COMSOL CONFERENCE 2017 BOSTON

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

Sandia National Laboratories

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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 $3 - 12\ \mu\mathrm{m}$

- Targeted Issue:

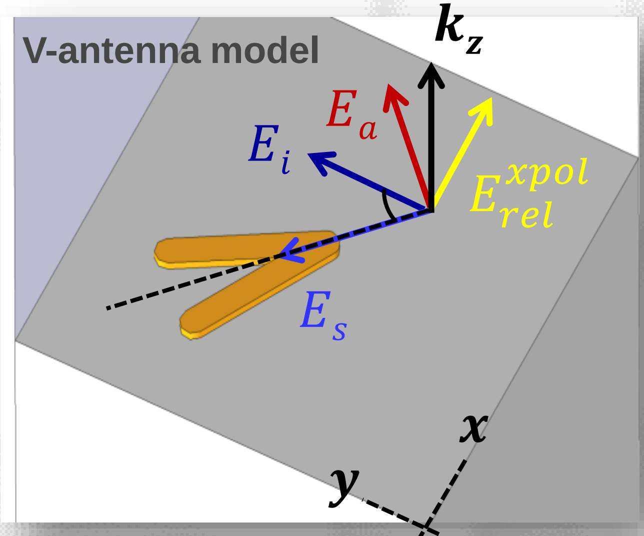
  Functionality suffers: 2-D plasmonic lens efficiency is **~1%–20%**

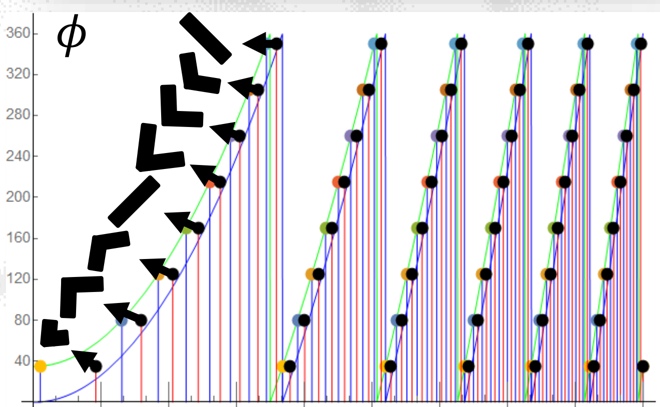
- Proposed Solution:

  Use COMSOL to create a design optimization tool that maximizes ***efficiency*** for M/LWIR metasurface optics

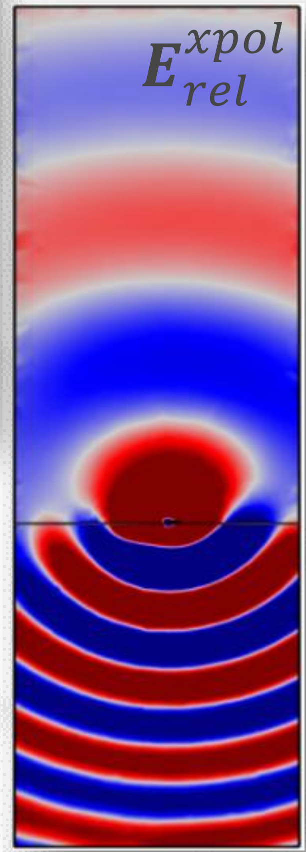
Validation of COMSOL-Based Metasurface Lens Design (2016)

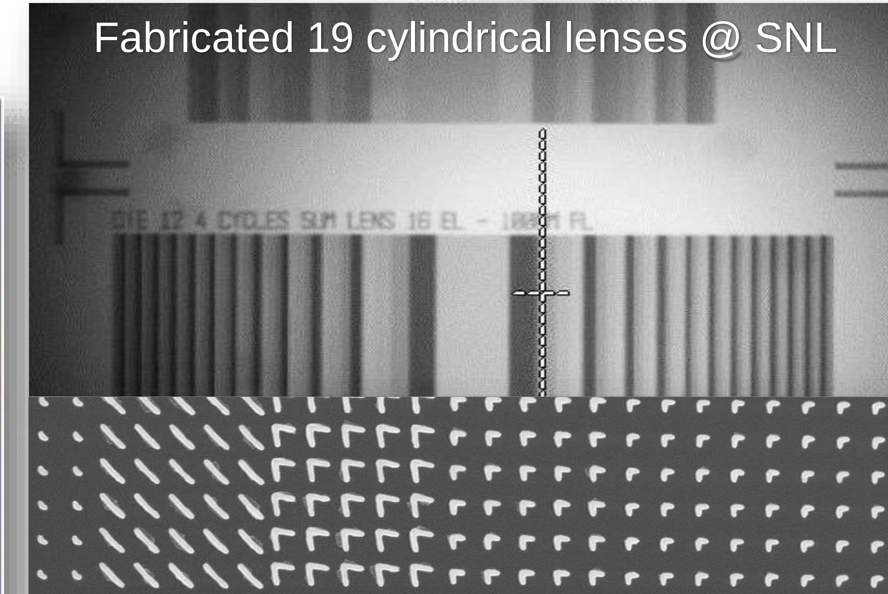
The AFIT of Today is the Air Force of Tomorrow.

