ECE 695
Numerical Simulations
Lecture 29: Finite-Difference Time Domain in MEEP

Prof. Peter Bermel

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Outline

- MEEP Tutorial examples:
  - Index-guided bent waveguide
  - Multimode ring resonators
  - Isolating individual resonances
  - Kerr nonlinearities
  - Quantifying third-harmonic generation
- Random and correlated random textured structures

Example: Index-Guided Bend

- Can create movie from this (as shown below):

Index-Guided Bend

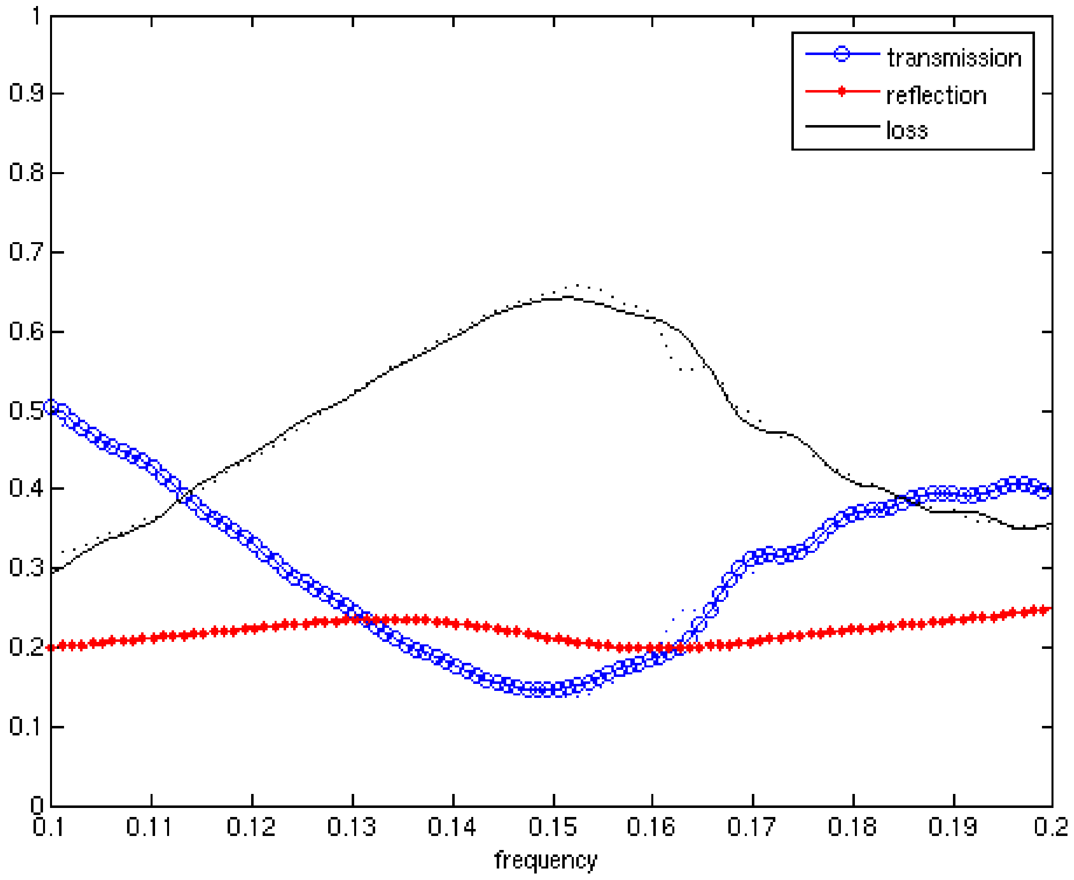
```
(define-param no-bend? false)
(set! geometry (if no-bend?
  (list (make block (center 0 wvg-ycen)
          (size infinity w infinity)
          (material (make dielectric (epsilon 12)))))
  (list (make block (center (* -0.5 pad) wvg-ycen)
         (size (- sx pad) w infinity)
         (material (make dielectric (epsilon 12))))
        (make block (center wvg-xcen (* 0.5 pad))
         (size w (- sy pad) infinity)
         (material (make dielectric (epsilon 12)))))))
```

Index-Guided Bend

```
(define-param nfreq 100)
(define trans ; transmitted flux
  (add-flux fcen df nfreq
      (if no-bend?
        (make flux-region
          (center (- (/ sx 2) 1.5) wvg-ycen) (size 0 (* w 2)))
        (make flux-region
          (center wvg-xcen (- (/ sy 2) 1.5)) (size (* w 2) 0)))))
(define refl ; reflected flux
  (add-flux fcen df nfreq
       (make flux-region
          (center (+ (* -0.5 sx) 1.5) wvg-ycen) (size 0 (* w 2)))))
```

Index-Guided Bend

Transmission, reflection, and loss spectrum for the bend



Example: Ring Resonators

- Ring resonators are essentially index-guided waveguides bent in on themselves
- Discrete resonant frequencies induced by periodicity
- Free spectral range between modes varies inversely with ring radius
- Radiative losses decay exponentially with ring radius

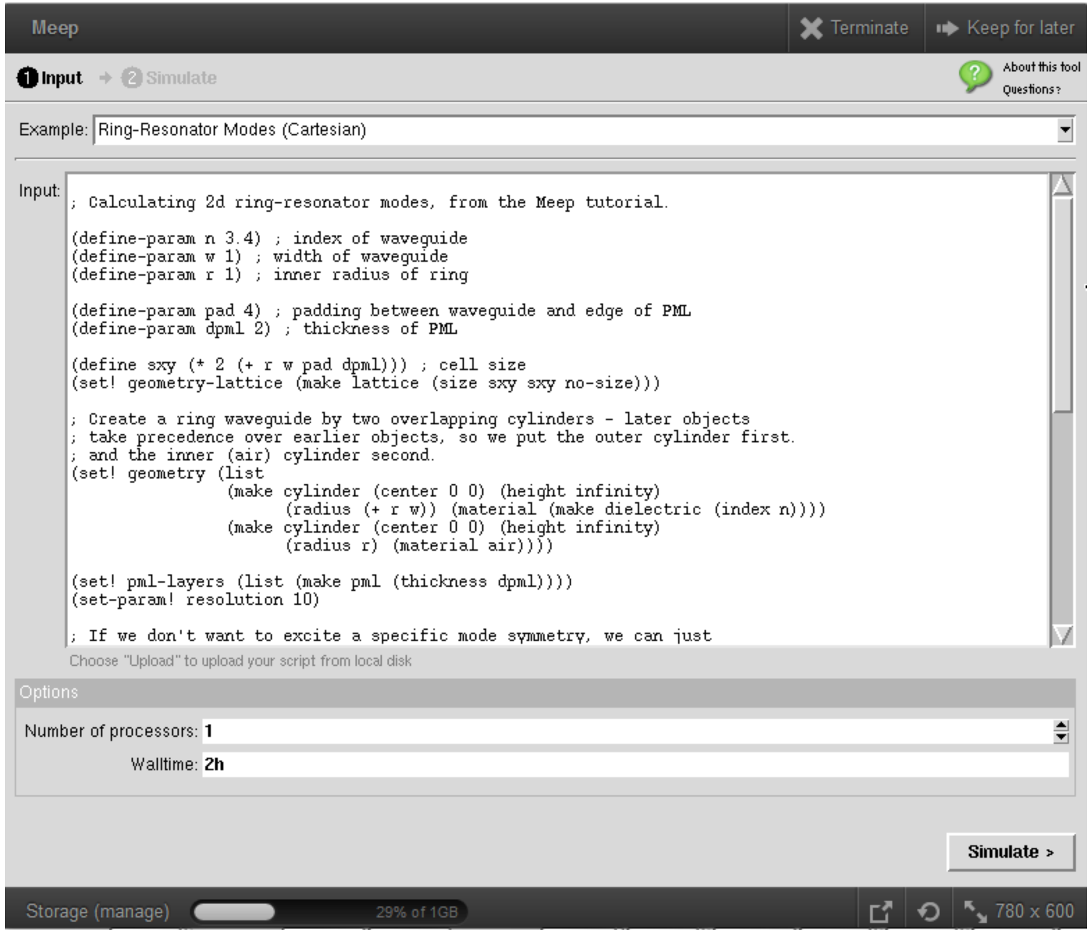
Ring Resonators

```
(define-param n 3.4) ; index of waveguide
(define-param w 1) ; width of waveguide
(define-param r 1) ; inner radius of ring
(define-param pad 4) ; padding from waveguide
(define-param dpml 2) ; thickness of PML
(define sxy (* 2 (+ r w pad dpml))) ; cell size
(set! geometry-lattice (make lattice (size sxy sxy no-size)))
(set! geometry (list (make cylinder (center 0 0) (height infinity)
                        (radius (+ r w)) (material (make dielectric (index n))))
                     (make cylinder (center 0 0) (height infinity)
                        (radius r) (material air))))
(set! pml-layers (list (make pml (thickness dpml)))) (set-param!
resolution 10)
```

