

ECE 595, Section 10

Numerical Simulations

Lecture 33: Introduction to Finite-Difference Time-Domain Simulations

Prof. Peter Bermel

April 3, 2013

Recap from Monday

- Numerical ODE solvers
 - Initial value problems
 - Boundary value problems
- nanoHUB Tool – CMTcomb3:
 - Rationale
 - Governing ODEs
 - User interface
 - Output analysis

Outline

- Recap from Monday
- Introduction to FDTD
- Special features of MEEP:
 - Perfectly matched layers
 - Subpixel averaging
 - Symmetry
 - Scheme (programmable) interface
- Examples:
 - Periodic light-trapping structures
 - Randomly textured structures

Equations for Light Propagation

$$\frac{dB}{dt} = -\vec{\nabla} \times \vec{E} - J_B - \sigma_B B$$

Fictitious magnetic current

$$\frac{dD}{dt} = \vec{\nabla} \times \vec{H} - \vec{J} - \sigma_D D$$

Fictitious magnetic conductivity

Material absorption

$$D = \epsilon E$$

Radiating dipole source

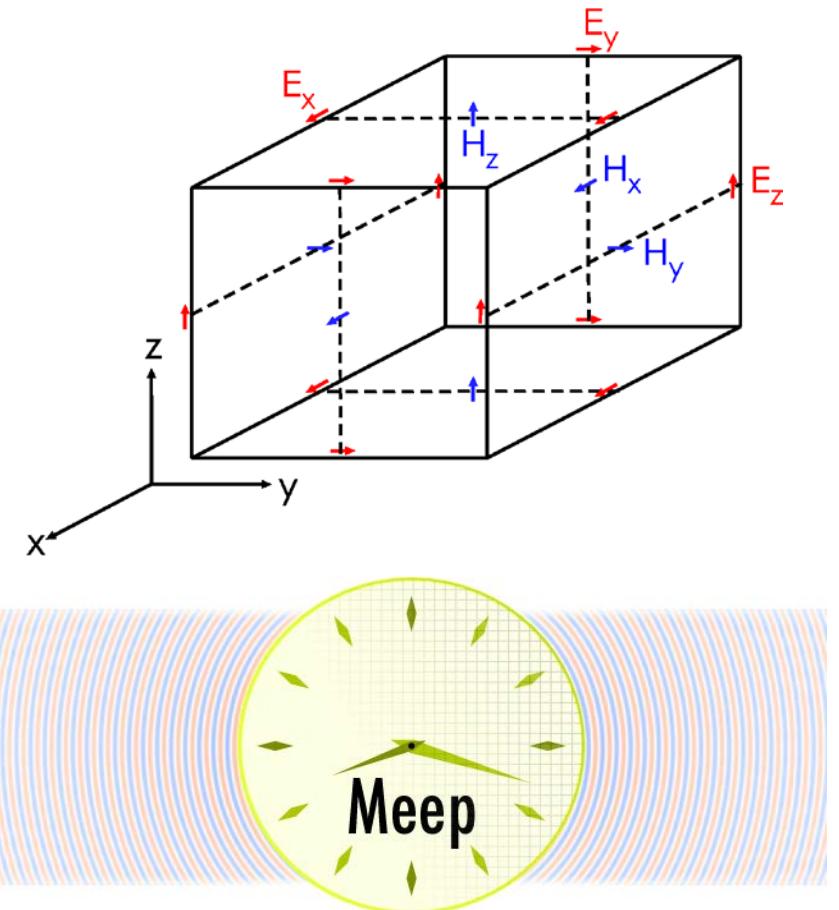
$$H = B / \mu$$

dielectric function $\epsilon(\mathbf{x}) = n^2(\mathbf{x})$

magnetic permeability $\mu(\mathbf{x})$

Finite Difference Time Domain

- Discretize space and time on a Yee lattice
- “Leapfrog” time evolution of Maxwell’s equations:
 - Alternate E and H fields in space & time
 - Accuracy $\sim 1/\Delta t^2$
- Implemented in MEEP (jdj.mit.edu/meep)



FDTD Stability

- Assume error is bounded after arbitrarily long time (von Neumann stability analysis)
- Leads to Courant condition:

$$\Delta t \leq \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

- Assuming uniform grid:

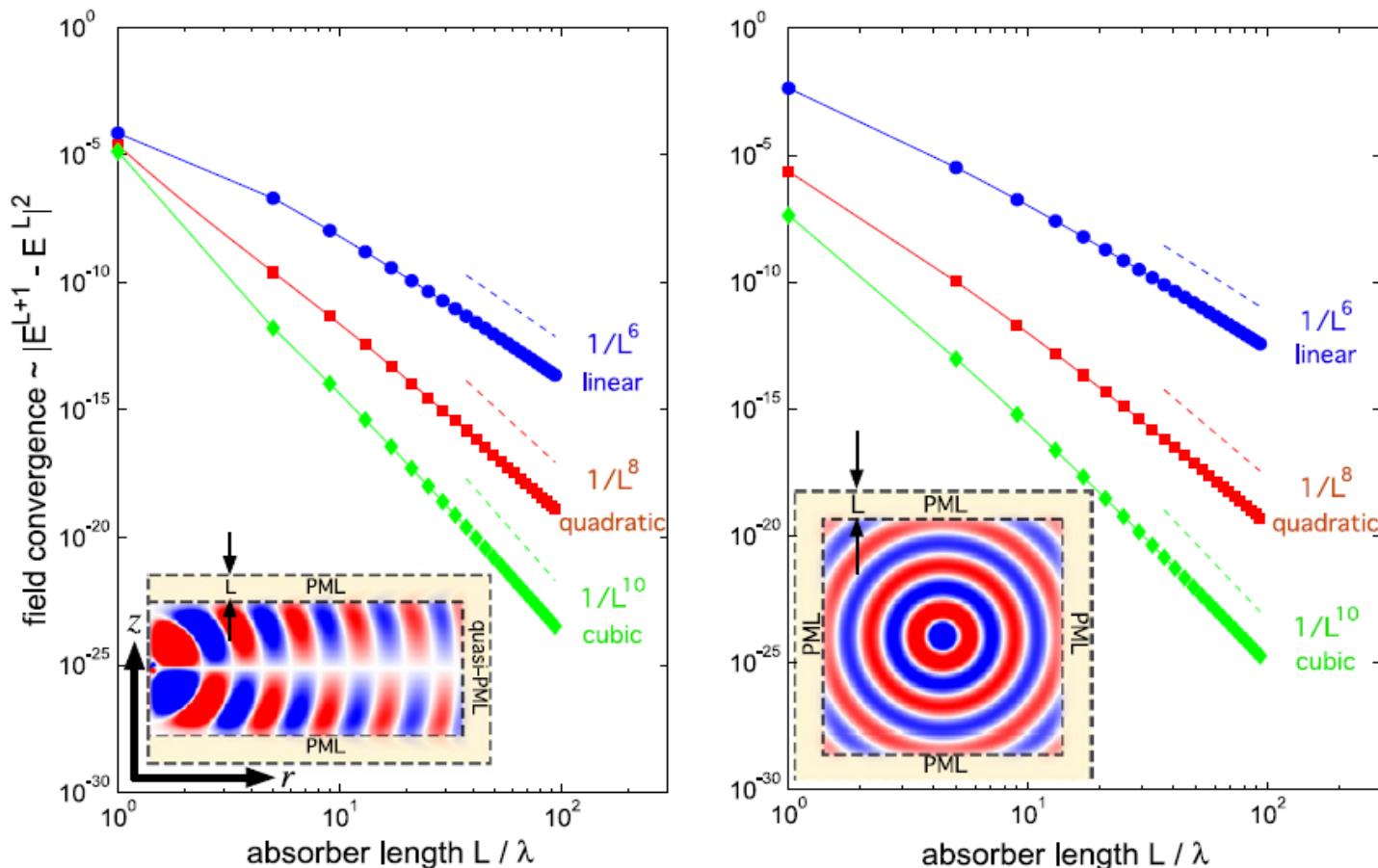
$$c \leq \frac{1}{\sqrt{3}} \frac{\Delta x}{\Delta t}$$

- Choose $\Delta x = \Delta t$ and $c = 1/2$ for simplicity

Special Features of MEEP

- Arbitrary dimensionality, boundary conditions
- Perfectly matched layers
- Subpixel averaging
- Symmetry and parallelization
- Fully programmable
- Nonlinear and saturable gain media
- Frequency-domain solver