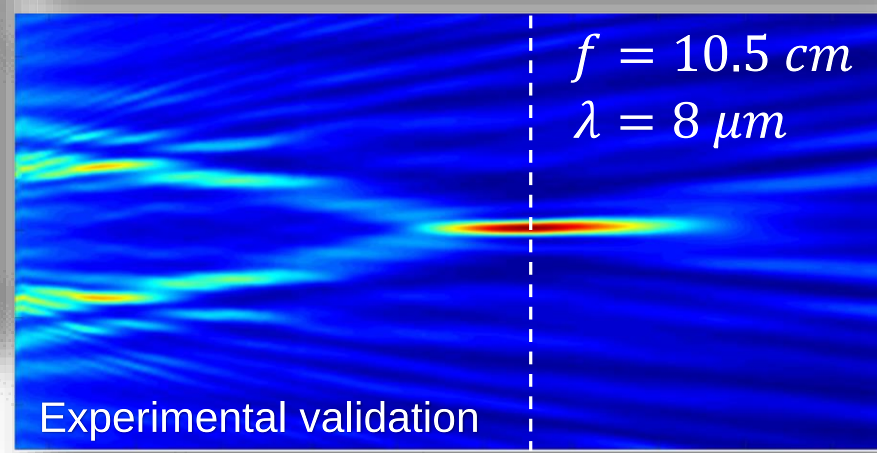




Phase calculation for
$5\ \mu\mathrm{m}$, $N = 8$, $f = 10$ cm

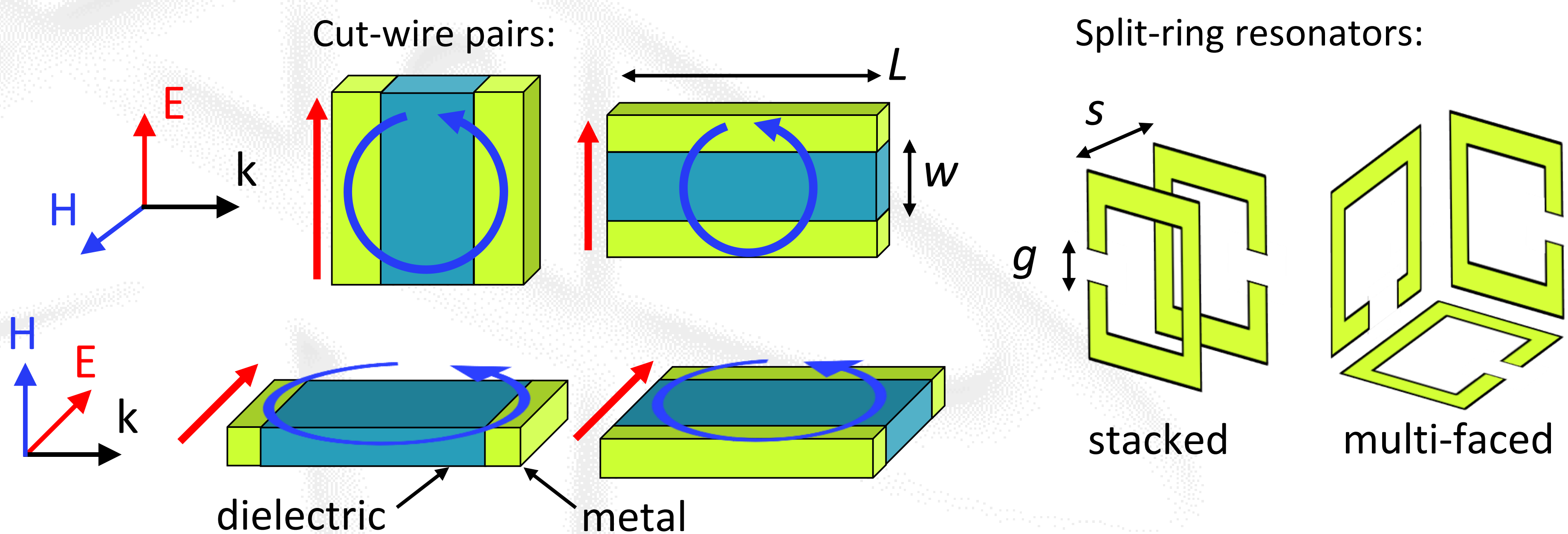






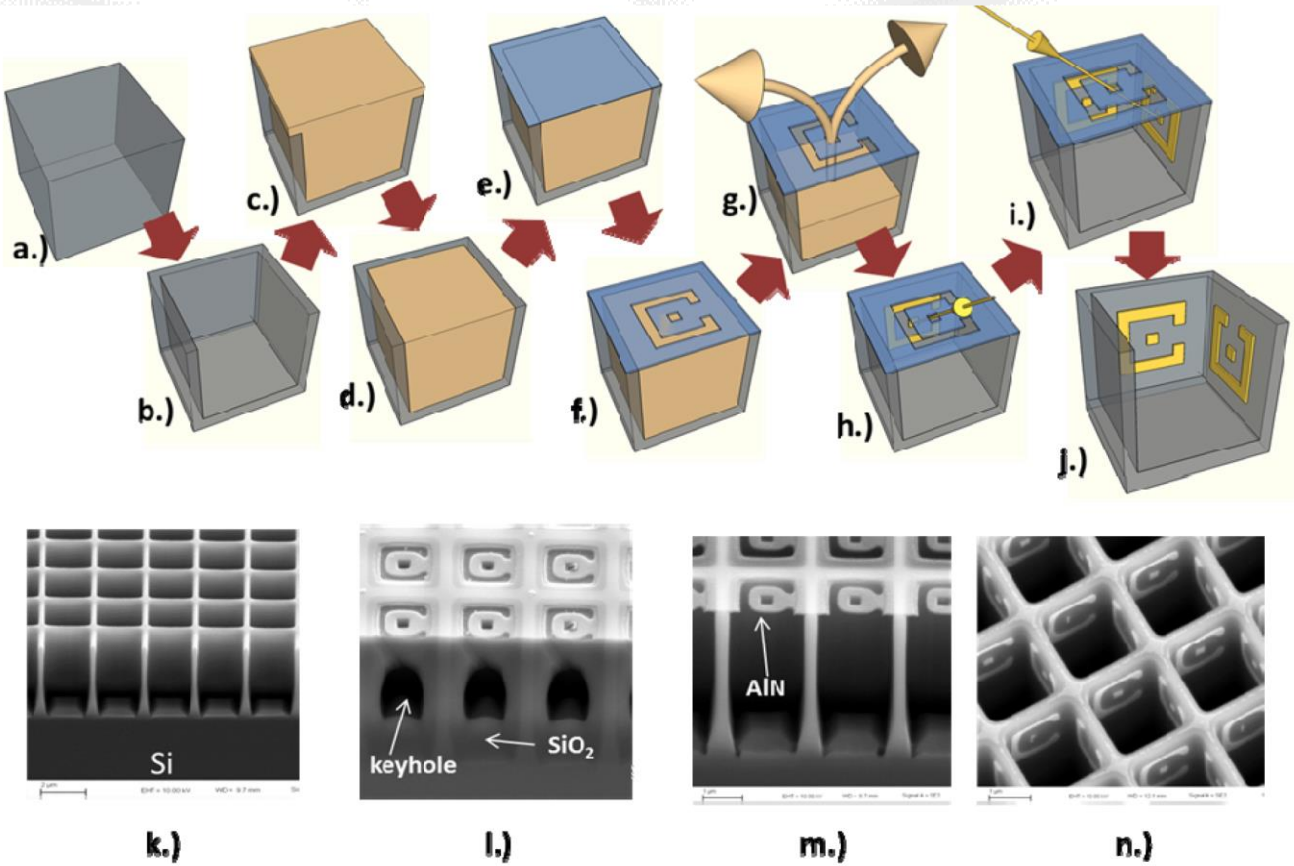
Potential Solution: 3-D Structures

- 3-D Structures offer:
  - Additional field coupling modes
  - Improved span of phase control
  - HUGE design space
- Issues:
  - Often non-analytical
  - More metal = more absorption loss
  - HUGE design space
  - Fabrication (!)



Membrane Projection Lithography

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



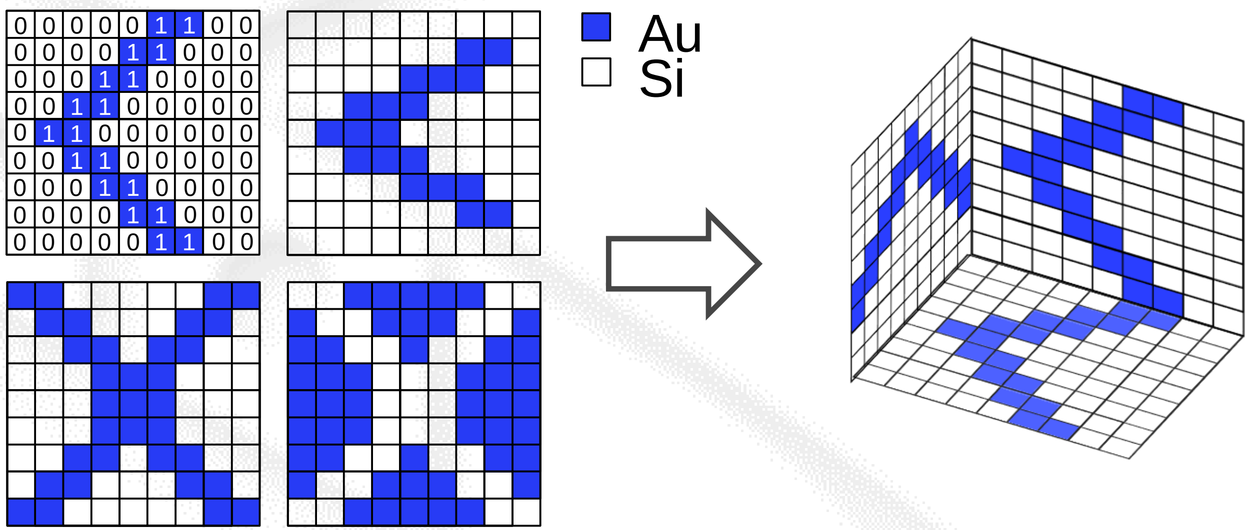
- Si/Air unit cells of arbitrary shape/periodicity
- Large area (wafer-scale)
- Metal deposition of any open shape…

Burckel et al., *Opt. Mater. Express*, **5**, 10 (2015)

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?



2D Planar
(not new, but limited)

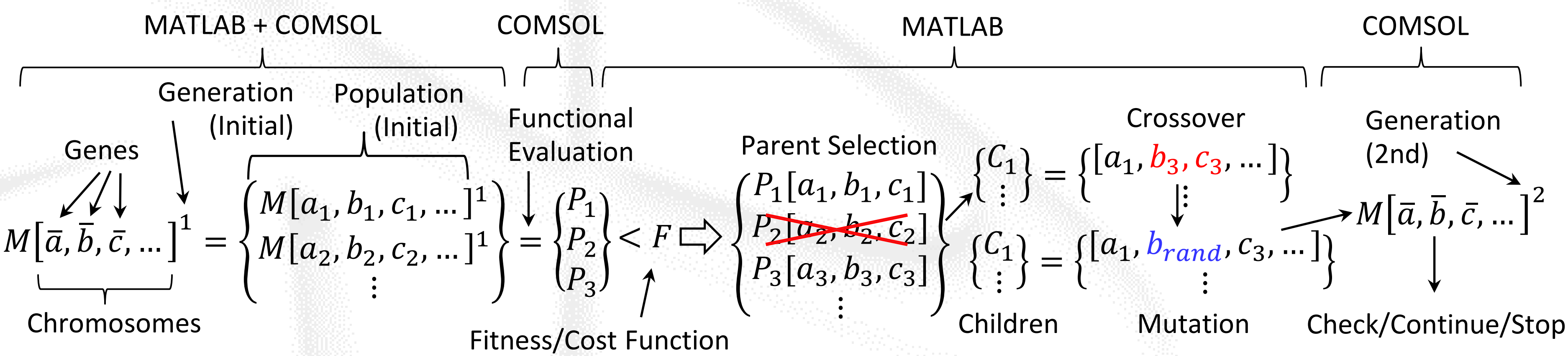
Full 3D
(new!)

