Thermal Radiation Modeling Workshop
For SPIE Optics+Photonics 2017

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## Brief History of Thermal Energy Harvesting

<table>
<thead>
<tr>
<th>Year</th>
<th>Discovery</th>
<th>Significance</th>
<th>Innovators</th>
</tr>
</thead>
<tbody>
<tr>
<td>1712</td>
<td>Atmospheric Engine</td>
<td>Pumping water out of mines</td>
<td>Thomas Newcomen</td>
</tr>
<tr>
<td>1776</td>
<td>Steam Engine</td>
<td>Mechanical workhorse of industrial revolution</td>
<td>James Watt</td>
</tr>
<tr>
<td>1870</td>
<td>Kirchoff’s law of thermal radiation</td>
<td>Establishing centrality of blackbody in thermal radiation</td>
<td>Gustav Kirchoff</td>
</tr>
<tr>
<td>1879</td>
<td>Stefan-Boltzmann law</td>
<td>Calculating total radiated power</td>
<td>Josef Stefan</td>
</tr>
<tr>
<td>1900</td>
<td>Planck’s law of blackbody radiation</td>
<td>Calculating radiation power spectrum</td>
<td>Max Planck</td>
</tr>
<tr>
<td>1956</td>
<td>Thermophotovoltaics</td>
<td>Converting thermal radiation into electricity</td>
<td>Henry Kolm</td>
</tr>
<tr>
<td>1960</td>
<td>Laser</td>
<td>Provides intense, monochromatic optical power</td>
<td>Schawlow &amp; Townes</td>
</tr>
<tr>
<td>1962</td>
<td>Solar Cell Efficiency Limits</td>
<td>Provided a target for PV and TPV research</td>
<td>Shockley &amp; Queisser</td>
</tr>
<tr>
<td>1979</td>
<td>Gallium antimonide cell</td>
<td>Provides suitable bandgap for TPV</td>
<td>Lew Fraas</td>
</tr>
<tr>
<td>2014</td>
<td>Photonic radiative cooling</td>
<td>Provides nearly ideal radiative cooling</td>
<td>Shanhui Fan</td>
</tr>
</tbody>
</table>
Key Concepts from Prior Research

- Carnot efficiency of heat engines
- Planck blackbody limit: centrality of blackbody in thermal radiation
- Shockley-Queisser limit of photovoltaics
- Additional losses at every step in practice
61% of raw energy wasted in 2013!
Energy Landscape Today

Too much parasitic loss in commonly used devices, like ovens and light bulbs.

The chart above lists values of overall luminous efficacy and efficiency for several types of general service, 120-volt, 1000-hour lifespan incandescent bulb.

<table>
<thead>
<tr>
<th>Bulb Type</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 W tungsten incandescent</td>
<td>1.9%</td>
</tr>
<tr>
<td>60 W tungsten incandescent</td>
<td>2.1%</td>
</tr>
<tr>
<td>100 W tungsten incandescent</td>
<td>2.6%</td>
</tr>
<tr>
<td>Glass halogen</td>
<td>2.3%</td>
</tr>
<tr>
<td>Quartz halogen</td>
<td>3.5%</td>
</tr>
<tr>
<td>Challenges</td>
<td>News</td>
</tr>
<tr>
<td>---------------------------------------------------------------------------</td>
<td>----------------------------------------------------------------------</td>
</tr>
<tr>
<td>Make solar energy economical</td>
<td>Provide energy from fusion</td>
</tr>
<tr>
<td>Manage the nitrogen cycle</td>
<td>Provide access to clean water</td>
</tr>
<tr>
<td>Advance health informatics</td>
<td>Engineer better medicines</td>
</tr>
<tr>
<td>Prevent nuclear terror</td>
<td>Secure cyberspace</td>
</tr>
<tr>
<td>Advance personalized learning</td>
<td>Engineer the tools of scientific discovery</td>
</tr>
</tbody>
</table>

August 6, 2017

SPIE Optics+Photonics, San Diego, CA - Peter Bermel
Make Solar Energy Economical
Make Solar Energy Economical

