COMSOL Multiphysics® Implementation of a Genetic Algorithm Routine for Metasurface Optimization

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Overview

Motivation
Previous Works
Theoretical Orientation
Motivation for Flat Lenses

• **Goal:**
  Create a **functional, single-interface, flat lens** in the infrared regime that mimics the refractive focusing function of a bulk curved lens in a sub-band between 3 – 12 μm

• **Targeted Issue:**
  **Functionality suffers:** 2-D plasmonic lens efficiency is ~1%–20%

• **Proposed Solution:**
  Use COMSOL to create a design optimization tool that maximizes **efficiency** for M/LWIR metasurface optics
Validation of COMSOL-Based Metasurface Lens Design (2016)

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- Phase calculation for $5 \mu m, N = 8, f = 10 \, cm$

- Fabricated 19 cylindrical lenses @ SNL

- Experimental validation

$\phi$

Position along optical axis $\sim 10.5 \, cm$

$\lambda = 8 \, \mu m$
Potential Solution: 3-D Structures

• 3-D Structures offer:
  o Additional field coupling modes
  o Improved span of phase control
  o HUGE design space

• Issues:
  o Often non-analytical
  o More metal = more absorption loss
  o HUGE design space
  o Fabrication (!)

Cut-wire pairs:

Split-ring resonators:

Stacked

Multi-faced
Membrane Projection Lithography

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- MPL produces out-of-plane scatterers with high fidelity

- Si/Air unit cells of arbitrary shape/periodicity

- Large area (wafer-scale)

- Metal deposition of any open shape...

MPL-Based 3-D Grid

• Assume we do not know which 3-D geometries are “best”…

Could we determine this via a grid of voxels?

• How do we choose the optimal grid layout of 1’s & 0’s?
Genetic Algorithm for MPL Grid Optimization

- **GA overview:** takes individual with best “fit”, evolves genes until optimal
  - Genes = voxel states → “1” for metal, “0” for dielectric
  - Individuals = models; population = set of models
  - Fitness = how well solution matches desired outcome (e.g., max/min or target value)

- **COMSOL** w/ LiveLink for MATLAB and Application Programming Interface
  - Create/solve models w/ random grids
  - Determine which voxel layout (genes) gives best fit (“parents”)
  - Evolve genes, create new population of “children” based on evolved genes
  - Iterate!

- **MATLAB + COMSOL**
  - Generation (Initial) Population (Initial)
  - Functional Evaluation
  - Fitness/Cost Function

- **COMSOL**
  - Parent Selection
  - Crossover

- **MATLAB**
  - Crossover
  - Mutation
  - Check/Continue/Stop

- **COMSOL**
  - Generation (2nd)
COMSOL Models

Validation Model
Membrane Projection Lithography (MPL) Model
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**Objective:** validate GA routine against multi-objective fitness function, seeking a Huygens-like scatter:

\[
F(w_\Delta, w_f) = w_\Delta \frac{\Delta|E|^2 - \min(\Delta|E|^2)}{\max(\Delta|E|^2) - \min(\Delta|E|^2)} + w_f \frac{|E^f|^2 - \min(|E^f|^2)}{\max(|E^f|^2) - \min(|E^f|^2)}
\]
COMSOL Validation of Huygens Source Model

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- What constitutes “best” in a multi-objective solution space?
  - Largest $|E_{far}^{fwd}|^2$ was $30\ dBv$, with $\Delta |E_{f-b}^{far}|^2 = |E_{fwd}^{far}|^2 - |E_{back}^{far}|^2 = 20\ dBv$
  - Largest $\Delta |E_{f-b}^{far}|^2$ was $-28\ dBv$, with $|E_{fwd}^{far}|^2 = 26\ dBv$
COMSOL Validation of Huygens Source Model

- **Best**: 26 dBv, −28 dBv
- **Modified**: 26 dBv, −24 dBv

Current density

Mirrored full structure

= flipped voxels

Strong forward propagation
MPL-Based Model: Unit Cell Analysis

Objective: use GA to identify voxel grid layout for maximum transmittance \( T \) at targeted phase points \( \Phi_0 \):

\[
F(w_\Phi, w_s) = w_\Phi \frac{\sigma_\Phi^2}{|\Phi - \Phi_0|^2 + \sigma_\Phi^2} + w_s \frac{\sigma_s^2}{|S_{21}|^2 - T_0} + \sigma_s^2
\]

Example MPL structures

Burckel et al., IEEE EDSSC (2015); Burckel et al., Adv Mater, 22, 5053 (2010)
Baseline of Undecorated MPL Si Boxes

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\[ T = |S_{21}|^2 \]

Diffraction edge = 2.33 \( \mu m \)

Design of interest:
\[ t_{wall} = 300 \text{nm} \]
\[ a = 2.3 \mu m \]
\[ \Phi = -113^\circ \]

