Project Goal

The goal of this project is the development of an optimization algorithm for use with numerical silicon solar cell models. By coupling an optimization algorithm with a solar cell model, it is possible to simultaneously vary design variables such as impurity concentrations, front junction depth, back junction depth, and cell thickness to maximize the predicted cell efficiency. An optimization algorithm has been developed and interfaced with the Solar Cell Analysis Program in 1 Dimension (SCAPID). SCAPID uses finite difference methods to solve the differential equations which, along with several relations from the physics of semiconductors, describe mathematically the operation of a solar cell. A major obstacle is that the numerical methods used in SCAPID require a significant amount of computer time, and during an optimization the model is called iteratively until the design variables converge to the values associated with the maximum efficiency. This problem has been alleviated by designing an optimization code specifically for use with numerically intensive simulations, to reduce the number of times the efficiency has to be calculated to achieve convergence to the optimal solution. Adapting SCAPID so that it could be called iteratively by the optimization code provided another means of reducing the cpu time required to complete an optimization. Instead of calculating the entire I-V curve, as is usually done in SCAPID, only the efficiency is calculated (maximum power voltage and current) and the solution from previous calculations are used to initiate the next solution. Optimizations have been run for a variety of substrate qualities and levels of front and back surface passivation. This was done to determine how these variables affect the optimized efficiency and the values of the optimized design variables. The sensitivity of efficiency to each of the design variables was investigated by changing one variable and reoptimizing the others. Work is progressing to include variables associated with the design of an anti-reflection coating in the optimization.

Problem Statement

How can all the inputs to a numerical model of a silicon solar cell be simultaneously varied to obtain the "optimal" design.
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Outline

I  Define the Optimization Problem.
   a) Objective, variables, and constraints

II  Solving the Optimization Problem
   a) Outline of optimization algorithm
   b) Calculating efficiency using SCAP1D
   c) Adapting SCAP1D for an iterative environment

III  Results of Optimization

IV  Future Work

Doping Concentration Versus Position
Use of Cerf Model for Doping

![Graph showing doping concentration versus position with net doping on the y-axis and position on the x-axis. The distance scale is exaggerated at junctions.]

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Optimization Model

MAX Efficiency( $D_0$, $X_F$, $D_B$, $X_B$, $D_L$, $X_L$ )

$14 \leq D_0 \leq 20.6$
$14 \leq D_B \leq 20.6$
$14 \leq D_L \leq 20.6$
$0.1 \leq X_F \leq 10.0$
$0.2 \leq X_B \leq 50.0$
$10.0 \leq X_L \leq 300.0$
$0.0 \leq D_L - D_B$
$0.1 \leq X_L - X_F - X_B$

$D_0 = \log[$Front surface doping concentration$] \text{ P atoms/cm}^3$
$D_B = \log[$Bulk doping concentration$] \text{ B atoms/cm}^3$
$D_L = \log[$Back surface doping concentration$] \text{ B atoms/cm}^3$
$X_F = $ Front junction depth $\mu$m
$X_B = $ Back junction depth $\mu$m
$X_L = $ Cell thickness $\mu$m
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Optimization Model Flow Chart

- Calculate the efficiency associated with the initial values of decision variables \((x^0, k=0)\) (1 call to SCAP1D)
- Calculate the numerical approximation of the gradient \((\nabla_{\text{eff}})\) at \(x^0\).
  (\(n\) calls to SCAP1D)
- Calculate the search direction.
  \(d^k = H^k \nabla_{\text{eff}}^k\)
- Enforce constraints to insure feasibility.
- Solve the 1-dimensional optimization problem along the direction \(d^k\).
  max eff \((x^k + \alpha^k d^k)\)
  (calls SCAP1D until converged to \(\alpha^k\))
  \(x^{k+1} = x^k + \alpha^k d^k\)

n-dimensional problem Converged??

yes \(\rightarrow\) DONE

no \(\rightarrow \)

\(k = k + 1\)
SCAP1D (Solar Cell Analysis Program in 1 Dimension)

Poisson's equation \[ \nabla^2 V = \frac{1}{\varepsilon} (n - p + N_D - N_A) \]

Electron Continuity Equation \( \nabla I_n = q (R - G) \)

Hole Continuity Equation \( \nabla I_p = -q (R - G) \)

Hole and Electron Carrier Transport Equations

\[ I_n = -q \mu_n n \left[ \nabla (V + \gamma \frac{\Delta \xi}{q}) \right] + q D_n \nabla n \]

\[ I_p = -q \mu_p p \left[ \nabla (V - (1-\gamma) \frac{\Delta \xi}{q}) \right] - q D_p \nabla p \]

where:

Effective gap reduction \( \Delta \xi = [\Delta E_g + \Theta_n + \Theta_p] \)

Effective asymmetry factor \( \gamma = \frac{\Delta \xi - \Theta_n}{\Delta \xi} \)

Several assumptions are required for the validity of these equations.