- Key Challenges:
  - Novel earth-abundant materials
  - Reliable, low-cost packaging techniques
  - Energy storage (daily and seasonal)

- How simulations can help:
  - Provide predictions of performance of realistic, novel PV materials (e.g., using DFT)
  - Predict and optimize lifetime energy production (e.g., using ADEPT)
  - Design electrolyzers and fuel cells (e.g., using FEM multi-physics)

SETUP FOR HANDS-ON WORK

- **Wireless ESSID:**
  - Left-hand side: UNITE-9980; password: 78841109
  - Right-hand side: 791L-8337; password: 68e8dc6d

- **Nanohub login:**
  - [https://nanohub.org/](https://nanohub.org/)
  - Create account via ‘Signup’ link in upper right
  - Login with institutional login, Facebook, or LinkedIn

- **Bug reporting site**
  - [https://nanohub.org/](https://nanohub.org/)
  - (upper right) help link

- **Get the hands-on files**
  - [https://nanohub.org/groups/photonics/thermal_rad_workshop](https://nanohub.org/groups/photonics/thermal_rad_workshop)
Step 1: Reach Maximum Temperature from Solar Heat

Key tool(s):
- S4sim
Selective Absorber: Maximum Thermal Transfer Efficiency

Thermal Transfer Efficiency

$$\eta_t = B\overline{\alpha} - \frac{\overline{\epsilon}\sigma T^4}{C}$$

Spectrally-averaged absorptivity

$$\overline{\alpha} = \frac{1}{I} \int_0^\infty d\lambda \int_0^{\theta_c} d\theta \left[ \epsilon(\lambda, \theta) \sin 2\theta \frac{dI}{d\lambda} \right]$$

Spectrally-averaged emissivity

$$\overline{\epsilon} = \frac{1}{\sigma T^4} \int_0^\infty d\lambda \int_0^{\pi/2} d\theta \left\{ \frac{2hc^2 \epsilon(\lambda, \theta) \sin 2\theta}{\lambda^5 \left[ e^{hc/\lambda kT} - 1 \right]} \right\}$$

Best Commercial Selective Solar Absorbers: $T=400 \text{ K} \ (1 \text{ sun})$

Almeco-TiNOX Solar

$\eta_t = 90\%$; $\alpha = 95\%$; $\varepsilon = 5\%$

Photonic Simulations with S^4

- Full-wave photonic simulations of arbitrary layered media, including thin-film and crystalline PV cells


https://nanohub.org/tools/s4sim/
What is nanoHUB and S4?

- An open-access science gateway for cloud-based simulation tools and resources in nanoscale science and technology.
- Stanford Stratified Structure Solver (S4) is a frequency domain code to solve layered periodic structures.

a major resource for computational nanotechnology

enabled by the HUBzero platform for simulation, learning, and collaboration
S-Matrix Method: Advantages

- No *ad hoc* assumptions regarding structures
- Applicable to wide variety of problems
- Suitable for eigenmodes or high-$Q$ resonant modes at single frequency
- Can treat layers with large difference in length scales
- Computationally tractable enough on single core machines
S-Matrix Method: Disadvantages

- Accurate solutions obtained more slowly as the following increase:
  - Number of layers
  - Absolute magnitude of Fourier components (especially for metals)
  - Number of plane-wave components (~N^3)
- Relatively slow for broad-band problems (time-domain is a good alternative)
Photonic Simulations with $S^4$

Accuracy improves systematically with computing power

S₄: Input

Can choose several pre-made examples drawn from the literature
S4sim: Output Window

Select output type
Label and coordinates of the selected curves
Click on x or y axis to select the parameter ranges and view option.
Select curves shown
Transmission through multilayer stack matches analytical expression
S^4: Output

Transmission through 1D square grating of silicon and air
Transmission from Fig. 4 of Tikhodeev et al., *Phys. Rev. B* **66**, 045102 (2002).
S⁴: Lua Control Files

- Obtain a new, blank simulation object with no solutions:
  
  ```lua
  S = S4.NewSimulation()
  ```

- Define all materials:
  