Ring Resonators

```
(define-param fcen 0.15) ; pulse center frequency
(define-param df 0.1)  ; pulse width (in frequency)
(set! sources (list (make source (src (make gaussian-src
(frequency fcen) (fwidth df))) (component Ez) (center (+ r 0.1)
0)))))
(run-sources+ 300 (at-beginning output-epsilon) (after-sources
(harminv Ez (vector3 (+ r 0.1)) fcen df)))
```

Ring Resonators



Can also access this example on MEEP tool:

https://nanohub.org/tools/meep

Ring Resonators

- Filter diagonalization (harminv) extract resonant frequencies and decay rates:

$$f(t) = \sum_{k=1}^{N} a_k e^{-j\omega_k t - \Gamma_k t}$$

- Where: $Q_k = \omega_k / 2\Gamma_k$
- Raw output:

harminv0:, frequency, imag. freq., Q, |amp|, amplitude, error harminv0:, 0.118101575043663, -7.31885828253851e-4, 80.683059081382, 0.00341388964904578, -0.00305022905294175-0.00153321402956404i, 1.02581433904604e-5

harminv0:, 0.147162555528154, -2.32636643253225e-4, 316.29272471914, 0.0286457663908165, 0.0193127882016469-0.0211564681361413i, 7.32532621851082e-7

harminv0:, 0.175246750722663, -5.22349801171605e-5, 1677.48461212767, 0.00721133215656089, -8.12770506086109e-4-0.00716538314235085i, 1.82066436470489e-7

Ring Resonators

- Add the following to ring.ctl:

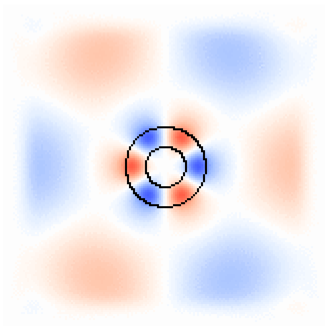
```
(run-until (/ 1 fcen) (at-every (/ 1 fcen 20) output-efield-z))
```

- Run the following from command line:

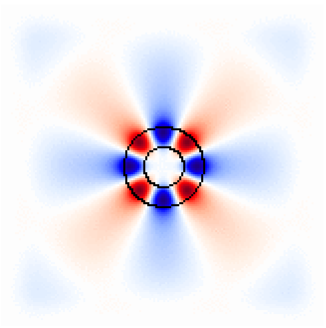
```
unix% meep fcen=0.118 df=0.01 ring.ctl
unix% meep fcen=0.147 df=0.01 ring.ctl
unix% meep fcen=0.175 df=0.01 ring.ctl
unix% h5topng -RZc dkbluered -C ring-eps-000000.00.h5 ring-ez-*.h5
unix% convert ring-ez-*.png ring-ez-0.118.gif
```

Ring Resonators

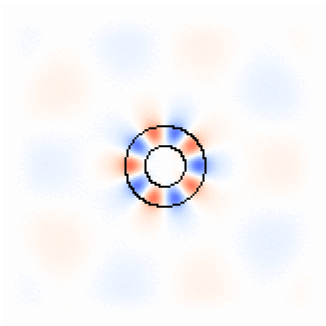
- End result is to create movies of single ring resonator modes:



$\omega = 0.118\ (2\pi c/a)$
$Q = 81$



$\omega = 0.147\ (2\pi c/a)$
$Q = 316$



$\omega = 0.175\ (2\pi c/a)$
$Q = 1682$

Example: Kerr Nonlinearities

- FDTD can simulate Kerr nonlinear media, where $n = n_o + k|\boldsymbol{E}|^2$
- Physically, four-wave mixing will result from this. Two key processes:
  - Sum/difference frequency generation
  - Third-harmonic generation
- Relative rates depend on field strengths, input profile overlaps, and output density of modes