- 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!



COMSOL Models

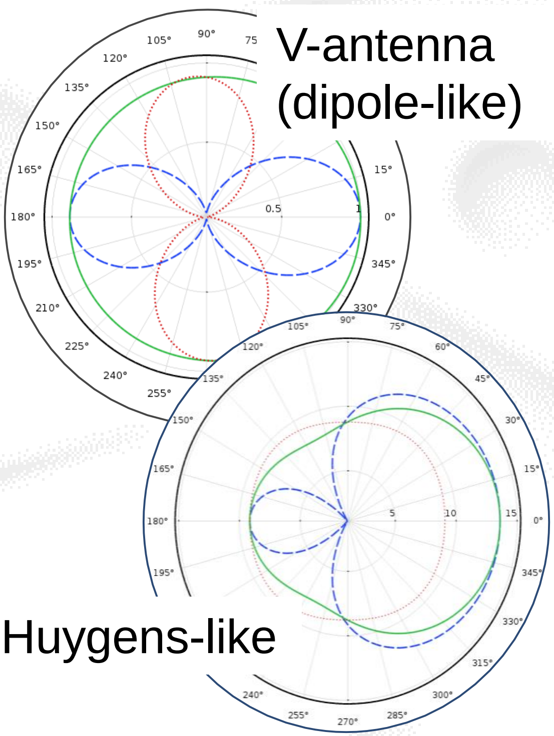
Validation Model

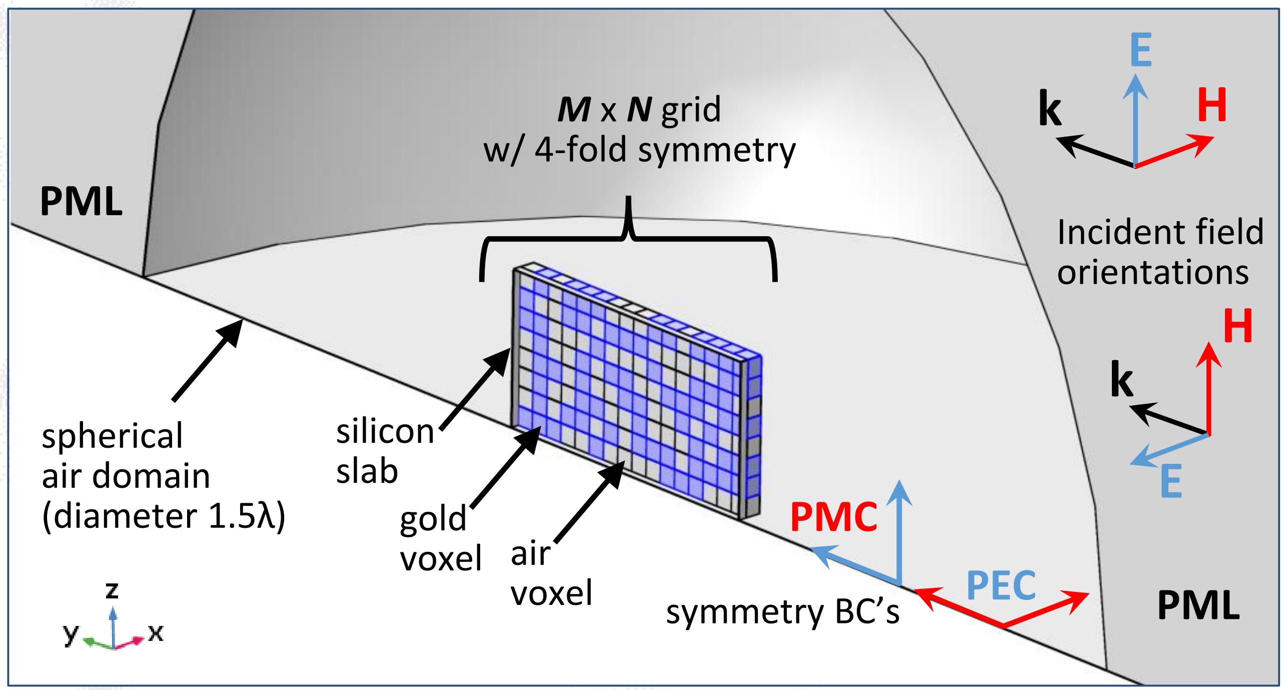
Membrane Projection Lithography (MPL) Model

Huygens Source Validation Model: Symmetric Scatterer in Air

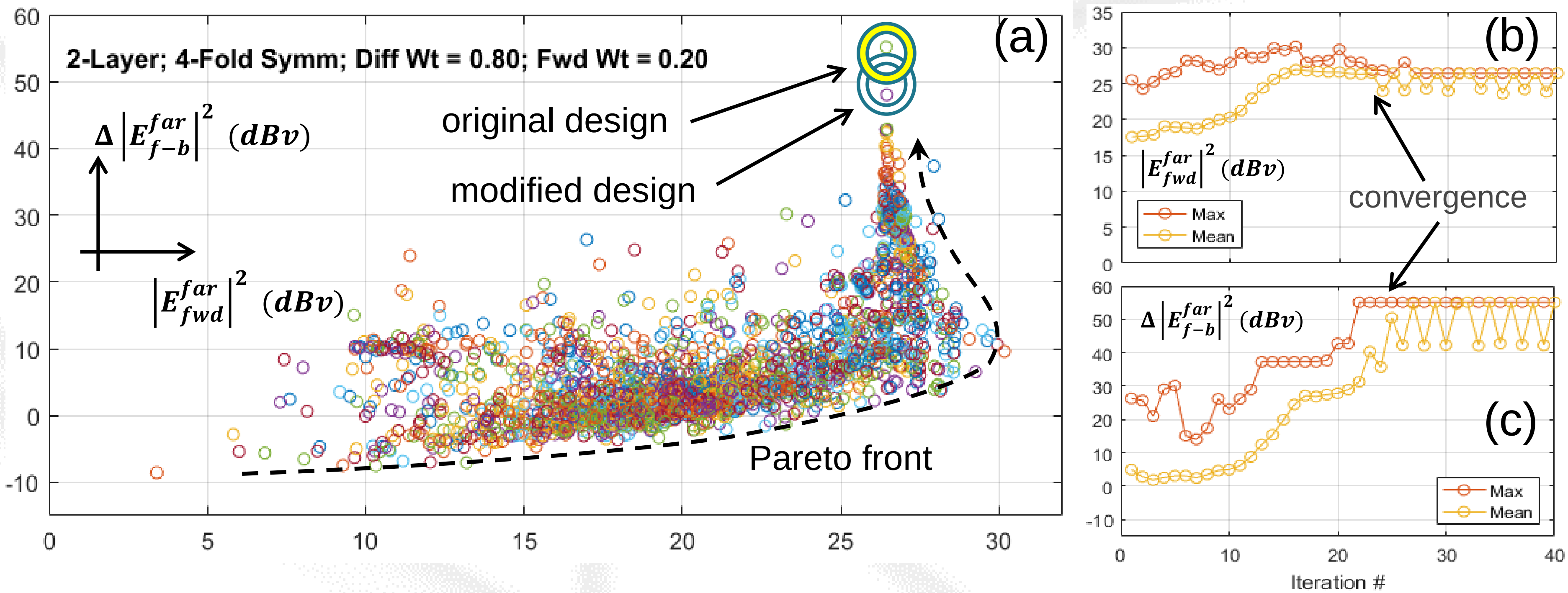
- **Objective**: validate GA routine against multi-objective fitness function, seeking a Huygens-like scatter:

$$F(w_\Delta, w_f) = w_\Delta \frac{\Delta|\boldsymbol{E}|^2 - \min(\Delta|\boldsymbol{E}|^2)}{\max(\Delta|\boldsymbol{E}|^2) - \min(\Delta|\boldsymbol{E}|^2)} + w_f \frac{|\boldsymbol{E}^f|^2 - \min\left(|\boldsymbol{E}^f|^2\right)}{\max(|\boldsymbol{E}^f|^2) - \min(|\boldsymbol{E}^f|^2)}$$