Undecorated Model

Wall Thickness
- 100 \( \mu m \)
- 120 \( \mu m \)
- 140 \( \mu m \)
- 160 \( \mu m \)
- 180 \( \mu m \)
- 200 \( \mu m \)
- 220 \( \mu m \)
- 240 \( \mu m \)
- 260 \( \mu m \)
- 280 \( \mu m \)
- 300 \( \mu m \)
- 320 \( \mu m \)
- 340 \( \mu m \)
- 360 \( \mu m \)
- 380 \( \mu m \)
- 400 \( \mu m \)
- 420 \( \mu m \)
- 440 \( \mu m \)
- 460 \( \mu m \)
- 480 \( \mu m \)
- 500 \( \mu m \)

Periodicity (nm)

1 1.5 2 2.5 3 3.5 4

1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0

180 150 120 90 60 30 0 -30 -60 -90 -120 -150 -180

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COMSOL Validation of MPL Model

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Target: $0^\circ$
Best: $\Phi = -0.15^\circ$
$T = 0.52$
Modified: $\Phi = 13.7^\circ$
$T = 0.49$

$\Phi = \arg[S_{21}]^2$ °

$\Delta \Phi \approx 113^\circ$

$
\begin{align*}
\Phi_{\text{target}} & = 0^\circ \\
T & = 0.746
\end{align*}$
COMSOL Validation of MPL Model
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- **Best:**
  \[ \Phi = -0.15^\circ \]
  \[ T = 0.52 \]

- **Modified:**
  \[ \Phi = 13.7^\circ \]
  \[ T = 0.49 \]
  \( \text{= flipped voxels} \)

Incident field

Propagated plane wave develops \( \sim 1 \text{um (}\lambda/8\text{)} \)

grid width/6

\( \Phi = \) best phase shift
\( T = \) best transmission

\( \text{Best:} \)
\[ \Phi = -0.15^\circ \]
\[ T = 0.52 \]

Propagated plane wave

\( \sim 1 \text{um (}\lambda/8\text{)} \)

grid width/6

\( \Phi = \) modified phase shift
\( T = \) modified transmission

\( \text{Modified:} \)
\[ \Phi = 13.7^\circ \]
\[ T = 0.49 \]
COMSOL Validation of MPL Model

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- **Repeatability:**
  - Accurately hit all 8 target phases
  - Transmittances typically between $T = 0.3 - 0.5$
  - Required 20 – 30 iterations for convergence

- **Flexibility:**
  - Dozens of designs per ° phase
  - 1° – 10° span in $\Phi_0$ may provide 10% – 20% increase in $T$
Early Fabrication

First Etch/Deposition
EBL Etch & Au Deposition

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• VERY early fabrication attempts @ 250nm resolution
  o First-ever use of e-beam lithographic mask for MPL process
  o Tested on low-quality cubic Si arrays—but not perfectly cubic!
    ▪ Poor deposition of metal on upper/side walls as result

• Verdict: clear corner/corner contact, sharp features
(VERY!) Recent Improvements

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<table>
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<th>T</th>
<th>R</th>
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Phase (°) | Δ Phase (°)
-------|-------|
113      | 134   |

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<td>0.17</td>
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Phase (°) | Δ Phase (°)
-------|-------|
0.01     | 113   |
**Conclusion**

**The AFIT of Today is the Air Force of Tomorrow.**

**COMSOL** demonstrated that a GA routine can generate a 3-D plasmonic structure capable of exceeding the physical limitations imposed by 2-D planar architectures for development of improved metasurface optics.

- From a performance/design standpoint, the **COMSOL**-based GA:
  - Delivered a solution that met technical goals in phase and amplitude
  - Demonstrated a robustness in reliability and flexibility

- From a computational standpoint, the **COMSOL**-based GA:
  - Successfully implemented a GA routine into a FEM computational software suite
  - Introduces a great savings for the user—no spectral sweep necessary!
    - We did not include a quantitative study on time savings, but it is easily inferred
  - Allows for optimal geometries that conventional intuition typically cannot predict

- **Thank you for your attention!** Contact: bryan.adomanis@us.af.mil
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Additional Material

Limitations of 2-D Metasurfaces
Results of “brick” grid MPL Design
Limitations of 2-D Planar Metasurfaces

- Fundamentally, thin 2-D metasurfaces cannot:
  - reach desired phase range in co-polarized states
  - reach high amplitudes in cross-polarized states

\[
|t_{co-pol}|^2 + \left| \sqrt{\frac{n_1}{n_2}} t_{co-pol} - 1 \right| \leq 1
\]

\[
|r_{co-pol}|^2 + \frac{n_2}{n_1} |r_{co-pol} + 1| \leq 1
\]

\[
|t_{x-pol}|^2 \leq \frac{n_1 n_2}{(n_1 + n_2)^2}
\]

\[
|r_{x-pol}|^2 \leq \frac{n_1^2}{(n_1 + n_2)^2}
\]

“Fabricate-able” Voxel Geometries

- Adjusted the square offset to include half-voxel edges. Makes for a ‘brick’ pattern
- Produces great results at the targeted phase point (0°), and is much more fabricable

### Table

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