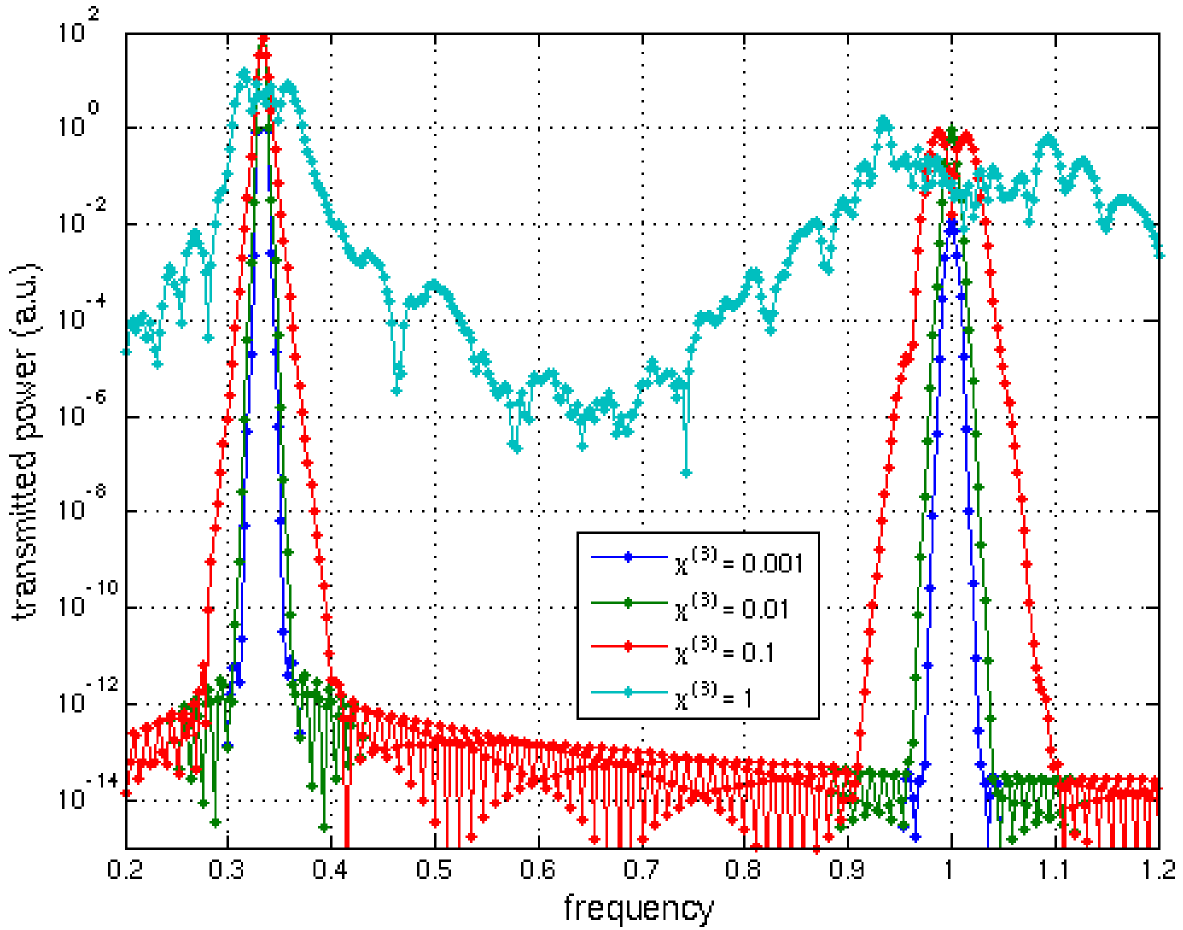
Kerr Nonlinearities

```
(define-param sz 100) ; size of cell in z direction
(define-param fcen (/ 1 3)) ; center frequency of source
(define-param df (/ fcen 20)) ; frequency width of source
(define-param amp 1.0) ; amplitude of source
(define-param k 1e-2) ; Kerr susceptibility
(define-param dpml 1.0) ; PML layer thickness
(set-param! dimensions 1)
(set! geometry-lattice (make lattice (size no-size no-size sz)))
(set! pml-layers (list (make pml (thickness dpml))))
(set-param! resolution 20)
(set! default-material (make dielectric (index 1) (chi3 k)))
```

Kerr Nonlinearities

```
(set! sources (list (make source (src (make gaussian-src (frequency fcen)
(fwidth df))) (component Ex) (center 0 0 (+ (* -0.5 sz) dpml)) (amplitude
amp)))) ; frequency range for flux calculation
(define-param nfreq 400)
(define-param fmin (/ fcen 2))
(define-param fmax (* fcen 4))
(define trans ; transmitted flux (add-flux (* 0.5 (+ fmin fmax (- fmax fmin)
nfreq (make flux-region (center 0 0 (- (* 0.5 sz) dpml 0.5)))))
(run-sources+ (stop-when-fields-decayed 50 Ex (vector3 0 0 (- (* 0.5 sz) dpml
0.5)) 1e-6))
(display-fluxes trans)
```

Kerr Nonlinearities



Third harmonic generation observed;
modulation instability for strong nonlinearities

Kerr Nonlinearities

- To quantify THG – add the following to our ctl file:

```
(define trans1 (add-flux fcen 0 1 (make flux-region (center 0 0 (- (* 0.5 sz) dpml 0.5)))))
(define trans3 (add-flux (* 3 fcen) 0 1 (make flux-region (center 0 0 (- (* 0.5 sz) dpml 0.5)))))
(print "harmonics:, " k ", " amp ", " (first (get-fluxes trans1)) ", " (first (get-fluxes trans3)) "\n")
```

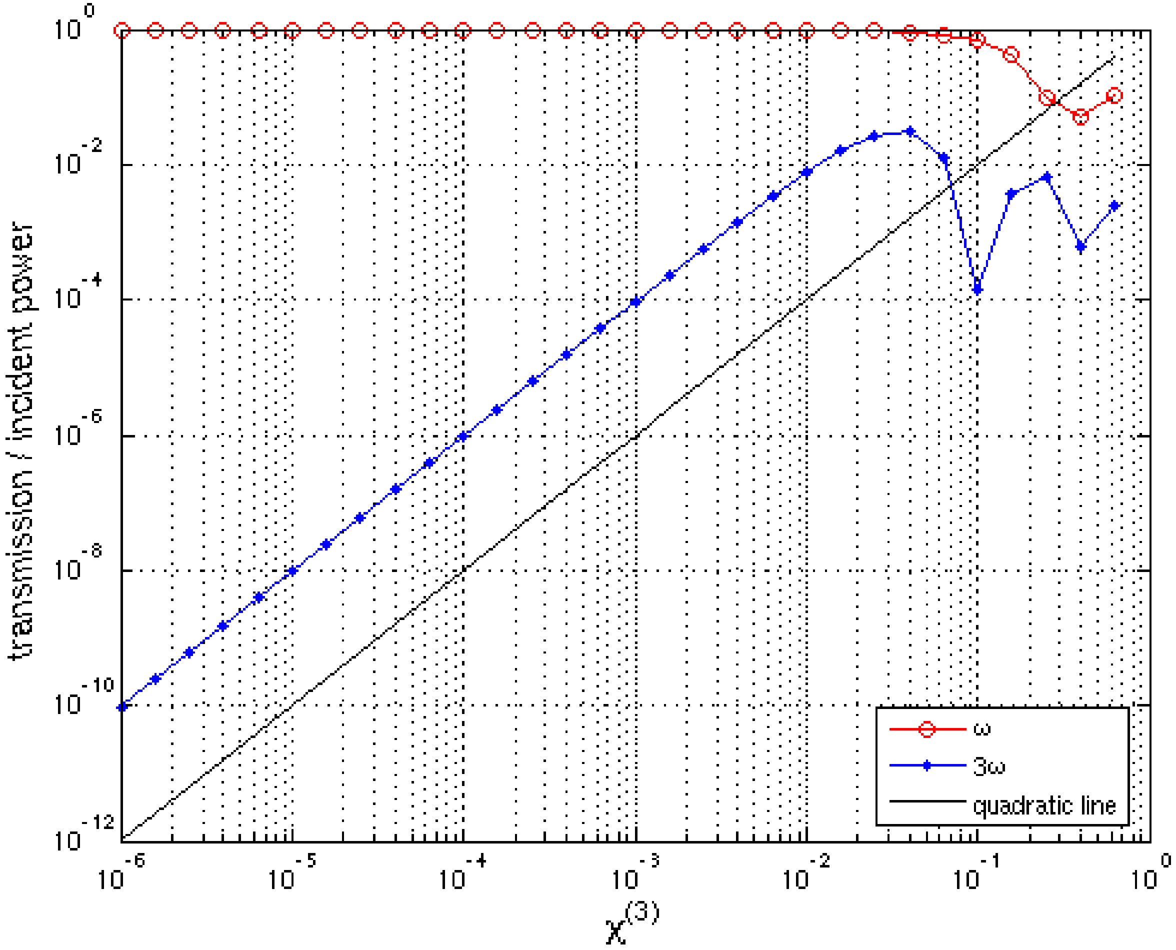
- From command line:

```
unix% (for logk in `seq -6 0.2 0`; do meep k="(expt 10 $logk)" 3rd-harm-1d.ctl |grep harmonics:; done) | tee harmonics.dat
```