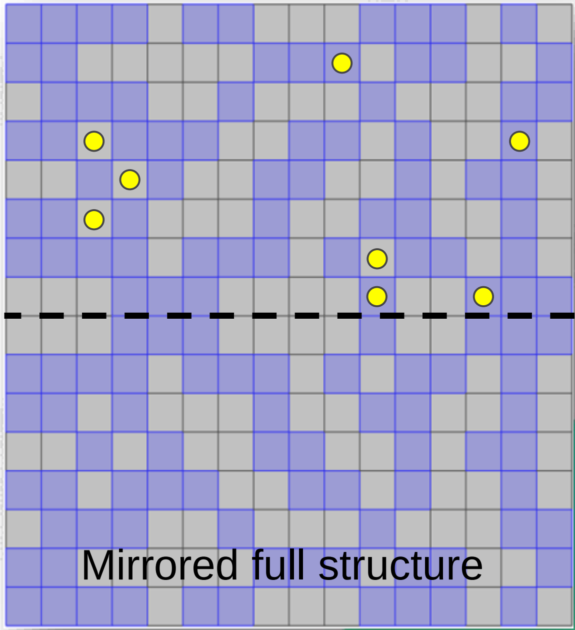


COMSOL Validation of Huygens Source Model



- What constitutes "best" in a multi-objective solution space?
  - Largest $\left|E_{fwd}^{far}\right|^2$ was $\mathbf{30\ dBv}$, with $\Delta\left|E_{f-b}^{far}\right|^2 = \left|E_{fwd}^{far}\right|^2 - \Delta\left|E_{back}^{far}\right|^2 = 20\ dBv$
  - Largest $\Delta\left|E_{f-b}^{far}\right|^2$ was $-28\ dBv$, with $\left|E_{fwd}^{far}\right|^2 = 26\ dBv$

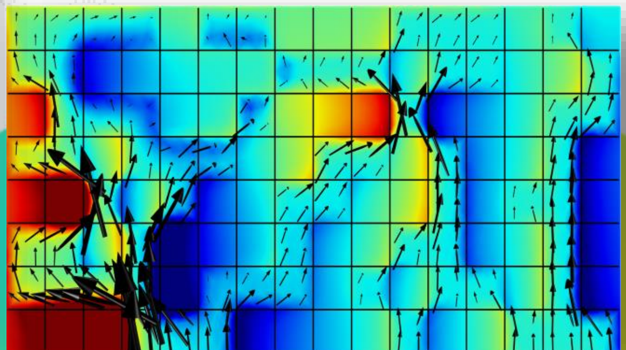
COMSOL Validation of Huygens Source Model



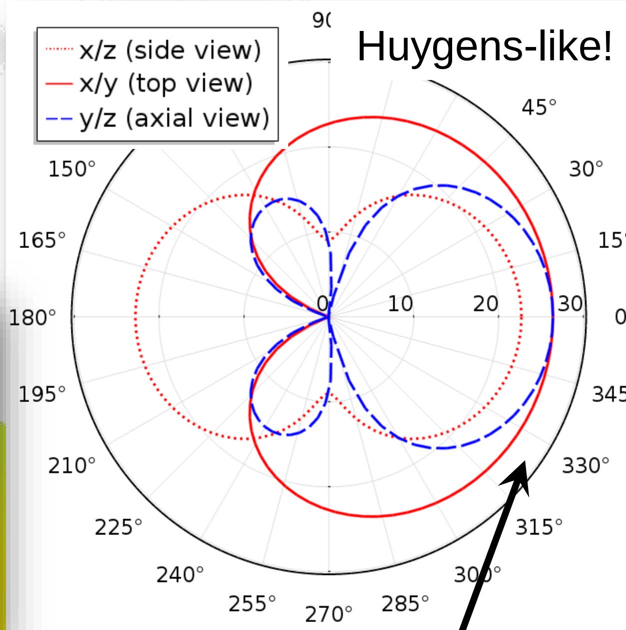
○ $= flipped\ voxels$

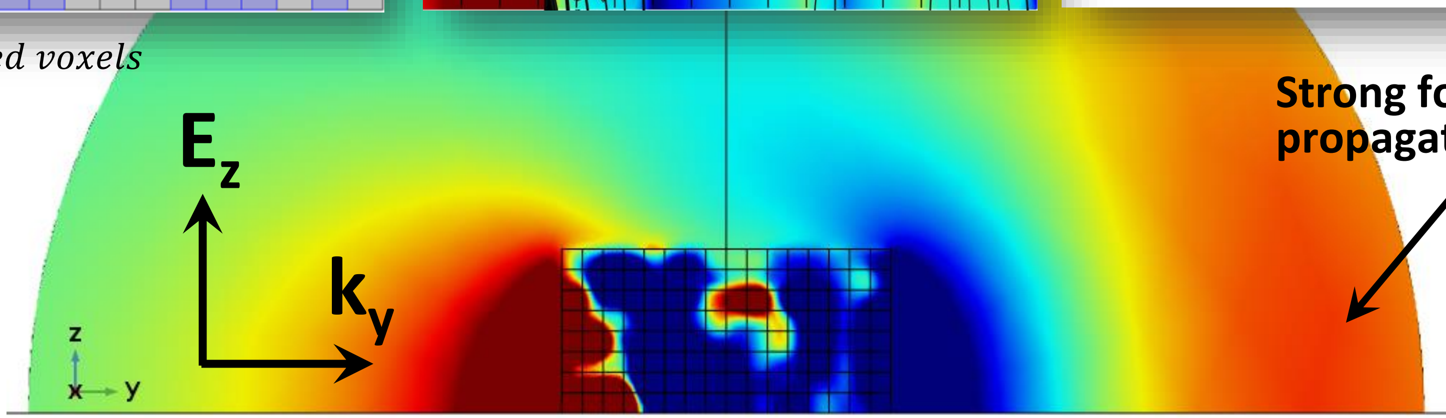
- $\boldsymbol{Best}$: $26\ dBv, -28\ dBv$
- $\boldsymbol{Modified}$: $26\ dBv, -24\ dBv$

Current density



Huygens-like!





Strong forward propagation

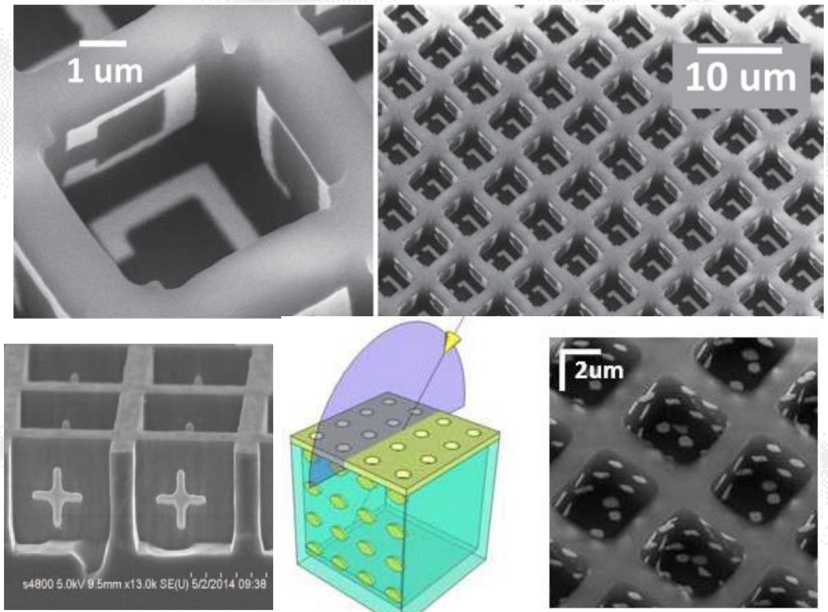
MPL-Based Model: Unit Cell Analysis

The AFIT of Today is the Air Force of Tomorrow.