  ```lua
  S:AddMaterial("Dielectric", {4,0.1}) -- real and imag parts
  S:AddMaterial("ARmat", {2,0})
  S:AddMaterial("Vacuum", {1,0})
  ```

- Add all layers:
  
  ```lua
  S:AddLayer('AirAbove',0,'Vacuum')
  S:AddLayer('ARcoat', art, 'ARmat')
  S:AddLayer('Slab', 2, 'Dielectric')
  S:AddLayerCopy('AirBelow',0,'AirAbove')
  ```

- Add patterning to layers:
  
  ```lua
  S:SetLayerPatternCircle('layer_name', 'inside_material', {0.0,0.0,0}, 0.2) -- centerx, centery, and radius
  ```
S⁴: FMM Formulations

- Specify the excitation mechanism:

  \[
  S:\text{SetExcitationPlanewave}(
    \{0,0\}, \text{--- phi and theta: phi in [0,180), theta in [0,360)}
    \{1.0,0.0\}, \text{--- s_pol_amp, s_pol_phase in degrees}
    \{1.0,0.0\}) \text{--- p_pol_amp, p_pol_phase in degrees}
  
  S:\text{SetNumG}(1)
  \]
S4: FMM Formulations

- Specify the operating frequency range and output:

```python
for freq=0.2, 0.4, 0.005 do
    S:SetFrequency(freq)
    forward_power, backward_power = S:GetPoyntingFlux(‘AirAbove’, 0)
    arf,arb = S:GetPoyntingFlux(‘ARcoat’,0)
    slab_forward, slab_backward = S:GetPoyntingFlux(‘Slab’, 0)
    E2 = S:GetLayerElectricEnergyDensityIntegral(‘Slab’);
    absorption = 1.0 - (math.abs(forward)+math.abs(abb))/math.abs(abf)
    avea=avea+absorption*(freq-oldfreq)
    denom=denom+freq-oldfreq
    oldfreq=freq
end
avea=avea/denom
print(art .. ‘\t’ .. avea);
```
Results

![Graph showing a plotted curve with x-axis labeled 'arl' and y-axis values ranging from 0.175 to 0.18. The curve has peaks and troughs indicating a periodic function.]

1 result

Clear
S4sim Example: PV Front Coating

<table>
<thead>
<tr>
<th>Number of front coating layers</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative permittivity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Layer 1</td>
<td>4.32</td>
<td>0</td>
<td>2.37</td>
</tr>
<tr>
<td>Layer 2</td>
<td>9.12</td>
<td>0</td>
<td>1.80</td>
</tr>
<tr>
<td>Layer 3</td>
<td>14.36</td>
<td>0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number of front coating layers</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (nm)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Layer 1</td>
<td>60</td>
<td>82.3</td>
<td>91.0</td>
</tr>
<tr>
<td>Layer 2</td>
<td>38.9</td>
<td>53.1</td>
<td>29.9</td>
</tr>
</tbody>
</table>
Selective Solar Absorbers

Schematic of the structure for selective absorber based on Si substrate with 215nm Si$_3$N$_4$ front anti-reflection coating (ARC) and 300nm Ag back reflection layer. Heights are not to scale.

The sample is heated by the heater, and the emitted light is collected and guided by the Cu tube, transmitted through a CaF₂ window, reflected by three off-axis parabolic mirrors (PM 1, 2, and 3, Edmund Optics) to a Fourier Transform InfraRed (FTIR) spectrometer with a mercury cadmium telluride detector and KBr beam splitter (Thermo Fisher Nicolet 670).

Measurement (solid lines) and simulation (dashed lines) of the emissivity of selective absorbers with (red lines) and without (black lines) front coating at room temperature. Measurements performed by a Lambda 950 spectrophotometer with an integrating sphere (Labsphere). The thicknesses of Si$_3$N$_4$, Si and Ag are 215nm, 300 $\mu$m and 300nm respectively.

High spectral selectivity is observed at 468 °C in both samples, with a cutoff wavelength of approximately 1.3 μm. Higher short-wavelength emittance is both predicted and observed for the structure with a Si₃N₄ AR coating.