- Resulting output:

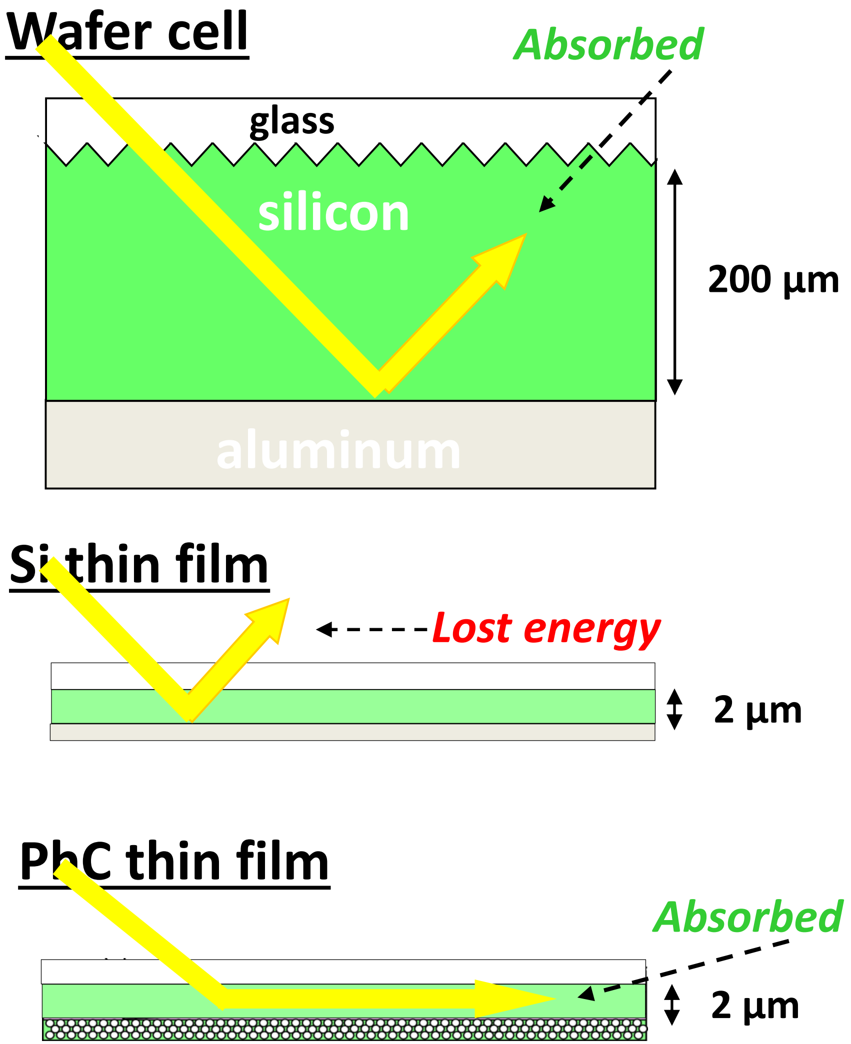
```
harmonics:, 0, 1.0, 112.62889036581, 1.20863942821229e-16
```

Kerr Nonlinearities

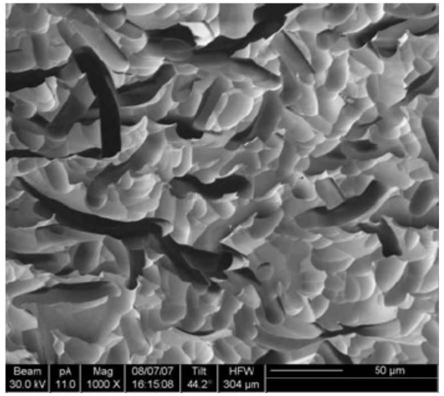
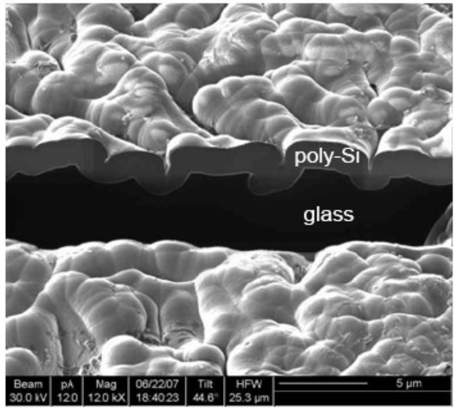


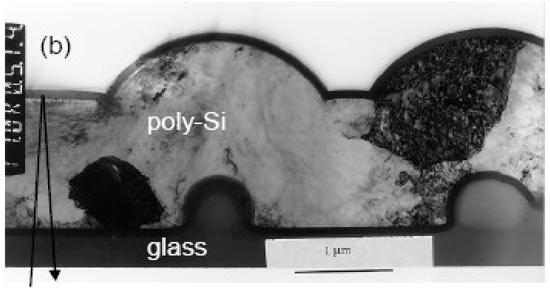
Third harmonic generation rate scales quadratically with nonlinearity

Example: Simulating Si PV Absorption



Different Geometric Light Trapping Approaches for Commercial μc-Si Cells



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

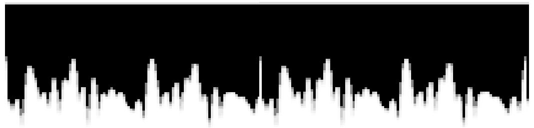
M.J. Keevers et al., “10% Efficient CSG Minimodules,”