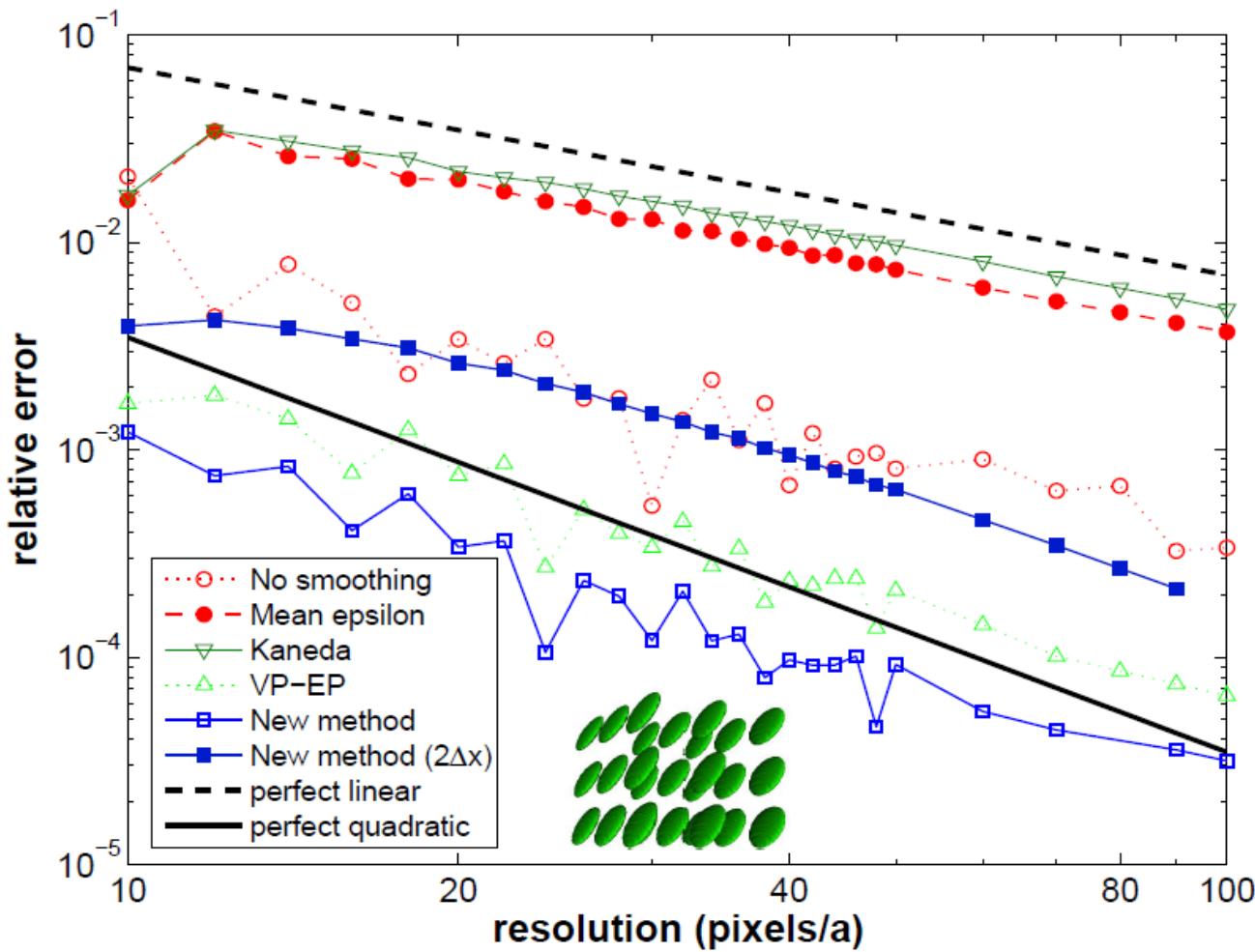
Perfectly Matched Layers



A. Farjadpour, D. Roundy, A. Rodriguez, M. Ibanescu, P. Bermel, J.D. Joannopoulos,
Johnson, *Comput. Phys. Commun.* (2009)

S.G.

