - Reproducibility
  - Easy parameter sweeps
  - Optimization

- Lumerical’s hierarchical group layout and script based parameterization makes almost anything possible

- It is worth the initial investment!
Material properties – broadband simulations

- Absorption bandwidth of typical solar cell materials is large

![Graph showing solar spectrum with absorption bands for c-Si, GaAs, P3HT:PCBM]  
Sun light spectrum. (AM1.5)

Material properties must be accurately modeled over a broad bandwidth
Material properties – broadband simulations

- Finite Difference Time domain (FDTD) simulation gives broadband result
- Solar cell devices utilize many dispersive materials
  - Well-known frequency domain relationship
  \[
  \vec{D}(\omega) = \varepsilon(\omega)\vec{E}(\omega)
  \]
  - Users can define their own model, or import from experimental data (real and imaginary \(\varepsilon(\omega)\))
  - FDTD is a time domain technique: relationship?
    \[
    \vec{D}(t) = \varepsilon(t) \ast \vec{E}(t) = \int_{0}^{t} \vec{E}(t')\varepsilon(t - t')dt'
    \]
Material properties – broadband simulations

- Common solutions are Lorentz or Drude models
  - Often insufficient for real materials
- Lumerical’s **Multi-Coefficient Model** (MCM) can solve for materials with arbitrary dispersion such as Si, GaAs, P3HT:PCBM, ITO...etc

![Graphs for Si, GaAs, P3HT:PCBM, ITO](images)
Boundary conditions

- In many cases, periodic boundaries can be used

- e.g. 2D Hexagonal lattice PCOSC

If we can further assume normal incidence, ...
Sources

- Sun light is modeled by a plane wave source.
- Results for incoherent, unpolarized light can be obtained from sum of two orthogonal polarization simulation.

\[
\left\langle |\vec{E}|^2 \right\rangle_{\text{unpolarized}} = \frac{1}{2\pi} \int_{0}^{2\pi} d\alpha |\vec{E}(\alpha)|^2 \\
= \frac{1}{2\pi} \int_{0}^{2\pi} d\alpha |\vec{E}_1 \cos(\alpha) + \vec{E}_2 \sin(\alpha)|^2 \\
= \frac{1}{2} \left( |\vec{E}_1|^2 + |\vec{E}_2|^2 \right)
\]
How do we incorporate the complicated spectrum of sun light into simulation result?

1. Calculate absorption rate as a function of wavelength for a flat spectrum. This is automatically done using CW normalization in FDTD Solutions.

2. Multiply the absorption with the solar spectrum as a post processing step.
Optical absorption calculation (1)

- Planar or sandwiched by lossless material
  - We use 2 planar power monitors.

Script function

\[
\text{transmission} = \frac{1}{2} \int_s \text{real}(P) dS
\]

\[
A(\lambda) = \text{transmission(”top”)} - \text{transmission(”bottom”)}
\]

\[
P_{\text{abs}}(\lambda) = A(\lambda) \times (\text{solar irradiance}) \quad [\text{W/m}^2/\text{nm}]
\]
Optical absorption calculation (2)

- Non planar structure sandwiched by loss material.
  - We use an Analysis group “pabs”
    - Electric field distribution => “field profile monitor”
    - Permittivity distribution => “index monitor”

- Calculate the normalized loss profile per unit volume $p_{abs}[1/m^3]$. 
  \[
  p_{abs}(\vec{r}, \lambda) = \frac{1}{2} \frac{|E(\vec{r}, \lambda)|^2 \text{imag}(\varepsilon(\vec{r}, \lambda))}{P(\lambda)_{\text{FDTD source}}} 
  \]

- Integrate $p_{abs}$ over the absorption region and multiply by the solar irradiance 
  \[
  P_{abs}(\lambda) = \left( \int_V p_{abs}(\vec{r}, \lambda) dV \right) \cdot \text{(solar irradiance)} [W/m^2/nm] 
  \]
Solar cell optical simulation examples
Simulation examples