Correlated Randomness

Combine gratings for each wavelength

inhomogeneous

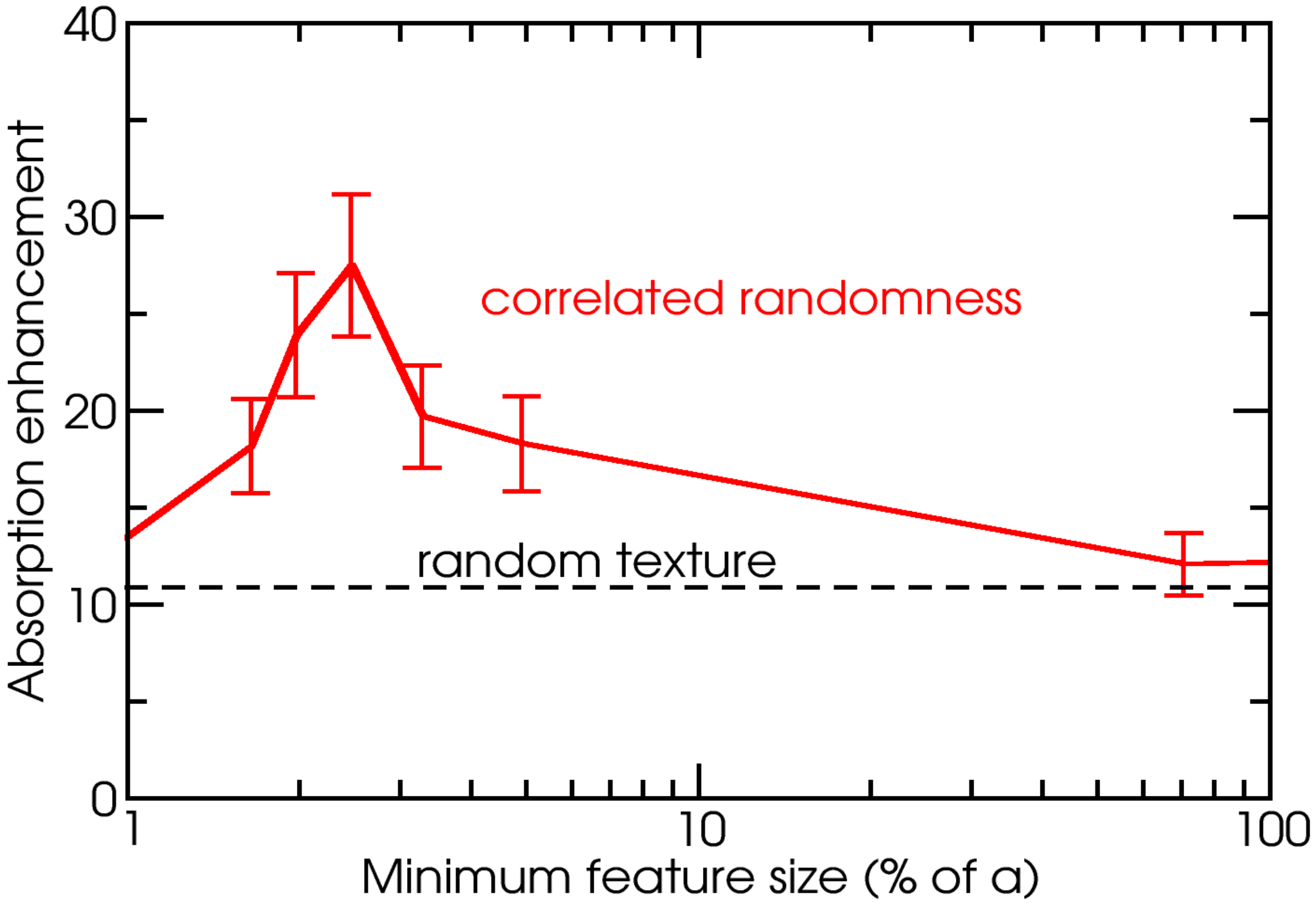
Combine periodicity with texturing in systematic fashion



homogeneous

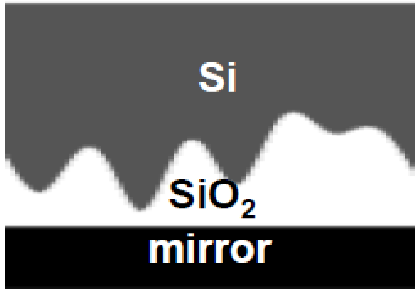
A.N. Bloch & P. Sheng, US Patent 4,683,160 (1987)
X. Sheng *et al*., *Opt. Express* **19**, A841 (2011)

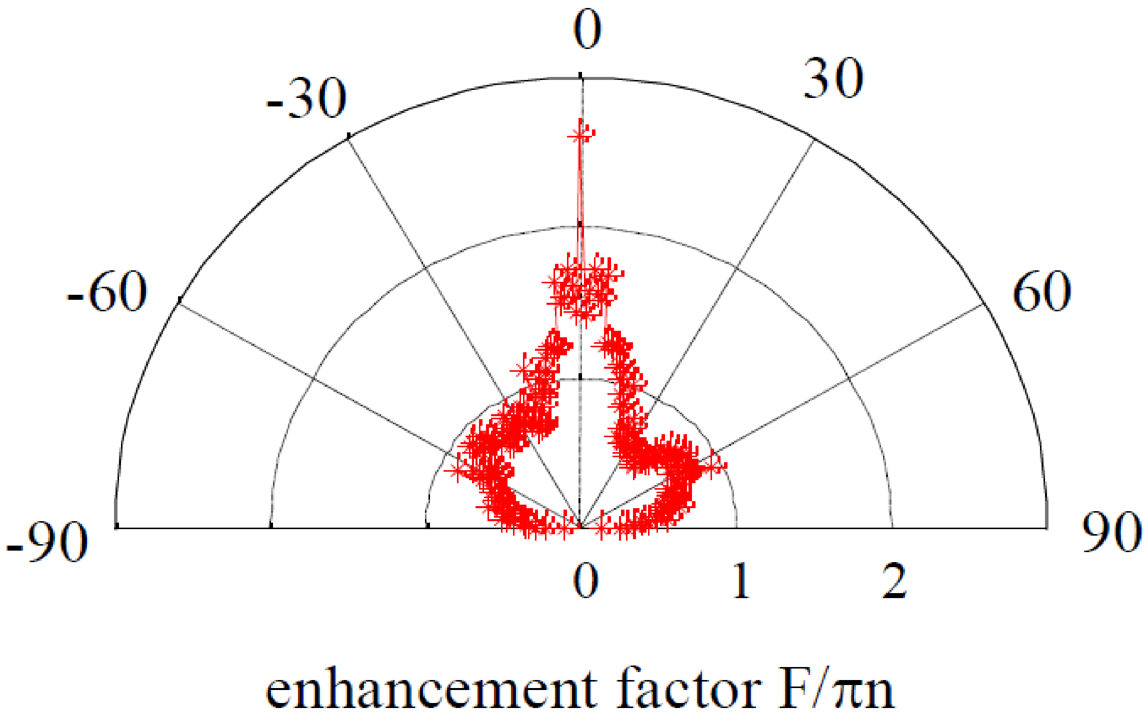
Correlated Randomness in 2D



For n=3.46 and 33% bandwidth (e.g., 500-700 nm)

