Simulation of Thin-Film Solar Cells

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Outline

1) Simulation Requirement
2) Calculation Method
3) Structure
4) Oblique Incident Light
5) Results
6) Outlook
Simulation Requirement

• Solve Maxwell’s equations
  \[ i\omega \hat{E} = \frac{1}{\epsilon} \nabla \times \hat{H} - \frac{\sigma}{\epsilon} \hat{E} \]
  \[ i\omega \hat{H} = -\frac{1}{\mu} \nabla \times \hat{E} - \frac{\sigma^*}{\mu} \hat{H} \]

• Calculate quantum efficiency \( QE(\lambda) := \frac{P_{\text{abs},\lambda}}{P_{\text{in},\lambda}} \)

• Calculate short-circuit current density
  \[ J_{SC} = \sum_\lambda QE(\lambda) P^{\text{AM1.5}}_\lambda \Delta \lambda \frac{e \lambda}{hc} \]
Calculation Method

- Finite Integration Technique (FIT)
- Staggered grid → periodic boundary conditions

1D staggered grid

3D staggered grid
3D - Simulation of Different Structures

- Flat, rectangular, pyramidal
- Integration of AFM scans

structure of a solar cell

AFM scan by Fraunhofer IST Braunschweig

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Structure

Discretization

- Size of the computational domain: $2.5\mu m \times 2.5\mu m \times 2.4\mu m$
- Number of points depend on wavelength ($\lambda = 550nm, \ldots, 1000nm$): between 6 and 50 million points
  → High Performance Computing
AFM Scan

- Original size: $5\mu m \times 5\mu m$
- Mirrored due to periodicity
  $\rightarrow$ computational domain: $10\mu m \times 10\mu m$
  $\rightarrow$ too large computational domain!
AFM Scan

- Size of random part of scan 1.2\( \mu m \times 1.2\mu m \)
- Mirrowed part → new simulation domain: 2.4\( \mu m \times 2.4\mu m \)
Oblique Incident Light

Until Now:
using periodic extension

New:
using phase shift
Comparison: Simulation vs. Experiment

Quantum efficiency of a flat structured solar cell for different incident angles $\alpha$

2D simulation

experimental data
Simulation Data

- Simulation with integrated AFM scan
- Size of simulation domain: $2.4\mu m \times 2.4\mu m \times 2.38\mu m$
- Wavelength range: $550 nm - 995 nm$
- Distance: $\Delta \lambda = 5 nm$
- Number of points: between 6 ($995 nm$) and 46 millions ($550 nm$)
- Number of MPI processors: 1000
- Average duration: 4 - 5 hours
Results

**Quantum Efficiency**

different random domains per wavelength

**Short-Circuit Current Density**

<table>
<thead>
<tr>
<th>$J_{SC}$ [mA/cm$^2$]</th>
<th>Rand01</th>
<th>Rand02</th>
<th>Rand03</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>8.982</td>
<td>9.242</td>
<td>9.125</td>
</tr>
</tbody>
</table>

→ max derivation: 2.9%

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Results

3D structure

$|E|^2 \ (\lambda = 800\text{nm})$
Outlook

Future Projects

- Integration of silver nanoparticle
- New implementation for oblique incident waves
- Less memory capacity and computing time
- Smaller wavelengths (start at 350 nm)
- Larger computational domain
- Tandem solar cell (with integrated AFM scan)
Tandem Solar Cell

Size of the computational domain:
2.5\(\mu m\) \(\times\) 2.5\(\mu m\) \(\times\) 3.55\(\mu m\)