Optimization and analysis of multilayer anti-reflection coating for thin-film Si selective solar absorber

Hao Tian
ECE695 Final Project
Instructor: Peter Bermel
4/26/2017
Introduction: Selective absorber

Goal: absorb most sun light while suppress thermal re-radiation

Kirchoff’s law \( \varepsilon(\lambda) = \alpha(\lambda) \)

Si\(_3\)N\(_4\): front anti-reflection coating
Si: selective absorbing layer
Ag: back reflector

Ideal Selective solar absorber emissivity/absorbtivity

Introduction: Selective absorber

Two ways to increase the efficiency of the absorber:
1. Reduce thermal re-radiation: decrease Si thickness

Mathematical Model for Selective Absorber

Maxwell’s equation in layer:
\[ \nabla \times \mathbf{H} = -i\omega\varepsilon_0\varepsilon \mathbf{E} \]
\[ \nabla \times \mathbf{E} = i\omega\mu_0 \mathbf{H} \]

S-Matrix:
\[
\begin{bmatrix}
\mathbf{u}^{(5)} \\
\mathbf{d}^{(0)}
\end{bmatrix}
= 
\begin{bmatrix}
T_{uu} & R_{ud} \\
R_{du} & T_{dd}
\end{bmatrix}
\begin{bmatrix}
\mathbf{u}^{(0)} \\
\mathbf{d}^{(5)}
\end{bmatrix}
\]

Material data (\(\varepsilon\)) are found from literatures:
- \(\varepsilon_{SiO_2}\): Malitson 1965 + Kischkat 2012
- \(\varepsilon_{TiO_2}\): Kischkat 2012
- Si: Green and Keevers 1995+Salzberg and Villa 1957+Bermel 2010
- Ag: Rakic 1998

Thermal transfer efficiency:
\[
\eta_t = \bar{\alpha} - \bar{\varepsilon} \sigma T^4 \\
\bar{\varepsilon} = \frac{\int_0^\infty d\lambda \varepsilon(\lambda) \lambda^5 \left[ \exp \left( \frac{hc}{\lambda kT} \right) - 1 \right]}{\int_0^\infty d\lambda \left[ \lambda^5 \left[ \exp \left( \frac{hc}{\lambda kT} \right) - 1 \right] \right]} \\
\bar{\alpha} = \frac{1}{C I} \int_0^\infty d\lambda \varepsilon(\lambda) \frac{dI}{d\lambda}
\]

\(\sigma\) - Stefan–Boltzmann constant,
\(T\) - temperature, \(C\) - solar concentration, \(I\) - solar intensity.

## Mathematical Model for optical property of Si at high temperatures

<table>
<thead>
<tr>
<th>Wavelength range</th>
<th>Semi-empirical equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4-0.8µm k</td>
<td>$k(h\nu, T) = k_0(h\nu)\exp(T / T_0(h\nu))$</td>
</tr>
<tr>
<td>1-10µm $\alpha_{BG}$</td>
<td>$\alpha_{BG}(h\nu, T) = \sum_{i=1}^{4} [\alpha_{ia}(h\nu, T) + \alpha_{ie}(h\nu, T)]$</td>
</tr>
<tr>
<td>$\alpha_{FC}$</td>
<td>$\alpha_{FC} = 4.15 \times 10^{-5} \lambda^{1.51} T^{2.95} \exp(-7000 / T)$</td>
</tr>
<tr>
<td>$\alpha_L$</td>
<td>$\alpha_L$ is assumed to be constant and can be deduced from the experimental results of Sato</td>
</tr>
<tr>
<td>0.4-1µm n</td>
<td>$n(h\nu, T) = \sqrt{4.386 - 0.00343 T + (99.14 + 0.062 T) / (E_g^2 - (h\nu)^2)}$</td>
</tr>
<tr>
<td>1-10µm n</td>
<td>$n(\lambda, T) = \sqrt{\varepsilon_r(T) + \frac{L(T)}{\lambda^2}(A_0 + A_1 T + A_2 T^2)}$</td>
</tr>
</tbody>
</table>


Numerical Approach and Validation

**S4:** the calculation of the reflection $R$ of the stratified structure.
The absorptivity is calculated by:

$$\alpha = 1 - R.$$  

The emissivity is calculated according to Kirchoff’s law:

$$\varepsilon = \alpha$$

S4 code:

```java
S = S4.NewSimulation()
S:SetLattice({1.000000, 0.000000}, {0.000000, 1.000000})
S:SetNumG(1)
S:AddMaterial("vacuum", {1.00000000000, 0.00000000000})
S:AddMaterial("SIO2", {2.161619071947, 0.00000000000})
S:AddMaterial("TIO2", {8.612985358210, 0.00000000000})
S:AddMaterial("SICR", {34.41845511694, 8.597409413696})
S:AddMaterial("AG", {-3.593775076486, 0.534195073204})
a = 1;
S:AddLayer('Layer_Above', 0.000000, 'vacuum')
S:AddLayer('layer_1', 0.1/a, 'SIO2')
S:AddLayer('layer_2', 0.05/a, 'TIO2')
S:AddLayer('layer_3', 20/a, 'SICR')
S:AddLayer('layer_4', 0.3/a, 'AG')
S:AddLayerCopy('Layer_Below', 0.000000, 'Layer_Above')
S:SetExcitationPlanewave({0.000000, 0.000000}, {1.000000, 0.000000}, {1.000000, 0.000000})
```

Assumptions:
Each layer is ideally flat without any fluctuation.

Normal incident light with both polarization

The S4 model is validated through our previous experimental results.
Numerical Approach and Validation

The optical property of Si at high temperature is calculated in Matlab using the empirical equations.

Optimization of TiO$_2$ and SiO$_2$ thickness

The targeted temperature is 550°C, Si 20um, Ag 300nm under 100 suns. Optimal TiO$_2$ and SiO$_2$ thicknesses are 50 nm and 100 nm, which generates thermal transfer efficiency 76.59%. 

![Diagram showing optimization of TiO$_2$ and SiO$_2$ thickness](image)
Optimization of TiO$_2$ and SiO$_2$ thickness

T = 550°C, C = 100 suns.

Comparison between one layer (Si$_3$N$_4$) and multilayer (SiO$_2$+TiO$_2$) anti-reflection coating
Efficiency under different temperatures for different Si thicknesses

The optimal temperature decreases as the concentration decreases.
For 20um Si, the optimal temperature at 100 suns is 480°C, with maximum efficiency 77.42%. 

As we increase the concentration, the optimal Si thickness increases, since the absorption will increase.
Conclusions

- Model based on S4 for the calculation of the reflection of the selective solar absorber is established.
- High temperature Si model is established using Matlab which is useful for the optical simulation of Si at high temperatures.
- To increase the absorption of sunlight, multilayer antireflection coating is designed and analyzed. The optimal thicknesses for SiO$_2$ and TiO$_2$ are 100nm and 50nm respectively.
- The optimized structure shows increased absorption while thermal re-radiation is not influenced.
- The thermal transfer efficiency at 550°C for 20um Si is increased to 76.59%.
- The Efficiency and optimal temperature increase as the concentration is increasing for 20um Si.
- The optimal Si thickness decreases as the concentration decreases.
Thank you very much!

Questions?