Angle-Sensitive Solar Absorbers

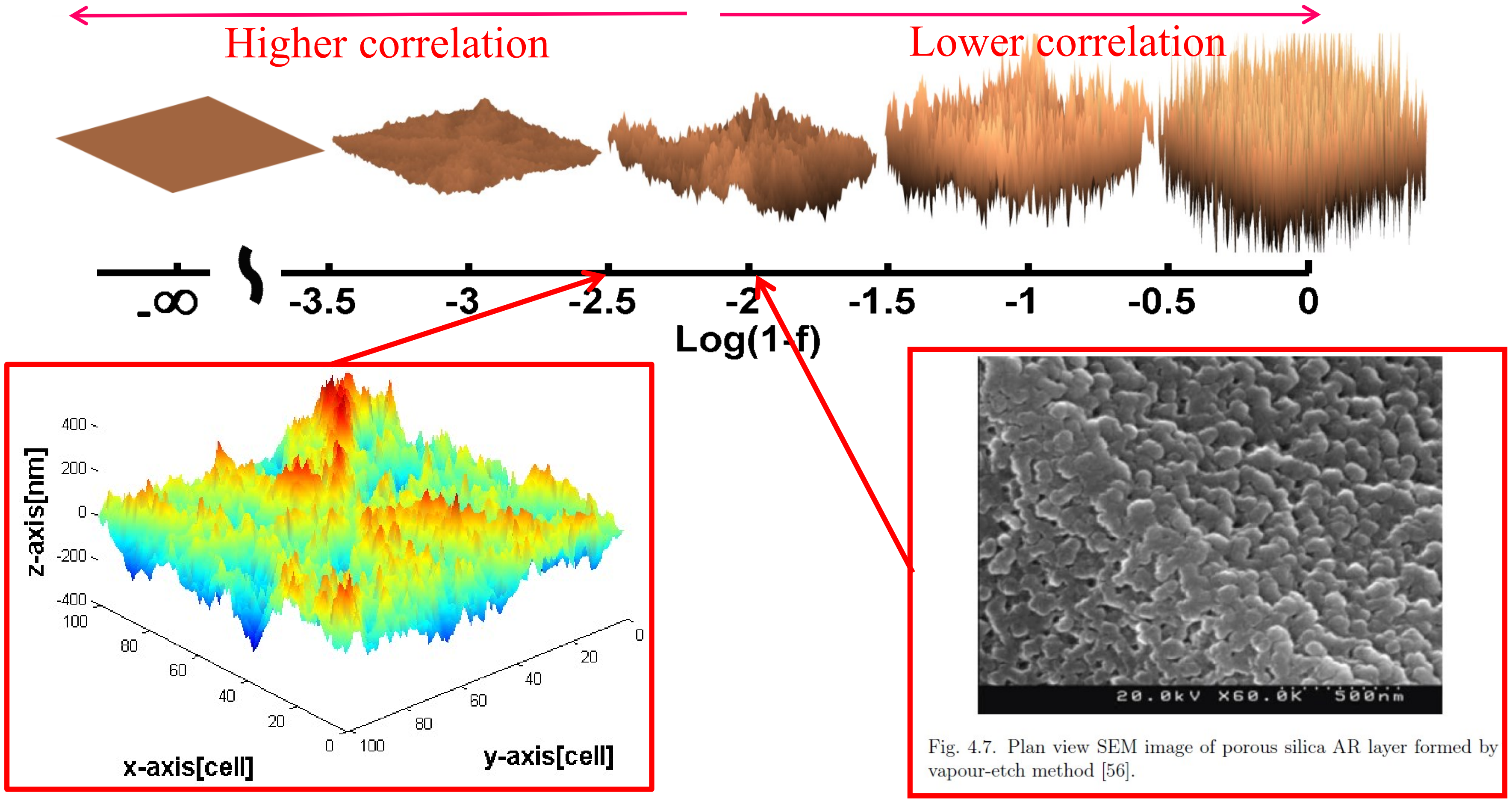




X. Sheng *et al.*, *Opt. Express* **19**, A841 (2011)

X. Wang et al., "Approaching the Shockley-Queisser Limit in GaAs Solar Cells", IEEE J. Photovolt. (2013).

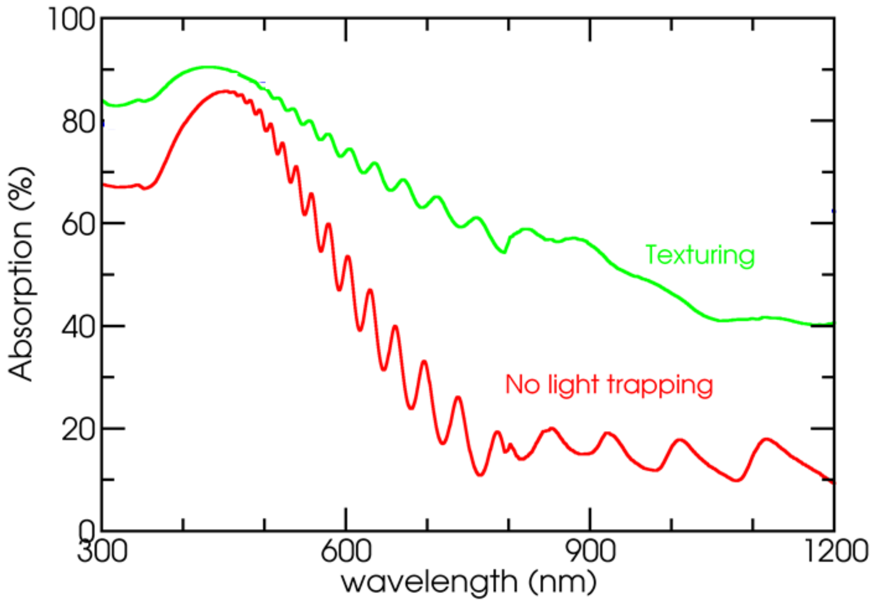
From flat to totally random structures via correlated random textures



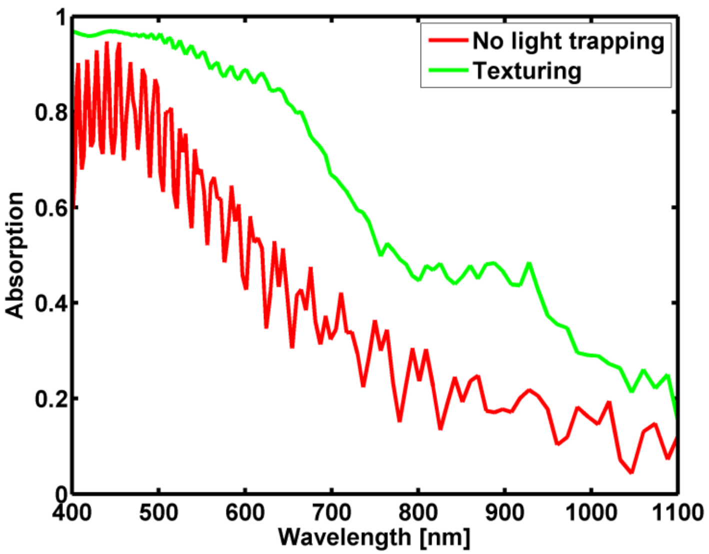
Keevers, M. J., et al. “10% efficiency CSG minimodules.” *Proceedings of the 22nd European Photovoltaic Solar Energy Conference.* (2007).

