Optimization of a nanostructured moth-eye anti-reflective coating in RSoft
Moth-eye anti-reflective structures

• Microscale structures on the surface of optical interfaces have been known for over a century as an effective method of reducing Fresnel reflections.

• The eyes of a moth are covered with a natural anti-reflective nanostructured film
  – The moth-eye pattern is a pattern of subwavelength “bumps”; reduces reflection by creating an effective refractive index gradient between the air and the medium.
  – The moth-eye structure is one of the most effective nanostructures to reduce reflection

Moth-eye anti-reflective structure applications

• Moth-eye nanostructures can be patterned on surfaces to give them antireflection properties

• Moth-eye structures have several advantages over traditional thin-film AR coatings
  – Environmental tolerance
  – Surface adhesion
  – Single-material fabrication
  – Minimal surface preparation
  – Higher laser-induced damage threshold
  – Self cleaning (lotus effect)

• Moth-eye structures are especially useful for reducing reflections from and increasing transmission between materials with a large refractive index contrast
  – Particularly important in high-power & low-loss applications

• Moth-eye AR structures have found uses in a number of applications, including laser systems, photovoltaics, LEDs, electronic displays, and fiber optics

Moth-eye patterns can be used to increase the extraction efficiency from OLEDs by breaking up the total internal reflection

Moth-eye anti-reflective structure design for $\text{As}_2\text{S}_3$ optical fiber

• In this work, we optimize the shape and dimensions of moth-eye structures for maximum output coupling through the endfaces of $\text{As}_2\text{S}_3$ ($\text{n}=2.45$) chalcogenide optical fibers.

• Rigorous computational EM propagation methods, like FDTD and RCWA, can be used to accurately simulate the transmission/reflection from the moth-eye surface.
  – For this particular moth-eye structure, RSoft’s DiffractMOD RCWA tool is utilized due to RCWA’s speed advantages over FDTD.

• RSoft’s MOST Optimization and Scanning Utility is used in conjunction with DiffractMOD to optimize the reflection/transmission for the moth-eye AR pattern.
# Moth-eye anti-reflective structure parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>Height of moth-eye cone</td>
</tr>
<tr>
<td>W1</td>
<td>Cone tip diameter</td>
</tr>
<tr>
<td>W2</td>
<td>Cone base diameter</td>
</tr>
<tr>
<td>Lattice</td>
<td>Hexagonal</td>
</tr>
<tr>
<td>Sx</td>
<td>Lattice packing constant</td>
</tr>
<tr>
<td>Sy</td>
<td>$\sqrt(3Sx)$</td>
</tr>
<tr>
<td>N</td>
<td>2.45 ($As_2S_3$)</td>
</tr>
<tr>
<td>Operating Wavelength</td>
<td>2-5um</td>
</tr>
</tbody>
</table>
Simulation Parameters

• The source is a plane wave, incident on the moth-eye surface from below.

• The index resolution and # of harmonics used in the DiffractMOD simulation is chosen to ensure converged transmission/reflection results

• A single unit cell of the moth-eye structure, with periodic boundary conditions, is used to replicate the moth-eye array

• Note that for a circularly symmetric structures in a square or hexagonal packing scheme with normal incidence, it is sufficient to study a single polarization of incoming light [2,3]
Parameter Scanning

• It is always best to use MOST for parameter scanning before beginning a MOST optimization study
  – Provides quickest validation of the simulation
  – Prevents time-consuming mistakes when setting up optimization studies!

• For this structure, some parameters to investigate include
  – Tip width (W1)
  – Base width (W2)
  – Height (H)
  – Lattice Period (Sx, Sy=√(3Sx))

R. J. Weiblen et al [1]
Parameter scanning

- DiffractMOD & MOST efficiently compute the moth-eye transmission vs. wavelength for a variety of individual simulation parameters.

- Parameter scans for W1, W2, H, Sx show good agreement with previous experimental and theoretical results [1]

- Simulation Parameters (unless scanned) are:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>0.2um</td>
</tr>
<tr>
<td>W2</td>
<td>0.7um</td>
</tr>
<tr>
<td>Sx</td>
<td>0.92um</td>
</tr>
<tr>
<td>Sy</td>
<td>1.59um</td>
</tr>
<tr>
<td>H</td>
<td>0.9um</td>
</tr>
</tbody>
</table>
Parameter Optimization

• Here, we will optimize the design parameters of the moth-eye structure to achieve maximum averaged transmission from 2-5μm.

• To achieve this, MOST’s Optimization features will be used, with DiffractMOD as the simulation engine.

• A MOST “User Simulator” is written to control the optimization. The user simulator completes the following tasks
  – Runs the DiffractMOD simulations
  – Computes the averaged transmission (from 2-5μm) from the DiffractMOD simulations
  – Using the averaged transmission as a target metric, the User Simulator uses MOST’s genetic optimization algorithm to vary the structure parameters until maximum transmission (minimum reflection) is achieved
User simulator

• The user simulator for this optimization (lam_avg_trans.py) is written in Python, but any scripting language could be used.

• This user simulator follows the standard RSoft user simulator calling conventions & syntax.

• The user simulator computes the averaged transmission, from 2-5 μm, as lam_avg_trans.

• 1-lam_avg_trans is then used as the MOST metric.
Optimization Results

• For faster optimization speed, W2 was set to be equal to Sx
  – Fits in with theoretical expectation, from graded-index model, of what W2 should be for maximum transmission

• Optimized structure is shown to the right, averages 99.804% transmission from 2-5um.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Optimized (Defined) Value</th>
<th>Optimization Range (if applicable)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2.973451636</td>
<td>0.8 ≤ H ≤ 3um</td>
</tr>
<tr>
<td>W1</td>
<td>0.2263061559</td>
<td>0 ≤ W1 ≤ 0.7um</td>
</tr>
<tr>
<td>W2</td>
<td>Sx</td>
<td></td>
</tr>
<tr>
<td>Lattice</td>
<td>Hexagonal</td>
<td></td>
</tr>
<tr>
<td>Sx</td>
<td>0.8980307418</td>
<td>0.7 ≤ Sx ≤ 0.9 um</td>
</tr>
<tr>
<td>Sy</td>
<td>$\sqrt{3Sx}$</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>2.45 ($A_{5}S_{3}$)</td>
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References