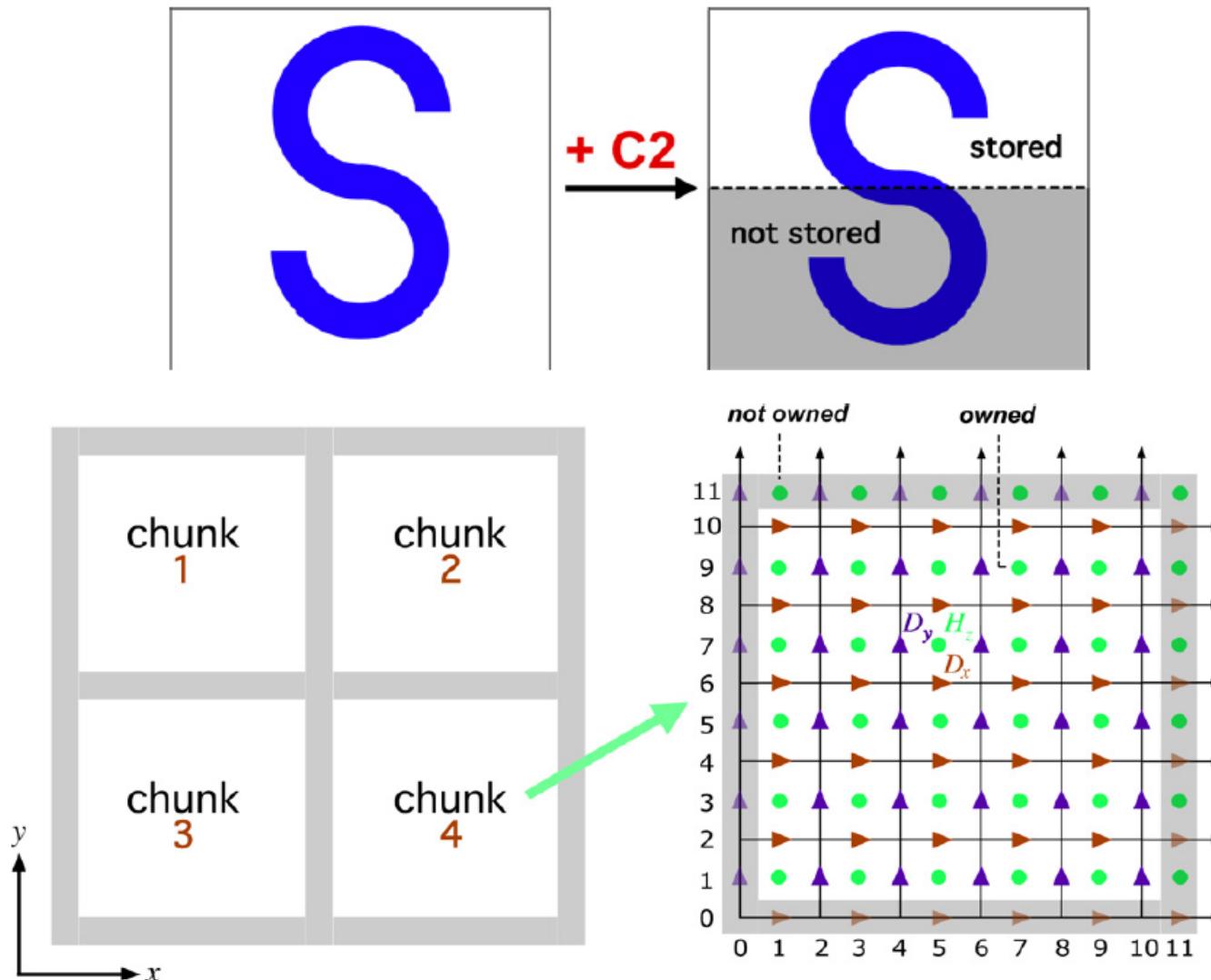
Subpixel Averaging



A. Farjadpour, D. Roundy, A. Rodriguez, M. Ibanescu, P. Bermel, J.D. Joannopoulos,
Johnson, *Proc. SPIE 6322*, 63220G (2006)

S.G.

Symmetry and Parallelization



Using the Scheme Interface

```
(set! geometry-lattice (make lattice (size 16 8 no-size)))
(set! geometry (list
                (make block (center 0 0) (size infinity 1)
                      (material (make dielectric (epsilon 12))))))
(set! pml-layers (list (make pml (thickness 1.0)))))

(set! sources (list
               (make source
                     (src (make continuous-src (frequency 0.15)))
                     (component Ez)
                     (center -7 0)))))

(set! resolution 10)
(run-until 200
          (at-beginning output-epsilon)
          (at-end output-efield-z))
```