Thin Si film optimization targeted @ 550 °C

Emissivity for selective absorbers with different Si thicknesses. Optimal Si$_3$N$_4$ thickness is used for each curve which is 80 nm. The temperature is set at 550°C and the F-P interference around the Mid-IR is smoothed out for more clear comparison. Less MWIR absorption is experienced for thinner layers of silicon because all samples are in the intrinsic regime, and free carrier absorption dominates.

Optimization Summary for 550 °C

Dependence of solar thermal transfer efficiency $\eta_t$ for different Si thicknesses on the concentration. The $\text{Si}_3\text{N}_4$ thickness is fixed at 80nm, and the temperature is 550C. Thinner layers of silicon experience less reradiation; however layers which are too thin have less absorption, which puts an upper bound on $\eta_t$.

Step 2: Reach Below-Ambient Temperatures under Sunlight

Key tools:
- RadCool
Radiative Cooling for Passive Thermal Management

Questions:
1. Any alternative coolers to PhCs?
2. What is the temperature reduction and performance improvement by applying radiative cooling to hybrid or STPV systems?

Most PV cells experience heating from sub-bandgap absorption

In c-Si cells, degradation processes with activation energy of 0.85 eV are accelerated almost a factor of 2 for every 10 K temperature difference

Radiative cooling on PV devices

Radiative cooling of solar absorbers using a visibly transparent photonic crystal thermal blackbody

Linxiao Zhu\textsuperscript{a,1}, Aaswath P. Raman\textsuperscript{b,1}, and Shanhui Fan\textsuperscript{b,2}

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Edited by John B. Pendry, Imperial College London, London, United Kingdom, and approved August 18, 2015 (received for review May 19, 2015)

- Silica/silica PhC layer should at least preserve the solar absorption of the absorber
- Silica/silica PhC layer is expected to enhance the thermal emittance at the IR window
Radiative cooling of solar absorbers using a visibly transparent photonic crystal thermal blackbody

Linxiang Zhu\(^h\), Aaswath P. Raman\(^h\), and Shanbin Fan\(^h\)

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Edited by John B. Pendry, Imperial College London, London, United Kingdom, and approved August 18, 2015 (received for review May 19, 2015)

Solar absorption of the three structures

Emissivity spectra of the three structures at the IR window
Experimental setup


Periodicity: 6 µm; Depth: 10 µm;

The container allows control over convection
Effects of radiative cooling

Without convection

With convection

Benefits of radiative cooling extend across many PV technologies and installations.

Enhanced thermal radiation

Radiative Cooler
Glass
Polymer
Solar Cell
Polymer
Tedlar
Radiative Cooler

\[ \Delta T_{PV} \text{ (K)} \]

S. Cooling
R. Cooling
S.&R. Cooling

Methods

- Radiative cooling – a passive technique that dissipates heat into remote space via thermal radiation
- Develop a simulation tool, RadCool, to model radiative cooling

Figure 3. Radiative cooling concept
Self-Consistent Modeling of Radiative Cooling for Passive Thermal Management

\[ P_{\text{emit}}: \text{emission power from thermal emitter at } T_E \]
\[ P_{\text{rad,cell}}: \text{radiative recombination of the PV diode at } T_C \]
\[ P_{\text{out}}: \text{electrical output power from PV diode (SQ Limit)} \]
\[ P_{\text{rad}}: \text{radiation power from the cooling emitter at } T_C \]
\[ P_{\text{atm}}: \text{radiation power from atmosphere (300 K)} \]
\[ P_{\text{conv}}: \text{convection power at the exposed surface} \]
\[ R = \frac{A_{\text{cooler}}}{A_{\text{cell}}} \ (\text{Area ratio}) \]
\[ P_{\text{emit}}(T_E, E > E_g) + R \cdot P_{\text{atm}} = P_{\text{out}}(T_C) + P_{\text{rad,cell}}(T_C) + R \cdot P_{\text{rad}}(T_C) + (2R - 1) \cdot P_{\text{conv}} \]

Radiative Cooling Reduces Temperature and Improves Performance Substantially

Simulation tool - input

Heat load phase

- Solar absorption power

\[ P_{\text{sun}} = \text{conc.} \times A \times \int_0^\infty d\lambda \varepsilon(\lambda) I_{\text{AM1.5}}(\lambda) \]