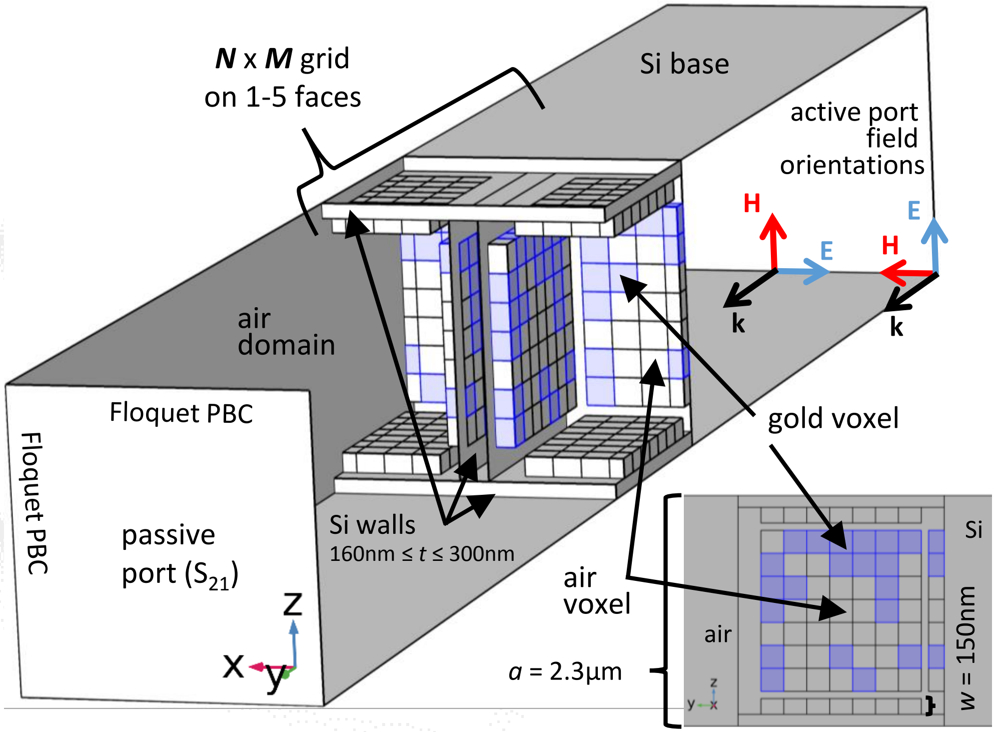
- **Objective**: use GA to identify voxel grid layout for maximum transmittance (T) at targeted phase points (Φ_0):

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

Example MPL structures

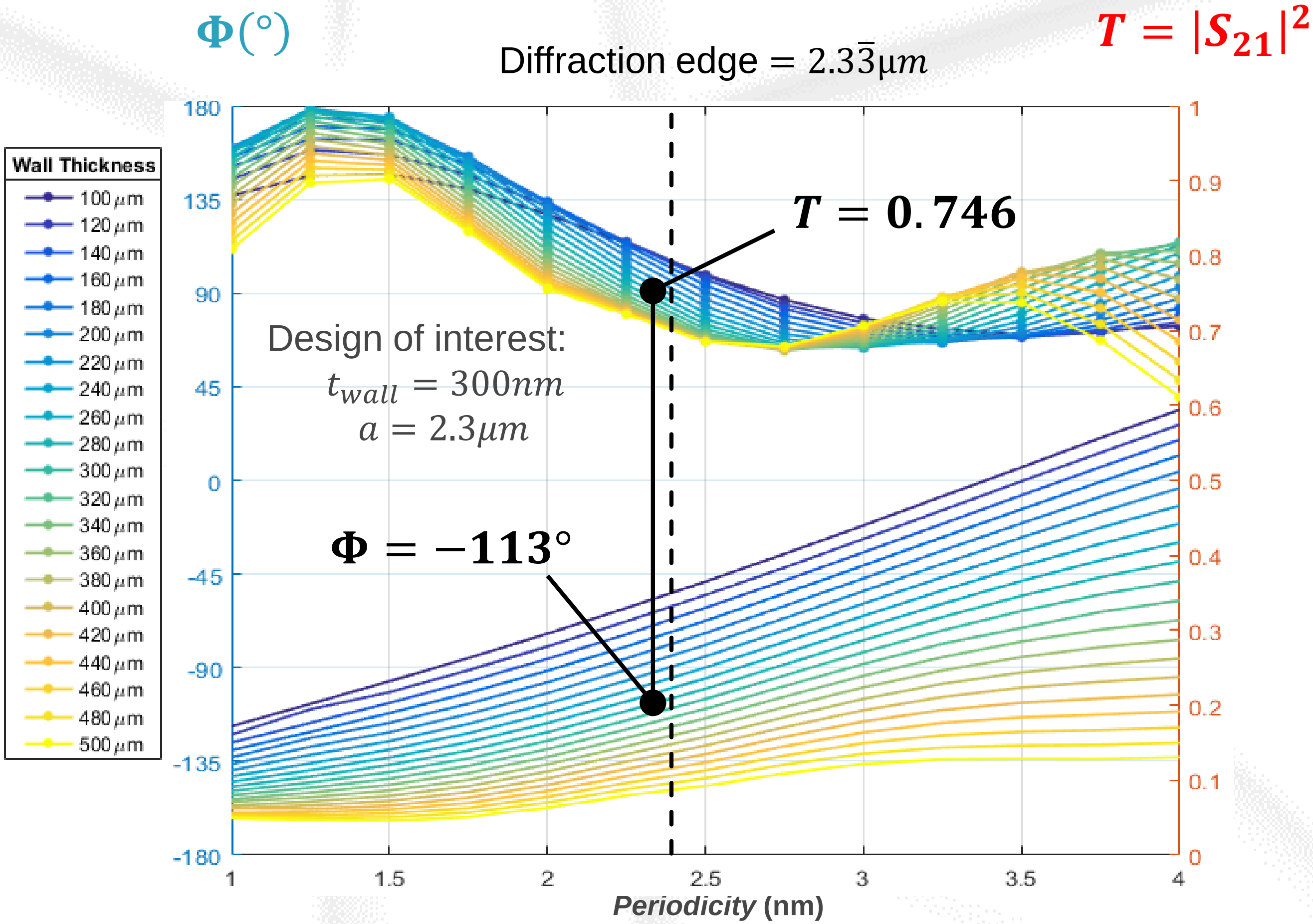


Burckel et al., *IEEE EDSSC* (2015);
Burckel et al., *Adv Mater*, **22**, 5053 (2010)

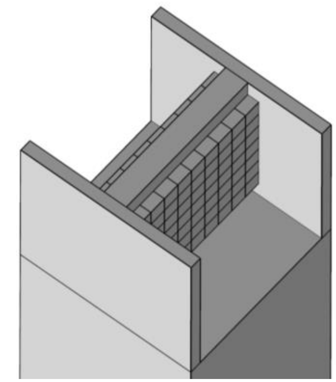


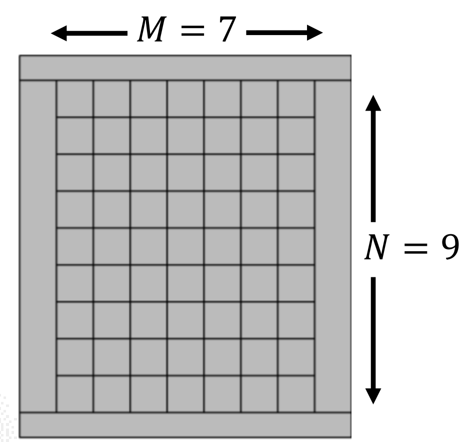
Baseline of Undecorated MPL Si Boxes

The AFIT of Today is the Air Force of Tomorrow.