1. Complete ionization of the dopants.
2. The heavily doped regions are quasi-neutral and in low injection.
3. The parameters \( \Delta \xi \) and \( \gamma \) are functions of the carrier concentrations.
4. \( \Delta \xi \) and \( \gamma \) do not change when the device is not in equilibrium.

I-V Curves
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Power Versus Voltage

Base Input Parameters

Constant Input Parameters

- Illumination: 100mW/cm² (AM 1.5)
- Temperature: 28 degrees C
- Doping Profile: erfc
- Shadowing (including reflection): 7%
- Auger Recombination: considered
- Band Gap Narrowing: Slookboom Degraff model

Inputs Vary Parametrically

Front surface recombination velocity ($S_f$)
Back surface recombination velocity ($S_b$)
Minority carrier lifetime (used same formulas as in last progress report)
$\tau_{e0}$ is electron minority carrier lifetime.
$\tau_{h0}$ is hole minority carrier lifetime (always taken as one half $\tau_{e0}$)
For 2 ohm-cm substrates the input $\tau_{e0} = 2$ ms, 1 ms, 4 ms gives bulk minority carrier lifetimes of 54, 30, and 13 micro seconds respectively.
$R_b$ (back surface reflection, 1.0 or 0.0)

Inputs Vary Parametrically or Optimized

- Front junction depth ($X_f$)
- Back junction depth ($X_b$)
- Cell thickness ($X_L$)
- Front surface doping concentration ($D_f$)
- Bulk doping concentration ($D_b$)
- Back surface doping concentration ($D_L$)
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Optimal Solution for Case 2

Parameters Held Constant During Optimization

- Front surface recombination velocity \( (S_f) \) = 1,000.0 cm/s
- Back surface recombination velocity \( (S_b) \) = 1,000.0 cm/s
- Electron minority carrier lifetime \( (\tau_e) \) = 1.0 ms
- Hole minority carrier lifetime \( (\tau_h) \) = 0.50 ms

Optimal Values of Decision Variables

- Front junction depth \( (X_f) \) = 0.10 \( \mu \)m (lower bound)
- Back junction depth \( (X_b) \) = 0.20 \( \mu \)m (lower bound)
- Cell thickness \( (X_c) \) = 280.1 \( \mu \)m
- Front surface doping concentration \( (D_f) \) = 2.153 \times 10^{19} \text{ P atoms/cm}^2
- Bulk doping concentration \( (D_b) \) = 1.989 \times 10^{16} \text{ B atoms/cm}^2
- Back surface doping concentration \( (D_b) \) = 3.214 \times 10^{19} \text{ B atoms/cm}^2

Cell Performance Parameters

- Efficiency = 21.871 \% 
- Open circuit voltage \( (V_{oc}) \) = 668.2 mV
- Short circuit current density \( (J_{sc}) \) = 39.063 mA/cm²
- Maximum power voltage \( (V_{mp}) \) = 584.86 mV
- Fill factor = 0.8379
- Collection efficiency = 99.23 \%
- Bulk resistivity = 0.74 ohm-cm
- Sheet resistance layer 1 = 988.0 ohm/\square
- Sheet resistance layer 2 = 23.37 ohm/\square

1 Values in lightly doped silicon.

Efficiency Versus Front Junction Depth

![Graph showing efficiency versus front junction depth](image-url)
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Optimal Front Surface Doping for Fixed Front Junction Depth

Efficiency Versus Back Junction Depth

Optimal Back Surface Doping for Fixed Back Junction Depth

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Efficiency Versus Back Junction Depth

Optimal Back Surface Doping for Fixed Back Junction Depth
Efficiency Versus $\tau$

at Different Levels of Surface Passivation

$\tau = \text{Intrinsic electron minority carrier lifetime}$

$sf (sb) = \text{front (back) surface recombination velocity}$
Optimal Efficiency Contours Versus SB and SF

Taun = 2.0 ms, cell thickness < 300

**SB** = effective back surface recombination velocity (cm/s)

**SF** = effective front surface recombination velocity (cm/s)
Optimal Efficiency Contours Versus SB and SF (Cont'd)

Taun = 2.0 ms, no BSF, cell thickness < 300

SB = effective back surface recombination velocity (cm/s)

SF = effective front surface recombination velocity (cm/s)
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Summary

(1) Significant computational savings can be realized by adapting a solar cell model for use with an optimization algorithm.

(2) Comparisons should only be made between different values of a design variable after the other variables are optimized.

(3) An optimization algorithm provides a systematic method for comparing different levels of technology and/or fabrication processes.

(4) A model coupled with an optimization algorithm provides a very powerful tool for analyzing the system modeled.

Future Work

(1) Analyze results of optimization runs.

(2) Investigate other models for the doping concentrations.

(3) Include a term for lateral resistance in the objective function.

(4) Include the design of the anti-reflection coating in SCAP1D and possibly in the optimization.