*Assuming incidence angle is 0
Simulation tool - input

Cooler phase
- Thermal radiated power

\[ P_{\text{rad}} = \int d\Omega \cos \theta \int_0^\infty d\lambda I_{BB} \epsilon(\lambda) \]

*\( I_{BB} \) is the spectral radiance of a blackbody at temperature \( T \)
Environment Phase

- Absorbed thermal radiation from the atmosphere

\[ P_{atm} = \int_0^\infty d\Omega \cos\theta \int_0^\infty d\lambda I_{BB}(\lambda, \Omega) \varepsilon(\lambda, \Omega) \varepsilon_{atm}(\lambda, \Omega) \]

- Conductive Power

\[ P_{cod} = K \times (T - T_{chamb}) \]

- Convective Power

\[ P_{cov} = 2 \times h_c \times A \times (T - T_{chamb}) \]
The steady-state temperature $T$ of the sample is determined by:

$$ P_{\text{rad}}(T) - P_{\text{atm}}(T_{\text{amb}}) - P_{\text{sun}} + P_{\text{cod}+\text{cov}} = 0 $$
Experimental verification

- Area ratio of the heat load and the cooler: 1
- Cooling material: silicon wafer with soda-lime glass
- Transmission spectrum: polyethylene film

Ambient temperature on the day of the experiment: ~290K
Conclusions/future work

- RadCool successfully models radiative cooling system in a graphical interface
- More experiments need to be done to confirm the generality of the system and modeling approach
- RadCool can be connected directly with the existing TPV model
- The radiative cooling technique is not limited to TPV systems
  - Potential applications include solar cell cooling, infrared detectors, and sensitive electronic devices that are used outdoors.
Step 3: Combine Hot and Cold Objects for Maximum Efficiencies

Key tools:
- TPXsim
- TPVexpt
What Makes TPV Different from PV?

Photovoltaics

- **Photon Source**: Sun
- **Distance**: 1.5 x 10^8 km
- **Receiver Type**: PV cell
- **Bandgap**: E_g = 1.1-1.4 eV
- **PV cell efficiency**

Thermophotovoltaics

- **Thermal emitter**: 1-10 mm
- **TPV cell efficiency**
- **TPV system efficiency**

TPV cell

E_g = 0.6-1.1 eV
23% Demonstrated TPV Electric Generation Efficiency with Spectral Control


Reflection spectrum for optical filter and receiver

Efficiency in converting radiation to electricity
Photon Recycling Can Greatly Reshape High Temperature Thermal Emission

TPV Efficiencies May Approach 52%* at Reasonable Temperatures†

Material Choices: GaSb 0.7 Si 1.1 GaAs 1.4

*Using highly selective emitters shown above, with MOVPE-grown GaSb TPV cells
†World record $\eta = 23\%$ at 1050 °C

Kirchhoff’s Law: 
\[ \text{Emissivity} = \text{Absorptivity} \]
\[ \varepsilon_{\lambda} = a_{\lambda} \]

\[
J(\nu) = \int_0^\infty d\lambda \frac{2\nu e(\lambda)\text{EQE}(\lambda)}{\lambda^4 \exp(hc/\lambda kT) - 1} - \left[ \frac{q(n^2 + 1)E_{\text{F}}^2kT_d}{4n^2\hbar^2c^2} e^{-\frac{E_{\text{F}}}{n kT_d}} + J_{\text{int}} \right] \left( e^{\frac{\hbar \nu}{n kT_d}} - 1 \right),
\]

(1)

**PV current**

**Dark Current**

\[ V_{\text{OC}}, \text{ open circuit voltage} \]
\[ I_{\text{SC}}, \text{ short circuit current} \]

**FF, fill factor = max. power rectangle**

\[
V_{\text{OC}} \cdot I_{\text{SC}}
\]

**Power conversion efficiency**

\[
\eta = \frac{V_{\text{OC}} \cdot I_{\text{SC}} \cdot FF}{P_{\text{inc}}}
\]

**Radiation Efficiency**

\[
\bar{\varepsilon} = \frac{\int_0^\infty d\lambda \varepsilon(\lambda) / \{ \lambda^3 \exp(hc/\lambda kT) - 1 \}}{\int_0^\infty d\lambda / \{ \lambda^3 \exp(hc/\lambda kT) - 1 \}}.
\]

**Average Emissivity**
TPXsim: A System-Level Modeling Tool
Unprecedented Efficiency of 35.4% is achievable for a filter band gap of 0.37 eV and PV band gap of 0.75 eV.