Experimental absorption versus simulated absorption

Experiment



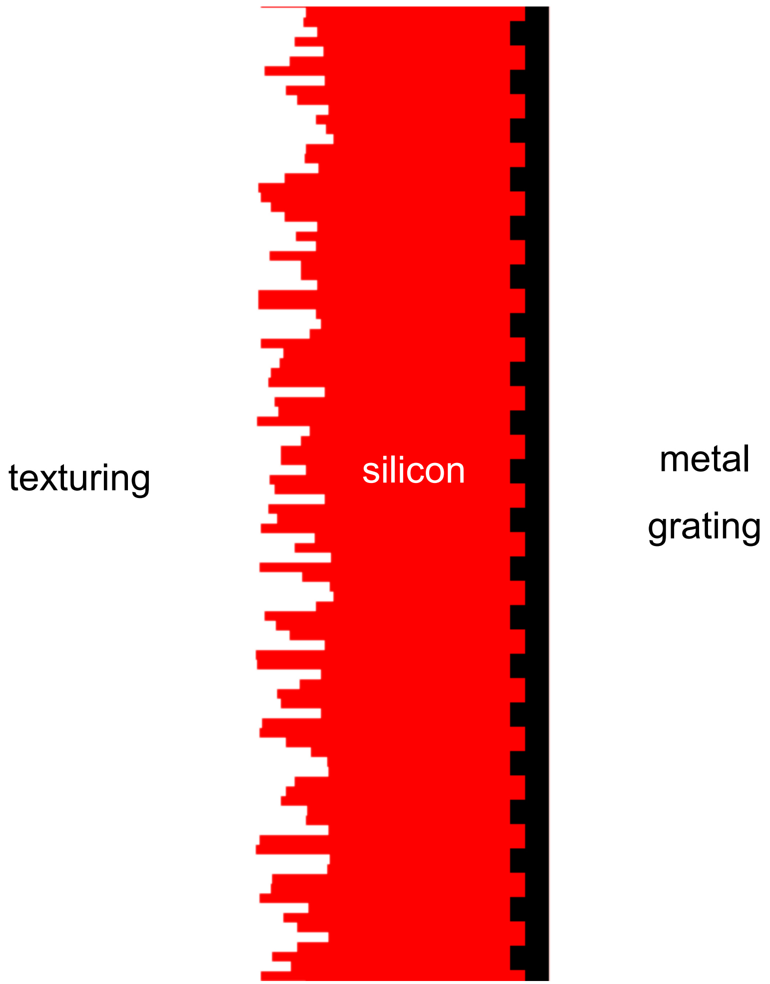
Simulation (3D QCRF-FDTD)



L. T. Varghese, Y. Xuan, B. Niu, L. Fan, P. Bermel, and M. Qi, "Enhanced photon management of thin-film silicon solar cells using inverse opal photonic crystals with 3d photonic bandgaps," *Advanced Optical Materials* **1**, 692–698 (2013).

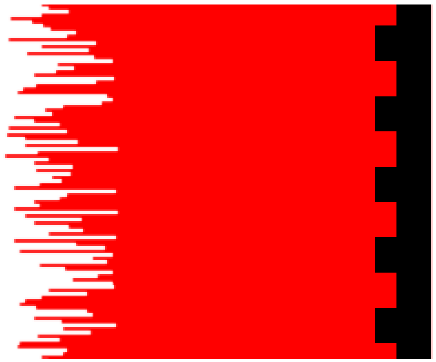
H. Chung, K-Y. Jung, X. T. Tee, and P. Bermel, "Time domain simulation of tandem silicon solar cells with optimal textured light trapping enabled by the quadratic complex rational function," *Opt. Express* **22**, A818-A832 (2014).

Computational Set-up

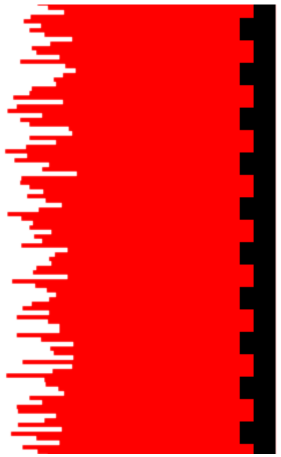


- Thickness of film = our experimental samples (1.47 μm)
- Four geometries tested
- Random texturing:
  - Uniform height distribution over 500 nm
  - Distance between features varies
- Photonic crystal:
  - Reflection captured by metal
  - Diffraction captured by grating (optimized for this thickness)