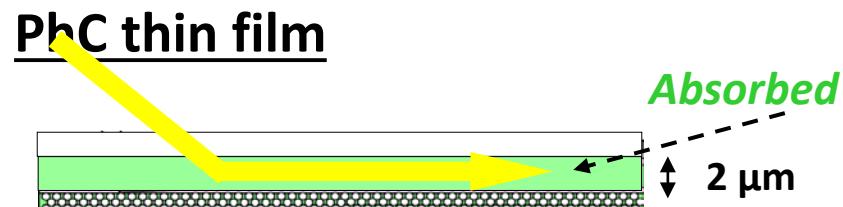
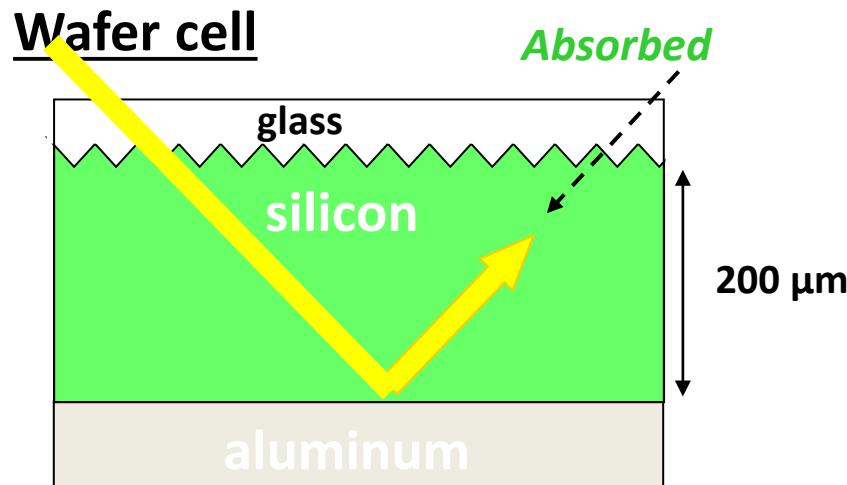
computational cell & materials

current source

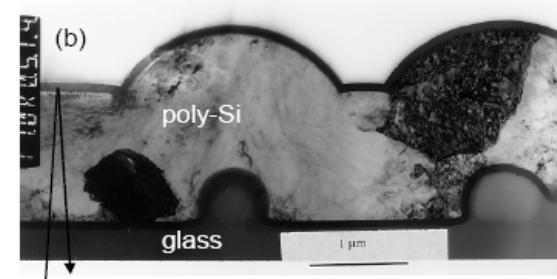
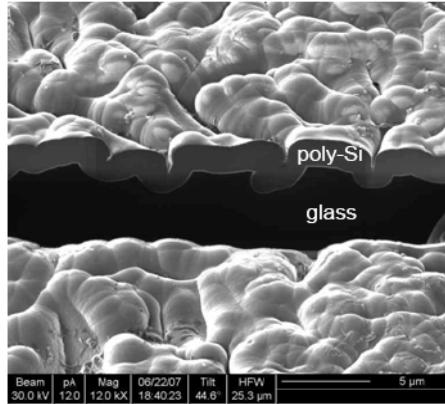
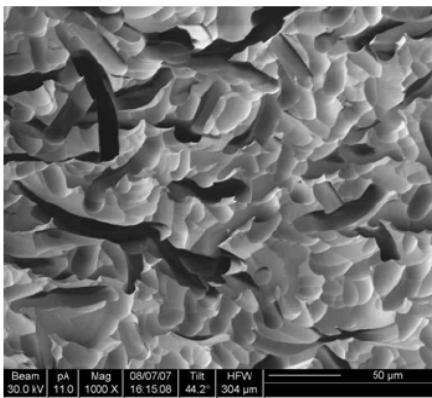
run & output