Why is this meaningful?
Ongoing Research in Birck Nanotechnology center will use these predictions to experimentally fabricate and characterize these structures.
TPVexpt

- Based on TPVtest
- Considers complex rectangular geometries for heater, emitter, and PV diode
- Considers non-idealities (e.g., series/shunt resistance)
- Phased GUI with overhauled “System” tab
View Factor/Geometry

- **View factor**: $F_{A \rightarrow B}$ is the proportion of the radiation which leaves surface $A$ that strikes surface $B$

Definitions: $X = x/z$; $N = \eta/z$; $Y = y/z$

$S = \xi/z$; $\alpha_{ii} = S_i - X_i$; $\beta_{kj} = N_k - Y_j$

$$F_{1-2} = \frac{1}{(X_2 - X_1)(Y_2 - Y_1)} \sum_{i=1}^{2} \sum_{k=1}^{2} \sum_{j=1}^{2} \sum_{l=1}^{2} (-1)^{i+j+k+l} G(\alpha_{ii}, \beta_{kj})$$

where $G(\alpha_{ii}, \beta_{kj}) = \frac{1}{2\pi} \left( \alpha_{ii}(1 + \beta_{kj})^{1/2} \tan^{-1} \left[ \frac{\alpha_{ii}}{(1 + \beta_{kj})^{1/2}} \right] - \beta_{kj} \tan^{-1} \beta_{kj} \right)$

View factor calculation for rectangle to rectangle in a parallel plane. All boundaries are parallel or perpendicular to $x$ and $\xi$ boundaries [2].
View Factor Implementation

- Heater, emitter, and cell modeled as rectangles
- Emitter physically attached to heater
- Heater area broken up into four rectangles for calculations
- Sum of rectangle view factors is equal to heater view factor
- Accounts for thickness of emitter and heater radiation

Method of calculating heater view factor. The back rectangle represents the heater (dark blue). The light blue rectangle represents the emitter.
View Factor Effect on Output

Simulation 1

Simulation 2

Efficiency results. Simulation 1 results in higher efficiency due to a greater view factor (better alignment)
Shunt/Series Resistance

- Fill factor (FF) determines the efficiency of PV cell
- Ideal cell has series resistance of 0 Ω and shunt of ∞ Ω
- Non-idealities decrease FF [6]

\[
\eta = \frac{V_{OC}I_{SC}FF}{P_{in}}
\]

\[
FF = \frac{V_{OC} - \ln(V_{OC} + 0.72)}{V_{OC} + 1}
\]

\[
r_s = \frac{R_S}{R_{CH}}, \quad r_{SH} = \frac{R_{SH}}{R_{CH}}
\]

\[
FF = FF_0 \left\{ \left(1 - 1.1r_s\right) + \frac{r_s^2}{5.4} \right\} \left\{ 1 - \frac{V_{OC} + 0.7FF_0}{V_{OC}} \frac{r_s}{r_{SH}} \left(1 - 1.1r_s\right) + \frac{r_s^2}{5.4} \right\}
\]
Shunt/Series Effect on Output

Efficiency values with varying series and shunt resistances. Default program values with emitter-cell distance of 0.1 mm.