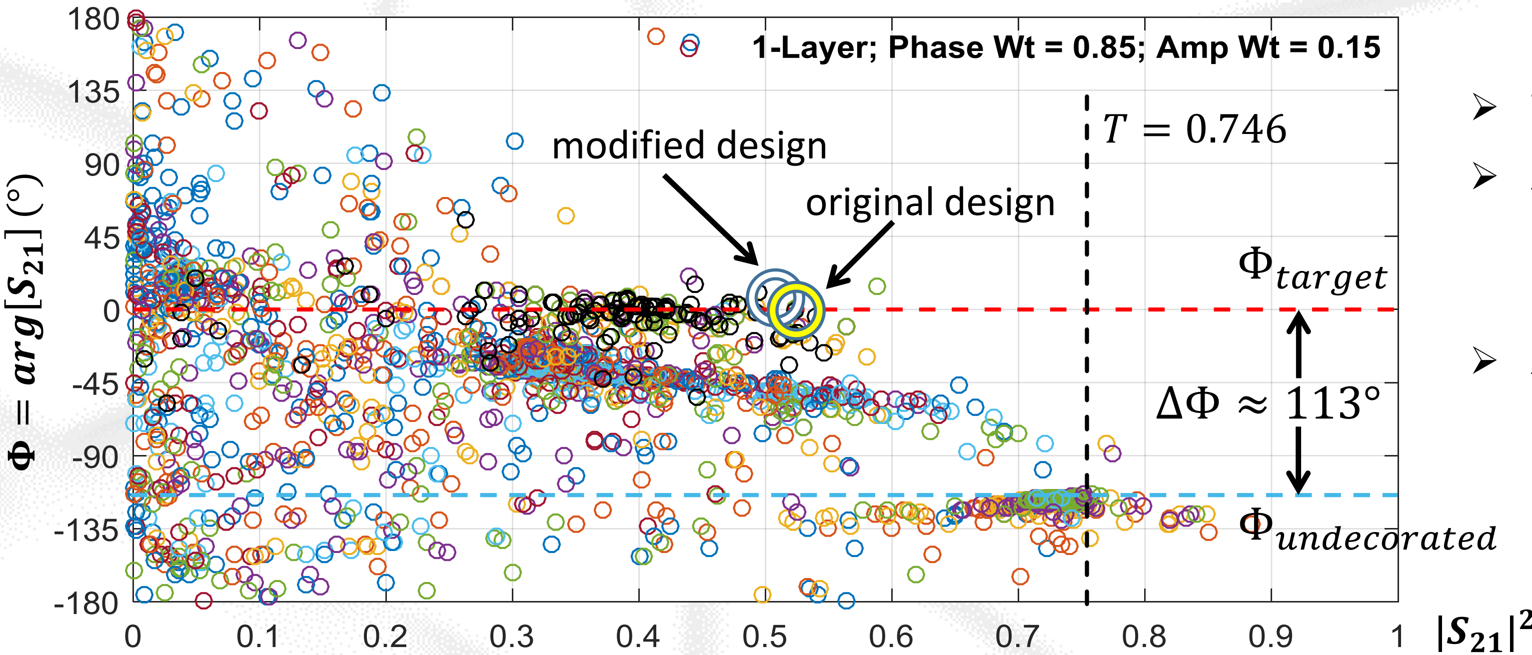
Undecorated Model



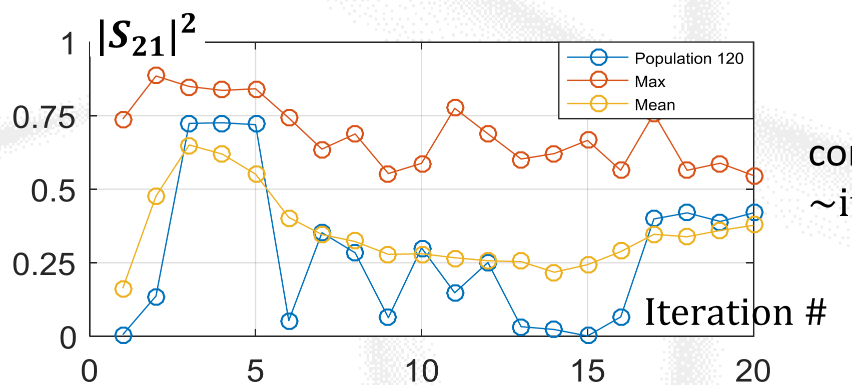


COMSOL Validation of MPL Model

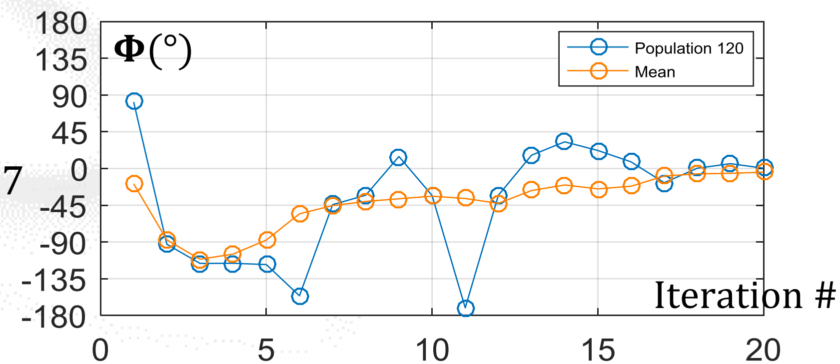
The AFIT of Today is the Air Force of Tomorrow.



- ***Target***: $0°$
- ***Best***:
  $\Phi = -0.15°$
  $T = 0.52$
- ***Modified***:
  $\Phi = 13.7°$
  $T = 0.49$



convergence
~iteration #17

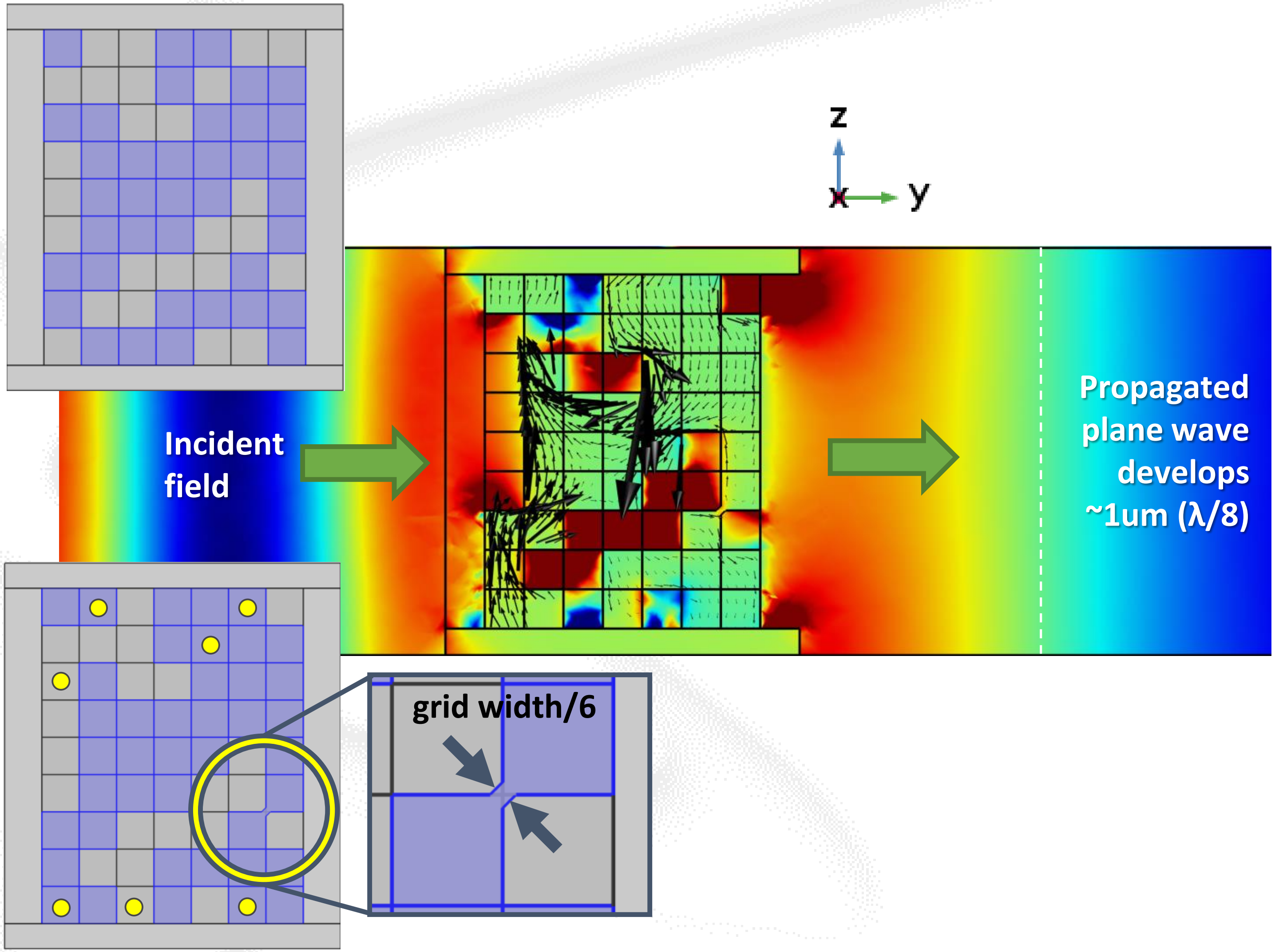


COMSOL Validation of MPL Model

- ***Best***:
  $\Phi = -0.15°$
  $T = 0.52$

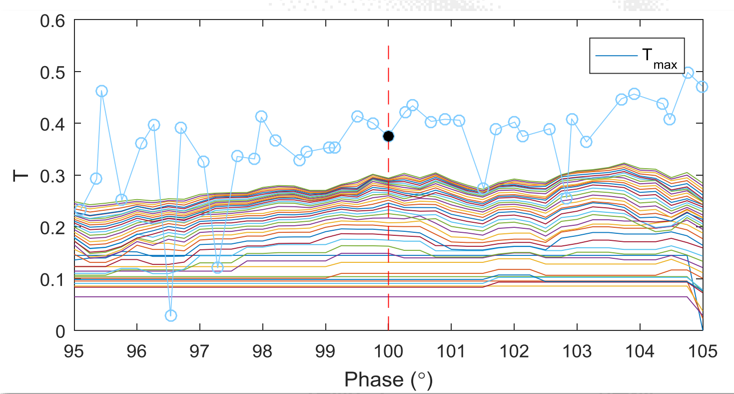
- ***Modified***:
  $\Phi = 13.7°$
  $T = 0.49$