HDF5 file → plotting program

Example: Simulating Si PV Absorption



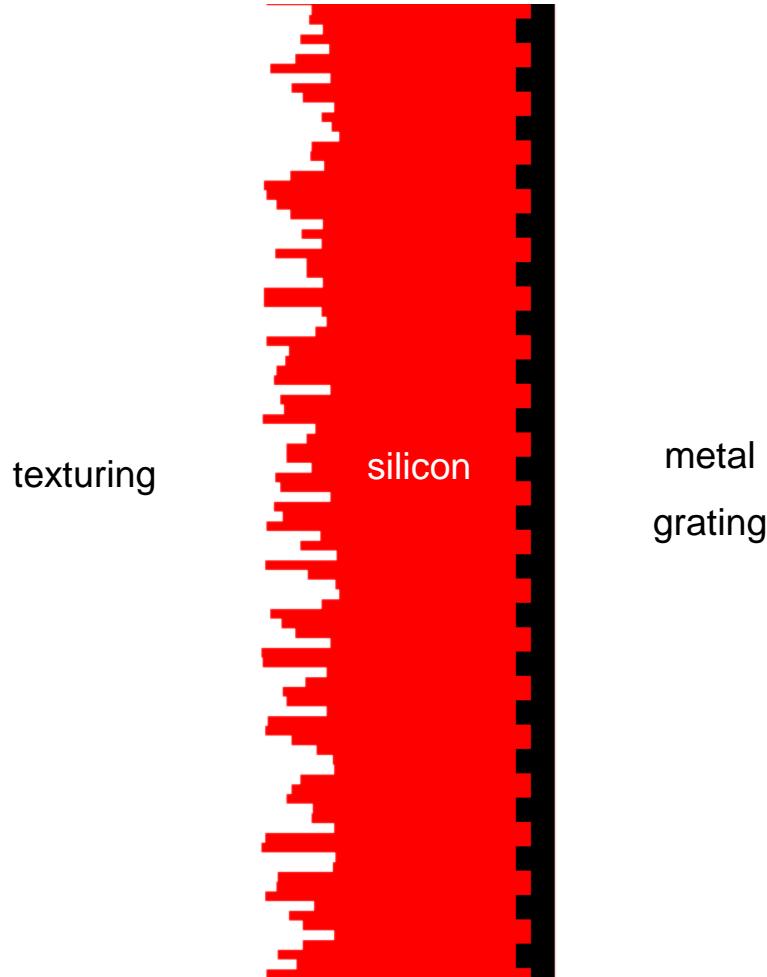
Different Geometric Light Trapping Approaches for Commercial μ -Si Cells



Treatment #1	Sand blast	Abrasion etch	Bead coat
Treatment #2	HF etch	HF etch	(used in our samples)
Feature depth	10-100 μ m	500 nm	500 nm
Feature width	10 μ m	1-5 μ m	500 nm

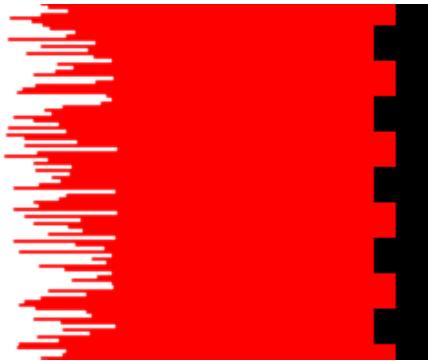
M.J. Keevers et al., “10% Efficient CSG Minimodules,”

Computational Set-up

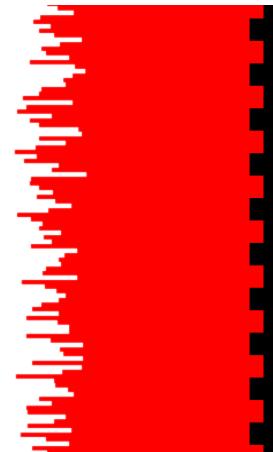


- Thickness of film = our experimental samples ($1.47 \mu\text{m}$)
- Four geometries tested
- Random texturing:
 - Uniform height distribution over 500 nm
 - Distance between features varies
- Photonic crystal:
 - Reflection captured by metal
 - Diffraction captured by grating (optimized for this thickness)