- Si Plasmonic solar cells

Nano particle (Au, Ag, Cu, ...) on Si


K. R. Catchpole and A. Polman, "Design principles for particle plasmon enhanced solar cells", APL 93, 191113 (2008)
Plasmonic solar cells

Spectral irradiance [W/m²/nm]

Wavelength [nm]

c-Si 300nm < λ < 1100nm

Silicon

Gold

Silver

Aluminum

Materials:

- Silicon
- Gold
- Silver
- Aluminum

Wavelength (microns)

Re(eps)

Im(eps)

FDTD model
Material data

Wavelength (microns)

Wavelength (microns)

Wavelength (microns)

Wavelength (microns)
Plasmonic solar cells

$E(t)$

$|E(\omega)|^2$

Fig. 1 Absorption profile of nano-particle on Si and bare Si surface.
Plasmonic solar cells

- Enhancement of absorption

\[ g(\lambda) = \frac{A_{\text{particle}}(\lambda)}{A_{\text{bare}}(\lambda)} \]
Plasmonic solar cell

- Optimization of 2 parameters, period and diameter.
- FOM = $\frac{OE_{\text{plasmonic}}}{OE_{\text{bare}}}$

Enhancements of 15% are possible.
Organic solar cell with photonic crystal

- 1D PCOSC

- 2D hexagonal lattice PCOSC


Organic solar cell with photonic crystal

- P3HT:PCBM
- PEDOT:PSS
- ITO
- nc_ZnO

Spectral irradiance [W/m²/nm] vs. Wavelength [nm]

P3HT:PCBM: 300nm < λ < 700nm

Graphs showing plots of Re( index) vs. Wavelength (microns) for different layers in the solar cell model.
Organic solar cell with photonic crystal

Absorption of 1D PCOSC

\[ A(\lambda) = \frac{P_{P3HT:PCBM}(\lambda)}{P_{in}(\lambda)} = \frac{\text{Absorbed power in P3HT:PCBM}}{\text{Incident plane wave power}} \]

Leaky (Quasi-waveguide) Modes

Planar Organic Solar Cell (PLOSC)

Absorption vs. wavelength

Absorbed power in P3HT:PCBM

Band-diagram of the 1DPCOSC

ITO (n=1.45) and PEDOT:PSS (n=1.8) => lossless
P=400nm, w=300nm, h=300nm, t=70nm

Leaky (Quasi-waveguide) Modes

Absorbed power in P3HT:PCBM

Absorption vs. wavelength

Absorbed power in P3HT:PCBM

Band-diagram of the 1DPCOSC

Absorbed power in P3HT:PCBM

Absorption vs. wavelength

Absorbed power in P3HT:PCBM

Band-diagram of the 1DPCOSC

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Absorption vs. wavelength

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Band-diagram of the 1DPCOSC

Absorbed power in P3HT:PCBM

Absorption vs. wavelength
Organic solar cell with photonic crystal

P=400nm, w=300nm, h=300nm, t=70nm

Absorption distribution
Parameter sweep demo

- Thickness $t$ from 0.1 to 0.2um
- Measure number of photons absorbed in P3HT:PCBM over 400nm and 700nm
Parameter sweep demo

- Number of absorbed photons as a function of thickness $t$. 

![Resource Configuration Table]

![Job Manager Panel]

![Figure 1: Graph of Number of Absorbed Photons vs. Thickness of ITO]
Concurrent computing

- Optimization and parameter sweep require many simulations
- Send them to many different workstations
  - Each workstation can run in distributed computing mode, using all cores

N computers means you can get your optimization or parameter sweep results N times faster!
Optimization demo

- 4 parameters (P, w, hf, t) optimization
- Figure of Merit (FOM) = \( \frac{OE_{PC}}{OE_{\text{flat}}} \)
  \[ OE_{PC} = \frac{(OE_{PC, TE} + OE_{PC, TM})}{2} \]
Optimization demo

Nearly 15% absorption enhancement
Simulation tips

- Use a coarse mesh (large values of dx)
  - Use conformal meshing
  - Use mesh grading if a fine mesh is required in a particular region
  - Always make any fine mesh simulations the last step!