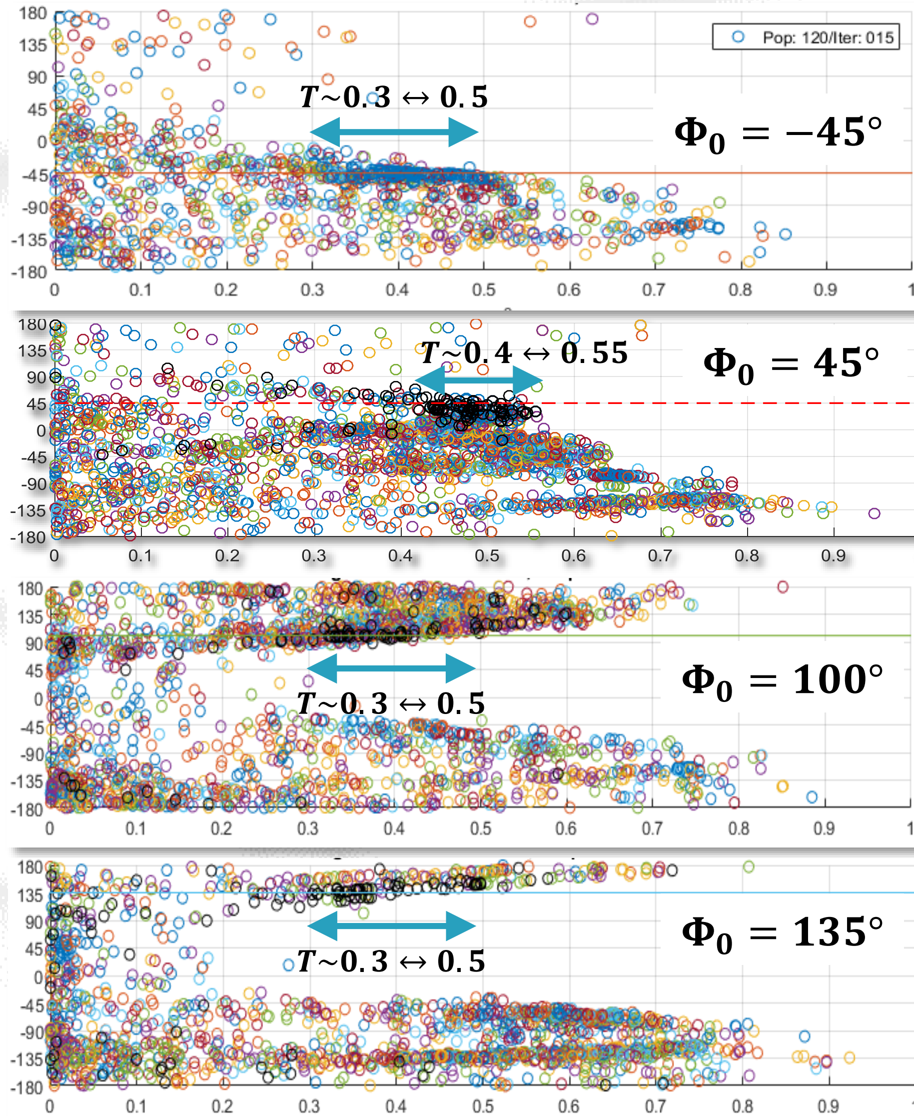
● = *flipped voxels*



COMSOL Validation of MPL Model

- Repeatability:
  - Accurately hit all 8 target phases
  - Transmittances typically between $\mathrm{T} = 0.3 - 0.5$
  - Required $20 - 30$ iterations for convergence
- Flexibility:
  - Dozens of designs per ° phase
  - $1° - 10°$ span in $\mathbf{\Phi_0}$ may provide $10\% - 20\%$ increase in T





Early Fabrication

First Etch/Deposition

EBL Etch & Au Deposition

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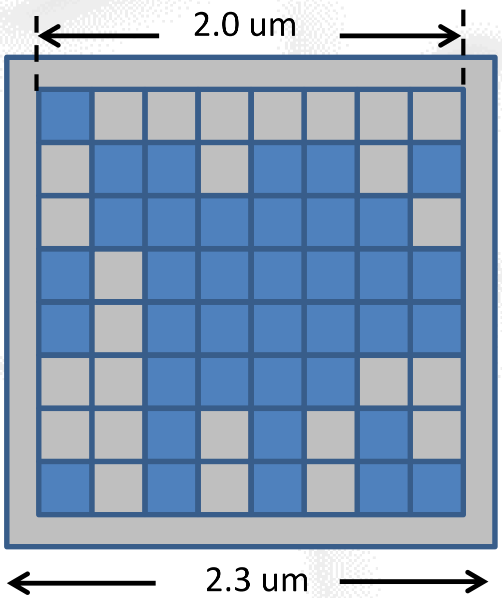
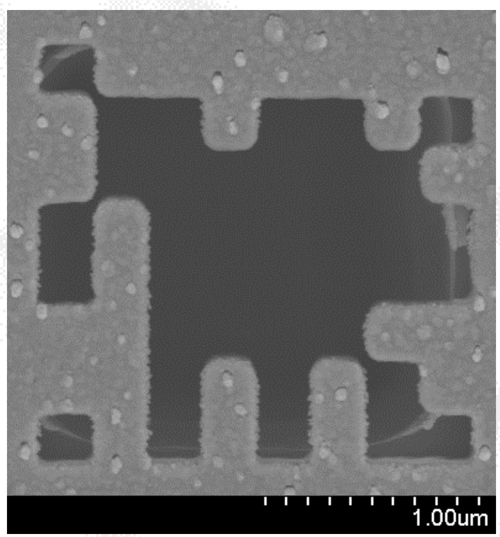
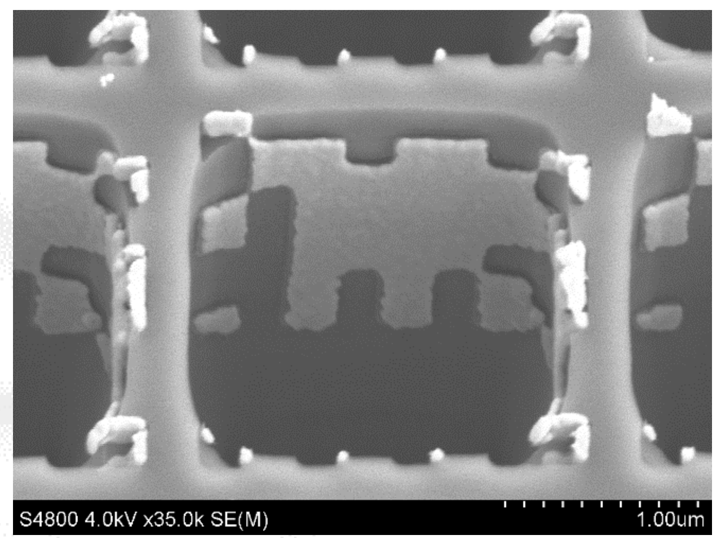
- VERY early fabrication attempts @ 250nm resolution
  - First-ever use of e-beam lithographic mask for MPL process
  - Tested on low-quality cubic Si arrays—but not perfectly cubic!
    - Poor deposition of metal on upper/side walls as result
- Verdict: clear corner/corner contact, sharp features

