Optical simulation of silver nanowire electrodes for thin film solar cells

Shuai Yan\textsuperscript{1,2}, Christoph Pflaum\textsuperscript{1,2}

\textsuperscript{1}Erlangen Graduate School of Advanced Optics Technologies (SAOT)

\textsuperscript{2}Department of Computer Science, LSS, Friedrich-Alexander-Universität Erlangen-Nürnberg
Outline

1 Motivation

2 Simulation

3 Results

4 Conclusion and Outlook
Motivation

Nanostructured metal electrodes (solution-processed silver nanowire (Ag NW) films) are introduced to replace indium tin oxide (ITO) in organic solar cells (OPV).
Motivation

The question marks refer to ...

- Extrordinary transmission;
- Plasmonic effects;
- Relation between transparency and conductivity;
- Other optical and electrical properties...
Cross sections in $x$-$y$ and $x$-$z$ plane (Left); Computational domain with boundary conditions (Right).
Simulation — Maxwell’s Equations

With time-harmonic source (plane wave) \( \mathbf{E} = \hat{\mathbf{E}} e^{i\omega t} \) and \( \mathbf{H} = \hat{\mathbf{H}} e^{i\omega t} \), we have

\[
\begin{align*}
i \omega \hat{\mathbf{E}} &= \frac{1}{\epsilon} \nabla \times \hat{\mathbf{H}} - \frac{\sigma}{\epsilon} \hat{\mathbf{E}} \\
i \omega \hat{\mathbf{H}} &= -\frac{1}{\mu} \nabla \times \hat{\mathbf{E}} - \frac{\sigma^*}{\mu} \hat{\mathbf{H}}
\end{align*}
\]

\( \hat{\mathbf{E}}, \hat{\mathbf{H}} \): Time-independent components of the electric and magnetic field.

\( \epsilon \): electric permittivity; \( \mu \): magnetic permeability;

\( \sigma, \sigma^* \): electric and magnetic conductivities
Simulation — Difficulties

- Dispersive material and negative permittivity;
  
  Classical FDTD method is unstable.
Simulation — Difficulties

- Dispersive material and negative permittivity; Classical FDTD method is unstable.
- Strong localisation of the field due to the plasmonics;

![Graph showing magnitude of electric field at an Ag/air interface involving plasmonic wave.](image)

Figure: Magnitude of electric field at an Ag/air interface involving plasmonic wave.
Simulation — Difficulties

- Dispersive material and negative permittivity;
  - Classical FDTD method is unstable.
- Strong localisation of the field due to the plasmonics;
- Multiscale problem (20μm vs 30nm).
Simulation — Difficulties

- Dispersive material and negative permittivity;
  Classical FDTD method is unstable.
- Strong localisation of the field due to the plasmonics;
- Multiscale problem (20µm vs 30nm).
  Large system!
Simulation — Method

Requirements?

FIT (Finite integration technique)/THIIM (Time harmonic inverse iterative method)
Inverse iteration in the metallic region;
As computational intensive as classical FDTD method;
Parallelizable

C. Pflaum, et al., Numerical Linear Algebra with Applications, 2010
Requirements?

Can deal with metal, less computational intensive, parallelisable.
Requirements?

Can deal with metal, less computational intensive, parallelisable.

FIT (Finite integration technique) / THIIM (Time harmonic inverse iterative method)
Simulation — Method

Requirements?

Can deal with metal, less computational intensive, parallelisable.

FIT (Finite integration technique)/THIIM (Time harmonic inverse iterative method)

- Inverse iteration in the metallic region;
- As computational intensive as classical FDTD method;
- Parallelisable
Simulation — Method

Requirements?

Can deal with metal, less computational intensive, parallelisable.

FIT (Finite integration technique)/THIIM (Time harmonic inverse iterative method)

- Inverse iteration in the metallic region;
- As computational intensive as classical FDTD method;
- Parallelizable

C. Pflaum, et al., Numerical Linear Algebra with Applications, 2010
Results: "Benchmark" — Single wire (in 2D)

\( \alpha \): polarizability of the dipole.
Results: TE/TM analysis of Extraordinary transmission

Table: Film transmittance for 1µm wide Ag NW films with different number of parallel-aligned and equally-spaced Ag NWs inside comparing to their geometric aperture. NUM = number of Ag NWs, GA = geometric aperture (%) and T = transmittance (%).

<table>
<thead>
<tr>
<th>NUM</th>
<th>GA</th>
<th>T (TE)</th>
<th>T (TM)</th>
<th>T (circular)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>70</td>
<td>70.8</td>
<td>94.6</td>
<td>82.7</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>41.6</td>
<td>87.8</td>
<td>64.7</td>
</tr>
<tr>
<td>30</td>
<td>10</td>
<td>25</td>
<td>36</td>
<td>30.5</td>
</tr>
</tbody>
</table>
Results: Approximating to the reality

Adding a binder layer

Optical simulation of silver nanowire electrodes for thin film solar cells / Shuai Yan, Christoph Pflaum
Results: Approximating to the reality

Adding a binder layer

Optical simulation of silver nanowire electrodes for thin film solar cells / Shuai Yan, Christoph Pflaum
Results: Approximating to the reality

**Experiment**
A sample Ag NW film with \( \sim 30\% \) surface coverage;

**3D Simulation**
A \( 1\mu m \times 1\mu m \) film containing randomly distributed Ag NWs, the surface coverage is 28.5%;

Conclusion and Outlook

- FIT/THIIM can be used to simulate the 3D large scale plasmonic structures with the help of parallel computation.

- The simulation of random Ag NW films (solution processed Ag NW films) shows a good agreement with the experimental results.

- Future work: improving the model and combining the electric aspect with the optical study.
Acknowledgement

Prof. Dr. C. J. Brabec
Dr. K. Forberich
J. Krantz

Erlangen Graduate School in Advanced Optical Technologies
Thank You for Your Attention!!!