**Ideal case (simulation 1)**

Series Resistance: 0
Shunt Resistance: 0

**Series only (simulation 2)**

Series Resistance: 1
Shunt Resistance: 0

**Shunt only (simulation 3)**

Series Resistance: 0
Shunt Resistance: 200

**Series and shunt (simulation 4)**

Series Resistance: 1
Shunt Resistance: 200

Efficiency values with varying series and shunt resistances. Default program values with emitter-cell distance of 0.1 mm.
Step 4: Improving Low-Bandgap Photovoltaic Cells

Key tool(s):

- ADEPT
- MEEPPV
Drift-Diffusion Model

- Electrostatics (Poisson’s equation):
  \[
  \nabla \cdot \varepsilon \nabla V = -\left( p - n + N_D^+ - N_A^- \right)
  \]

- Charge conservation:
  \[
  \frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + U_n
  \]
  \[
  \frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + U_p
  \]

- Current from drift & diffusion terms:
  \[
  J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx}
  \]
  \[
  J_p = qp(x)\mu_p E(x) - qD_p \frac{dn}{dx}
  \]

Solar Cells: Ideal IV Characteristics

\[ I_D = I_0 \left( e^{qV_D/k_BT} - 1 \right) \]

\[ I_{TOT} = I_0 \left( e^{qV_D/k_BT} - 1 \right) - I_{SC} \]

\[ P_{out} = I_{TOT} V_{OC} = 0 \]

\[ P_{out} = I_{SC} V_D = 0 \]

\[ P_D = I_{TOT} V_D < 0 \]

\[ P_{out} = I_{mp} V_{mp} = I_{SC} V_{OC} FF \]
Maximum Short Circuit Current

Example: Silicon $E_g = 1.1 \text{eV}$. Only photons with a wavelength $< 1.12 \mu\text{m}$ will be absorbed.

$$\frac{hc}{E_g} < \lambda$$

Solar spectrum (AM1.5G)

$J_{SC}\big|_{\text{max}} = 44 \text{ mA/cm}^2$

$P_{in} = 100 \text{ mW/cm}^2$
Open-circuit Voltage and Efficiency

\[ I_{TOT} = I_0 \left( e^{\frac{qV}{k_B T}} - 1 \right) \]

\[ I_{SC} \quad V_{OC} = \frac{k_B T}{q} \ln \left( \frac{I_{SC}}{I_0} \right) \]

\[ = \frac{P_{out}}{P_{in}} = \frac{I_{SC} V_{OC} FF}{P_{in}} \]

Example for silicon photovoltaics:

\[ I_0 = 1 \times 10^{12} \text{ A} \]

\[ I_{SC} = 0.90 \times 44 \times 10^{-3} = 40 \text{ mA} \]

\[ V_{OC} = 0.026 \ln \left( \frac{40 \times 10^{-3}}{1 \times 10^{-12}} \right) = 0.63 \]
Increasing the Efficiency

\[ \frac{P_{\text{out}}}{P_{\text{in}}} = \frac{I_{\text{SC}}V_{\text{OC}}FF}{P_{\text{in}}} \]

1) Increase the short circuit current from 40 towards 44

2) Increase \( V_{\text{OC}} \) (decrease \( I_0 \))

\[ V_{\text{OC}} = \frac{k_B T}{q} \ln\left( \frac{I_{\text{SC}}}{I_0} \right) \]

\[ I_0 = qA \left( \frac{D_n n_i^2}{W_P N_A} \right) \]
Efficiency of Silicon Solar Cells (PERL Architecture)

Martin Green Group UNSW – Zhao et al., 1998 (25% at 1 sun)

$J_{SC} = 41.5 \text{ mA/cm}^2$ (94%)

$V_{OC} = 0.703$  \hspace{1cm} $FF = 0.81$

$I_0 = 0.075 \times 10^{-12} \text{ A}$

August 6, 2017

SPIE Optics+Photonics, San Diego, CA - Peter Bermel
1) Smaller bandgaps give higher short circuit current

2) Larger bandgaps give higher open-circuit voltage

3) For the given solar spectrum, an optimum bandgap exists.

“Shockley-Queisser Limit”
ADEPT 2

Available on nanoHUB.org via:
https://nanohub.org/tools/adeptnpt/
ADEPT: Input deck

- Upon opening ADEPT 2, a blank input page will appear, awaiting your input file.
- If upload/download does not work, one reason could be “pop-up” blocking by your internet browser.