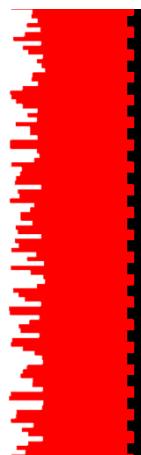
Varying spacing between features



5 periods

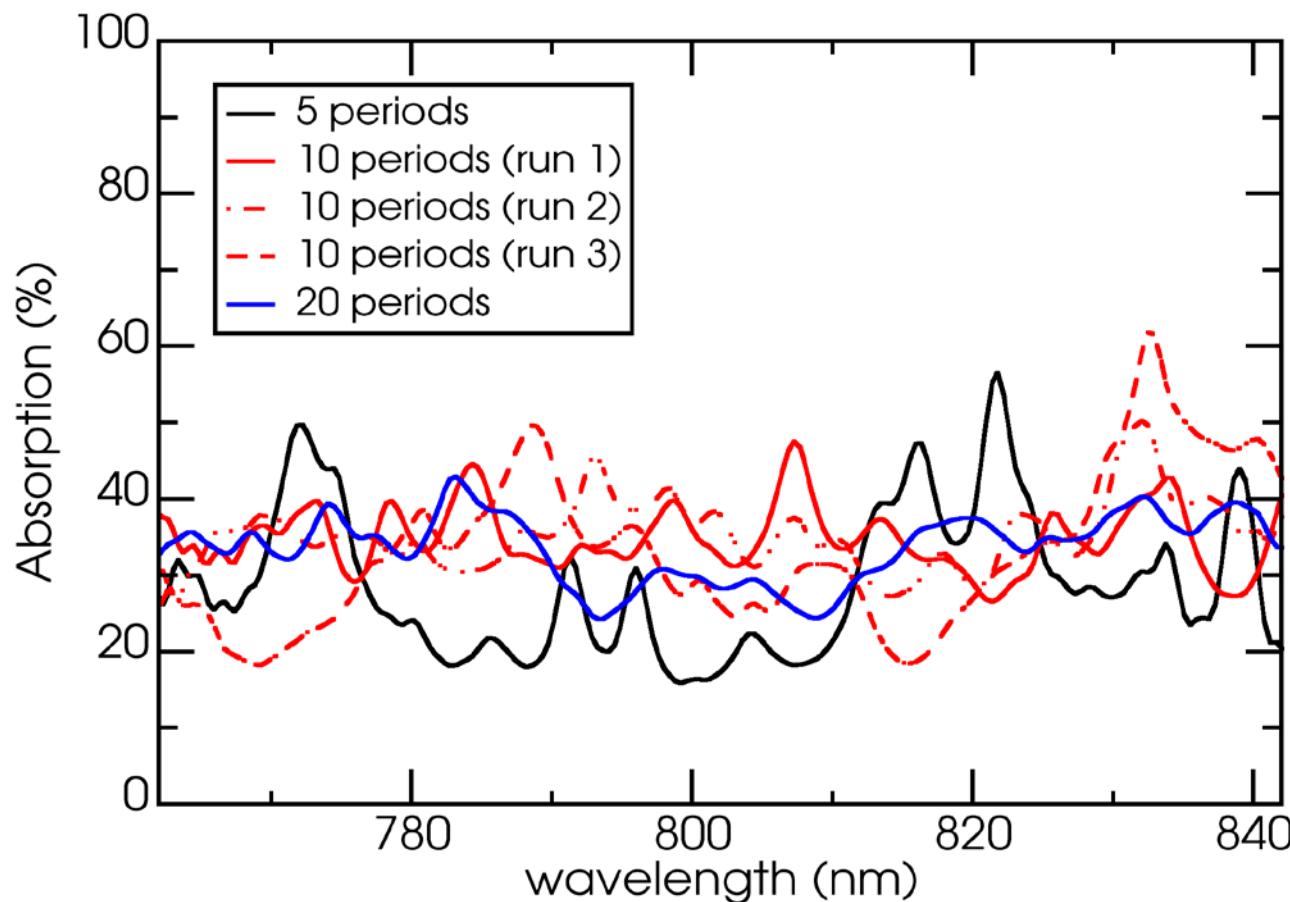


10 periods



20 periods

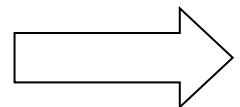
Varying spacing between features: absorntion