- Multi-wavelength calculations
  - Check material fits!

- Reduce memory and simulation time
  - Store only necessary data to keep file sizes smaller
  - Remove movie monitors for faster simulations
Tip: Use a coarse mesh

- Memory scales as $dx^3$
- Simulation time scales as $dx^4$
- Example convergence tests from silicon absorption in CMOS image sensors
Tip: Conformal meshing

- Devices can be extremely sensitive to certain dimensions
- Can we define dimensions to better than the mesh size?
  - Yes
  - Conformal meshing

Potential problems with finite sized mesh
Electrical simulation

With some simple assumptions the J-V curve is analytic

- Assume no recombination

\[
J(V) = J_0 (e^{qV/k_BT} - 1) - J_{ph} \approx A \exp\left(\frac{eV - E_g}{kT}\right) - J_{ph}
\]

\[
J_{ph} = e \int \frac{\lambda}{hc} \text{OE} (\lambda) I_{AM1.5}\, d\lambda = \text{charge on electron} \times \text{number of absorbed photon}
\]

\[
A = \frac{e(n^2 + 1)E_g^2kT}{4\pi^2h^3c^2}
\]
Electrical simulation

Beyond simple assumptions to accurate results

- We need to solve Poisson and Continuity Equation numerically

Lumerical DEVICE, coming soon...
http://www.lumerical.com/tcad-products/device/

DEVICE Preview
Optoelectronic TCAD Device Simulator
Preview Webinar  March 6, 2012

DEVICE: Coming March 2012
Powerful semiconductor device simulation for the design, analysis and optimization of silicon-based optoelectronic structures
## Challenges and solutions

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<th>Challenge</th>
<th>Solutions and best practices</th>
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<tr>
<td>Wavelength scale microscopic patterning</td>
<td>Full vectorial 3D Maxwell solver can capture all physical effects</td>
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<tr>
<td>Complex 3D geometries</td>
<td>• Parameterize designs</td>
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<tr>
<td>Simulation time</td>
<td>• 3D simulations are often necessary for realistic results</td>
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<td>• Take advantage of symmetry and periodicity to reduce the size of simulations</td>
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<td>• Store only necessary field data</td>
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<td>• Use coarse mesh size where possible</td>
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<td>• Always for initial simulations</td>
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<td>• Do convergence testing of mesh size last!</td>
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<td></td>
<td>• Use distributed parallel computation to take advantage of modern hardware</td>
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<tr>
<td>Broadband simulation</td>
<td>• Time domain gives broadband results</td>
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<td>• Highly dispersive materials require multi-pole material models</td>
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<td>• Check the material fit before running the simulation!</td>
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<tr>
<td>Optimization and parameter sweeps</td>
<td>• Using a global search algorithm that significantly reduces the number of simulations required</td>
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<td>• Use concurrent computing to use all your available computer resources optimally</td>
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<td>Opto-electronic modeling</td>
<td>Combine optical and electrical modeling</td>
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<tr>
<td></td>
<td>• Bring optical generation rate into electrical models</td>
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<td>• Lumerical DEVICE coming soon!</td>
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**Sales representatives (other regions)**

http://www.lumerical.com/company/reps.html

Free, 30 day trial at www.lumerical.com
Appendix

Poisson and Continuity Equation

- Poisson equation
  \[ \nabla \cdot (\varepsilon \nabla \psi) = q \left( p - n + N_D^+ - N_A^- \right) \]

- Continuity equation
  \[
  \begin{cases}
    \frac{1}{q} \nabla J_n = G_n - U_n \\
    \frac{1}{q} \nabla J_p = G_p - U_p
  \end{cases}
  \]

  Drift current
  \[ J_n = -q n \mu_n \nabla \psi + q D_n \nabla n \\
  J_p = -q p \mu_p \nabla \psi - q D_p \nabla p \]

Inputs from the optical simulation