List of pre-loaded example input decks. Try them for some quick simulation samples!
ADEPT: Running a simulation

- Keep in mind that ADEPT 2 is FORTRAN 77 based. The format of certain input may cause unexpected error.
- Please refer to “ADEPT 2 User Manual” for more information regarding how to write an ADEPT input deck.
ADEPT: While simulation is running

- In ADEPT, an entire simulation consists of two parts: ADEPT simulation and PLOTA output generation.

This window dynamically displays output. Sometime, an error occurs and a notification will be shown here.

This is a simulation progress bar. It shows approximately how much simulation is done.
ADEPT: Output

Click “input” to go back to input page. Worry not! Your old simulation results will be saved until you close ADEPT 2.0.

Click here for a complete list of output plots

You can review your old simulations results here

Click “clear” to clear out all output plots
ADEPT: Output

- Click on the plot and drag to "Zoom"
- Download the plot as CSV or PDF image
- "Zoom" reset
- Click "play" to look at this output quantity at different bias
ADEPT: Output

Click on axis to format it

Curve formatting

Bias sequence display option
ADEPT: Output

- Outputs include electrostatic (Poisson) solution:
ADEPT: Output

- Energy band diagram
ADEPT: Output

- Carrier concentrations:

![Graph showing carrier concentrations](image)
ADEPT: Output

- And finally, realistic I-V curves:
MEEPPV: User Interfaces
https://nanohub.org/tools/meeppv

- Upon opening MEEPPV, a simulation option page will appear, allowing users to select between using a graphical user interface and uploading a control file.

- Click on the button below to proceed to the second page.
Graphical User Interface

You will be directed to this page if the graphical user interface (first option) is selected.

Users can input parameters that describe the solar cell features as well as the simulation domain.
Solar cell schematic
Feature tabs will appear when the on/off button is turned on. Click on each tab to input more solar cell’s features.

Click on the on/off button to include the features to the solar cell for simulation.

Click here to go back to the first page.

- The solar cell image shown on the left changes with respect to feature’s on/off button.
Graphical User Interface

- More input parameters under each feature tab

Finally, click here to begin simulation.
Text-Based (Scheme) Interface

- Create new input
- Upload a control file from your computer
- Download this control file to your local computer
- Pre-loaded examples of control files. Try them for some quick simulation samples.

- This interface will appear if the second option (upload control files) from the first page is selected.

- If upload/download does not work, one reason could be “pop-up” blocking by your internet browser.
This is your entire control file. You can edit it here.

Click here to begin simulation

- Note that the input file is written in Scheme language.
- For more details and tutorial on writing control file with Scheme, please refer to: [http://ab-initio.mit.edu/wiki/index.php/Meep_Tutorial](http://ab-initio.mit.edu/wiki/index.php/Meep_Tutorial)
This window dynamically displays output. Sometimes, an error occurs and a notification will be shown here.
Click here for different output figures.

Click “clear” to clear all or one of the simulation results.

You can review your old simulation results here.

Click here to go back to input page.
Generating Graphics

Click play to see the animation of fields propagating through the solar cell.

Image sequence display option
MEEPPV: [https://nanohub.org/tools/meeppv](https://nanohub.org/tools/meeppv)

Output animations
Absorption Spectrum

- Green line: randomness = 0
- Red line: textured
- Blue line: decayf = 10e-6

Absorption

Wavelength (nm)

400 500 600 700 800 900 1000 1100

0.2 0.4 0.6 0.8 1.0

MEEPPV Output
Downloading Data

Download current results to your local computer

Click on axis to format it

“Zoom”
MEEPPV: Post-processing in MATLAB
Summary

- MEEPPV performs full-wave electromagnetics simulations of photovoltaic devices
- Two interfaces to control the input:
  - Graphical user interface – allows graphical feedback on device design
  - Text-Based (Scheme) interface – allows greatest degree of control, designed for experts
- Output
  - Can generate graphics, including line plots (with adjustable axes) and field distributions (either at a single time, or as a movie)
  - Can download raw data as text or csv for further analysis
- Any problems handled through nanoHUB help interface
Future Capabilities

- Jupyter Notebooks
- MATLAB-based version of ADEPT