Sharp spectral features smoothed out with greater # periods and
feature spacing

Propagation of Light in Planar Geometry

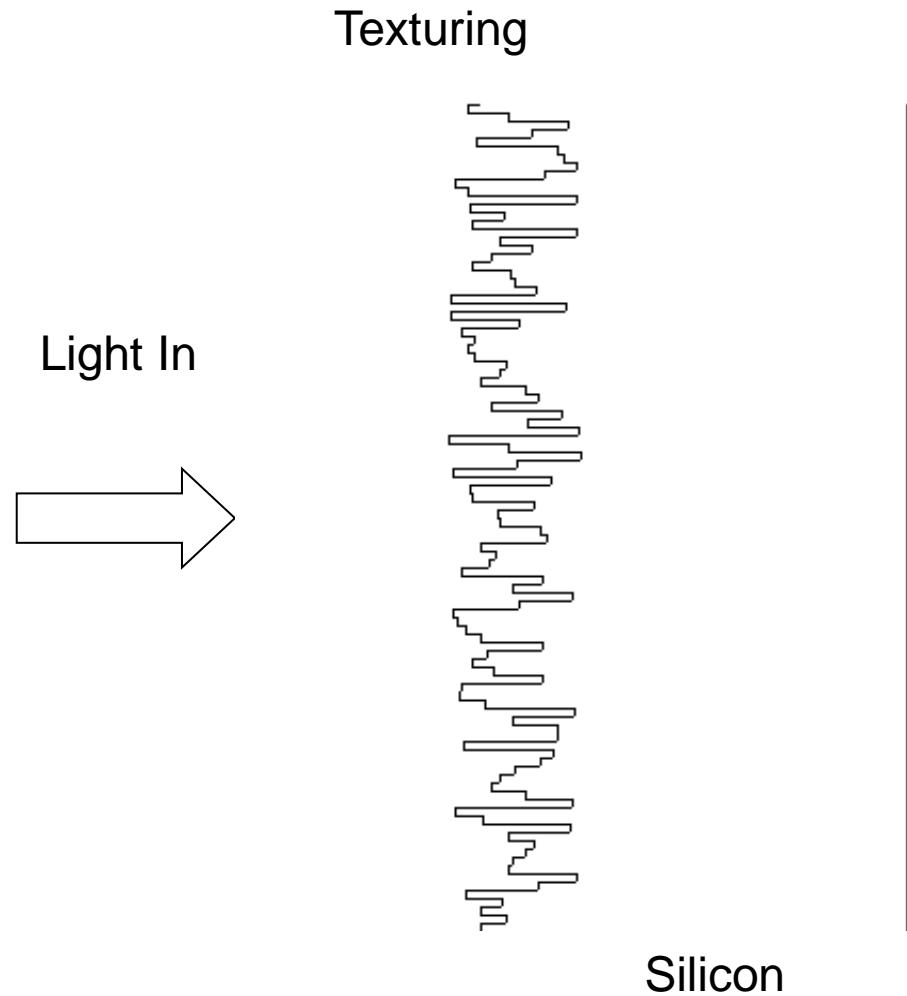
Light In



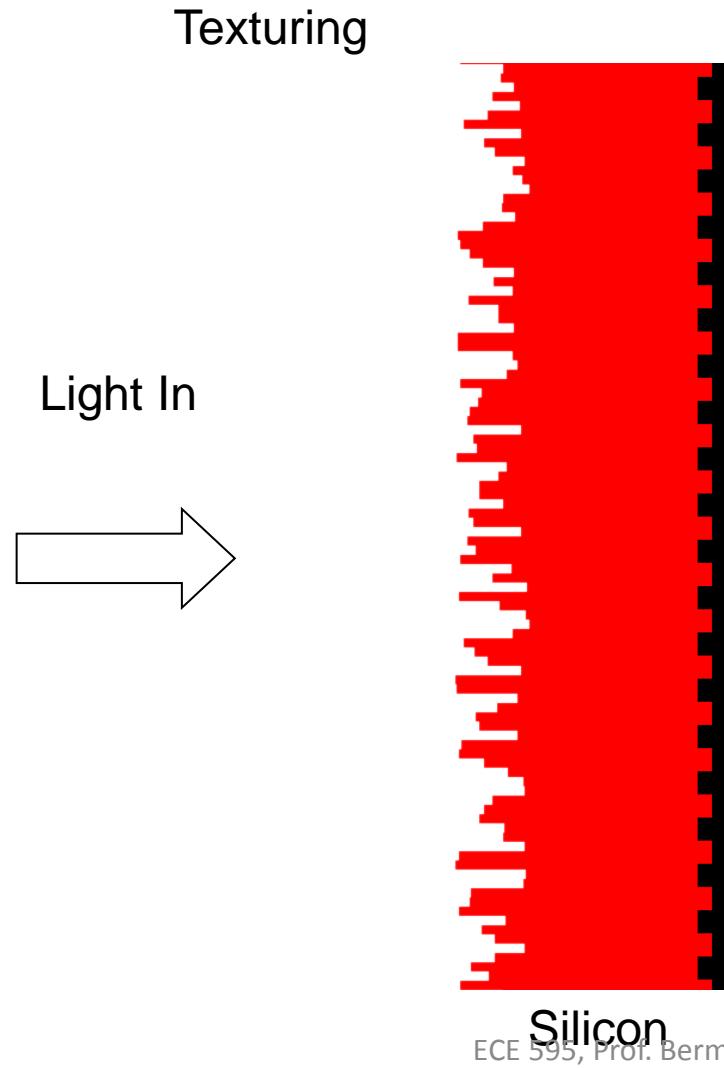
Metal
backing

Silicon

Propagation of Light in Textured Geometry (no backing)



Propagation of Light in Textured Geometry + Metal Grating



Next Class

- Is on Wednesday, April 3
- Next time: we will discuss finite-difference time domain techniques
- Suggested reference: S. Obayya's book, Chapter 5, Sections 4-6