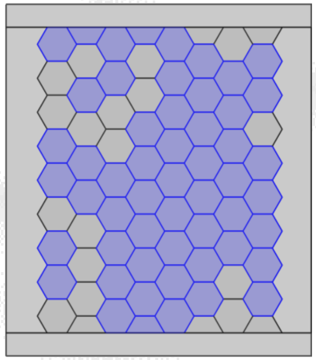


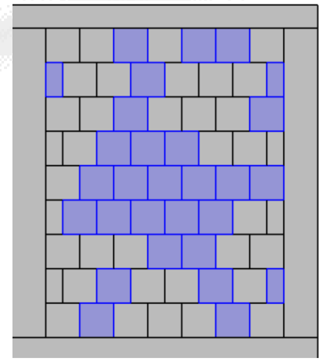




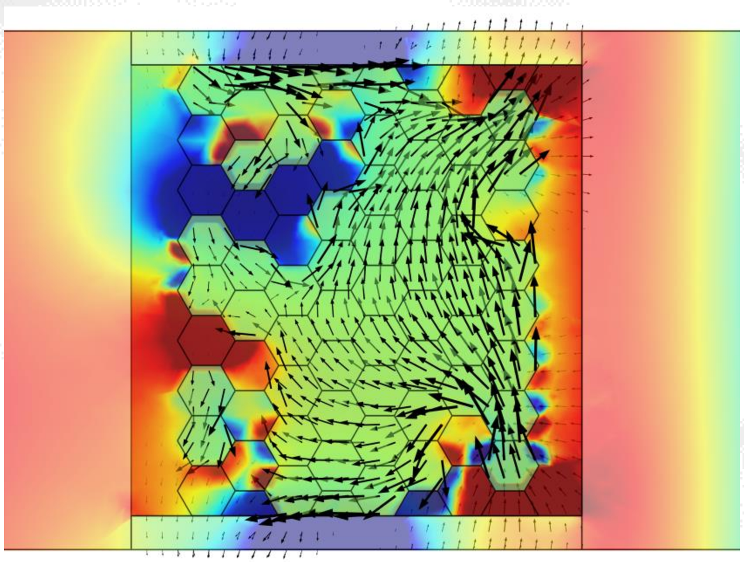
(VERY!) Recent Improvements

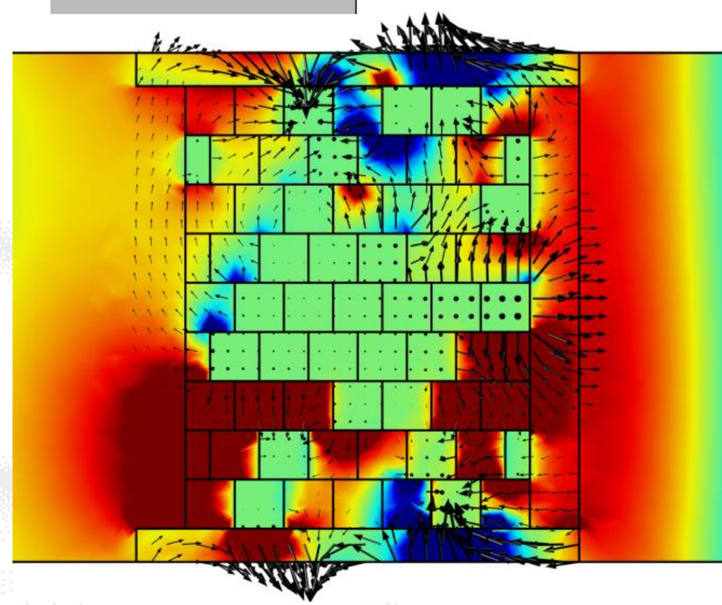
T	R
0.61	0.08
Phase (°)	Δ Phase (°)
113	134





T	R
0.46	0.17
Phase (°)	Δ Phase (°)
0.01	113





Conclusion

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

Additional Material

Limitations of 2-D Metasurfaces

Results of “brick” grid MPL Design

Limitations of 2-D Planar Metasurfaces

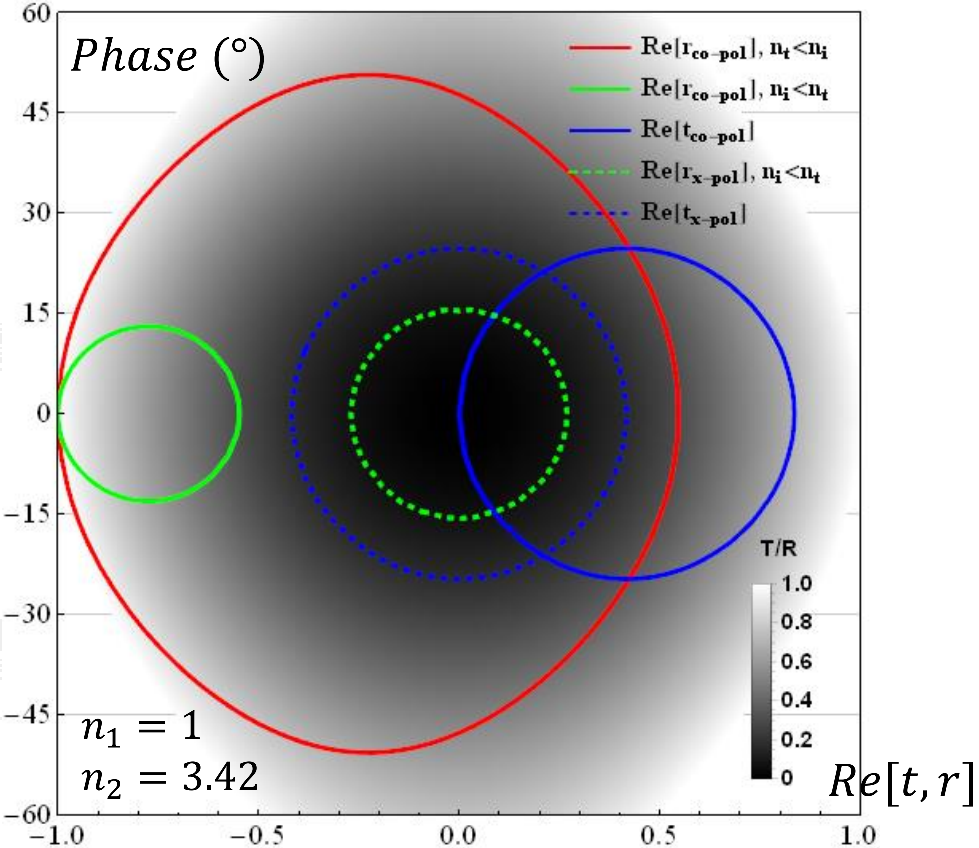
- Fundamentally, thin 2-D metasurfaces *cannot*:
  - reach desired phase range in co-polarized states
  - reach high amplitudes in cross-polarized states

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

$$\left|r_{co-pol}\right|^2 + \frac{n_2}{n_1}\left|r_{co-pol} + 1\right| \leq 1$$

$$\left|t_{x-pol}\right|^2 \leq \frac{n_1 n_2}{(n_1 + n_2)^2}$$

$$\left|r_{x-pol}\right|^2 \leq \frac{n_1^2}{(n_1 + n_2)^2}$$

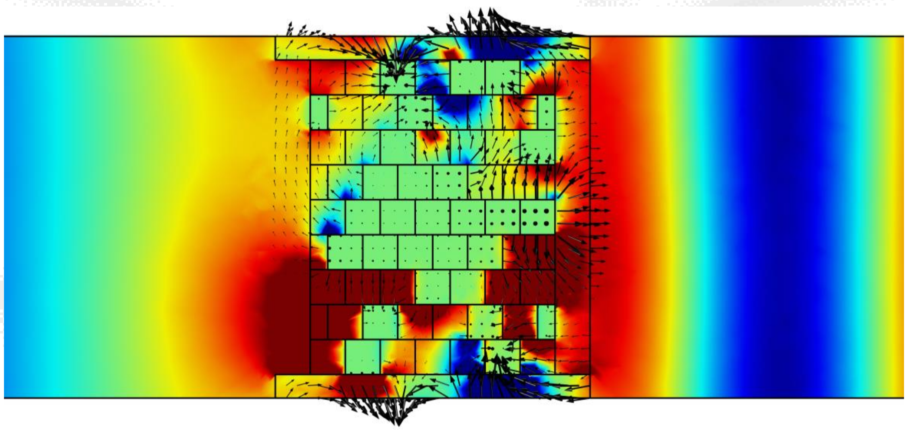


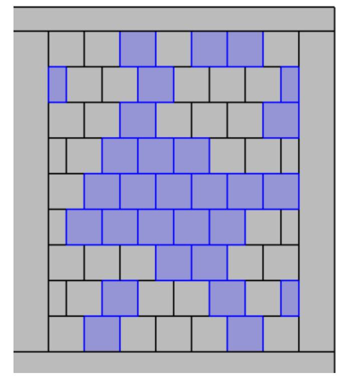
A. Arbabi and A. Faraon, Sci Rep, **7**, 43722 (2017)

“Fabricate-able” Voxel Geometries

The AFIT of Today is the Air Force of Tomorrow.

- 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





T	R
0.46	0.17
Phase (°)	**Δ Phase (°)**
0.007	113