Varying spacing between features



5 periods

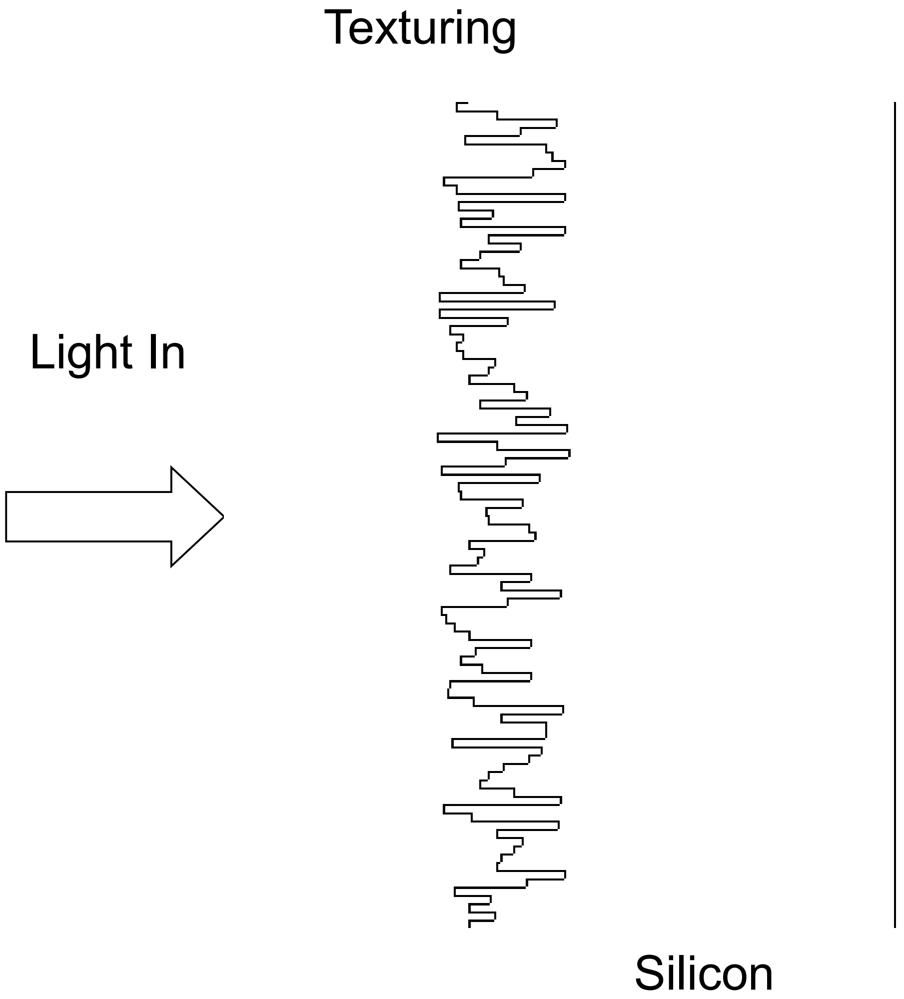


10 periods

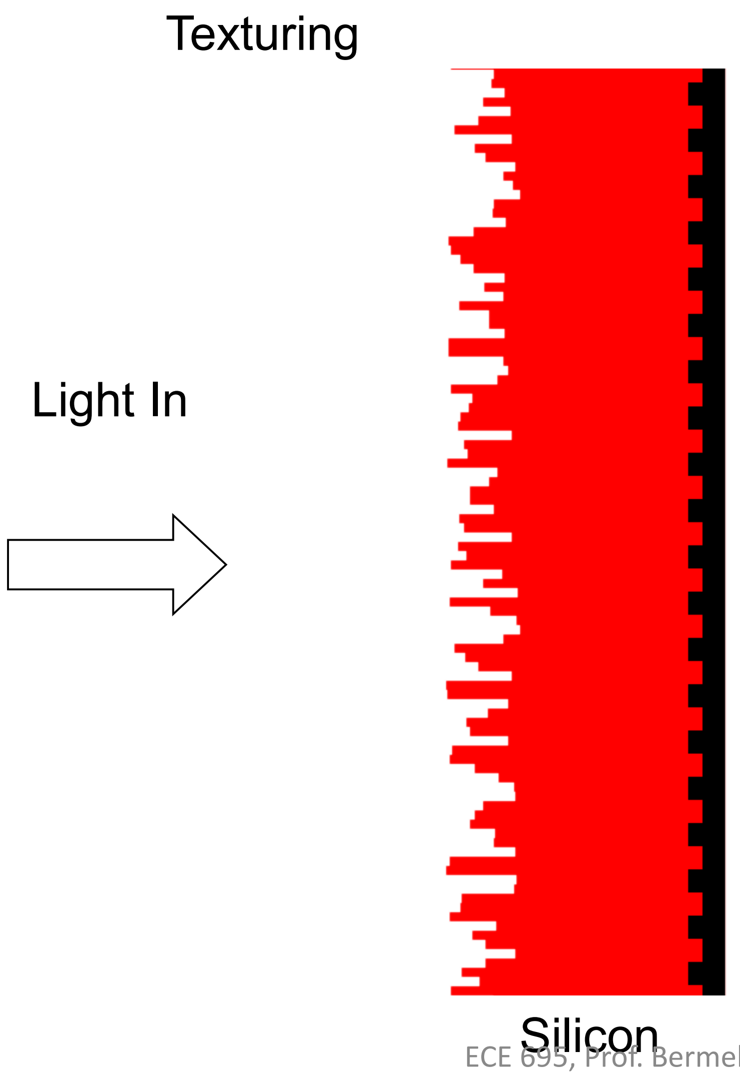
20 periods

Propagation of Light in Planar Geometry

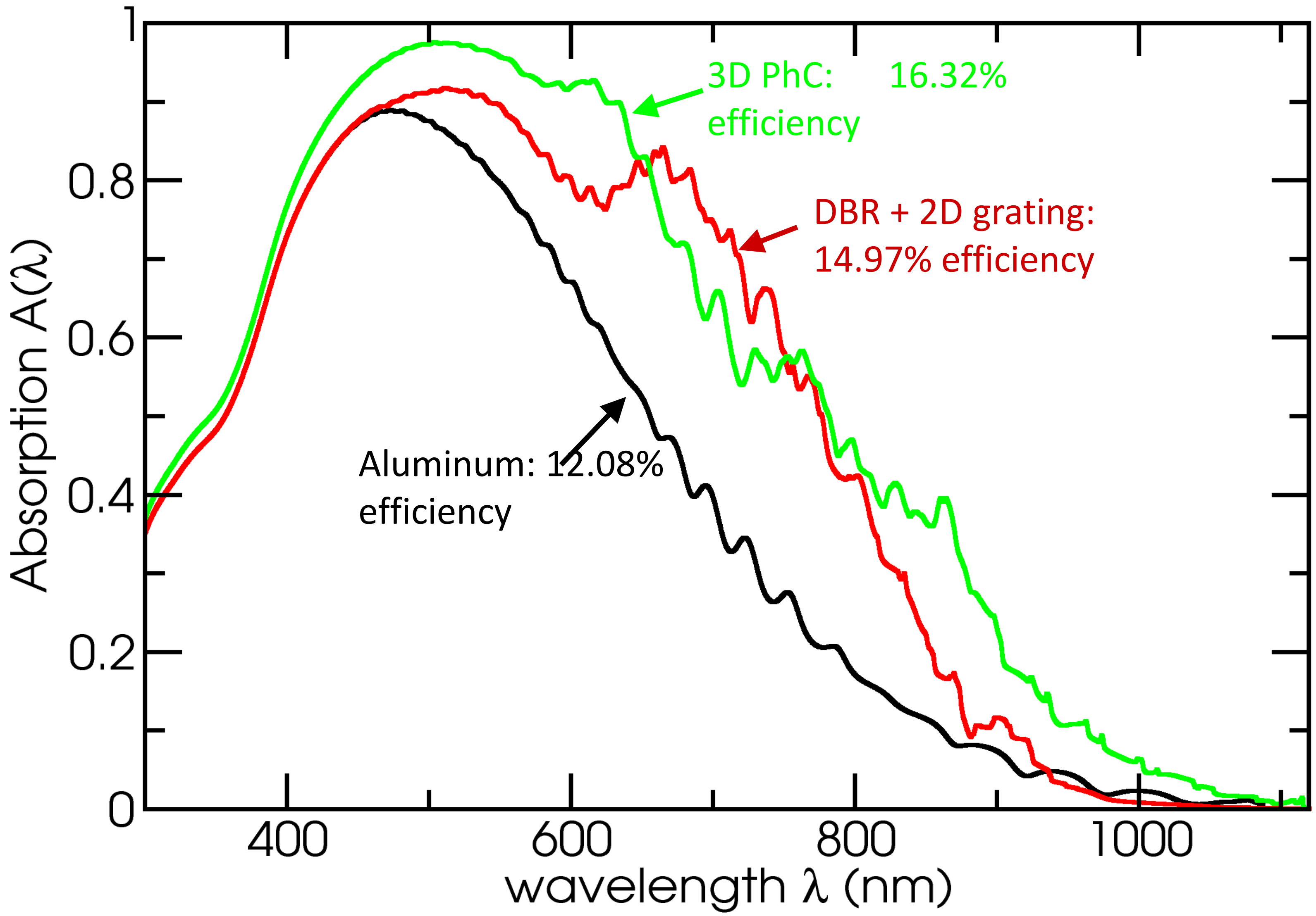
Propagation of Light in Textured Geometry (no backing)



Propagation of Light in Textured Geometry + Metal Grating

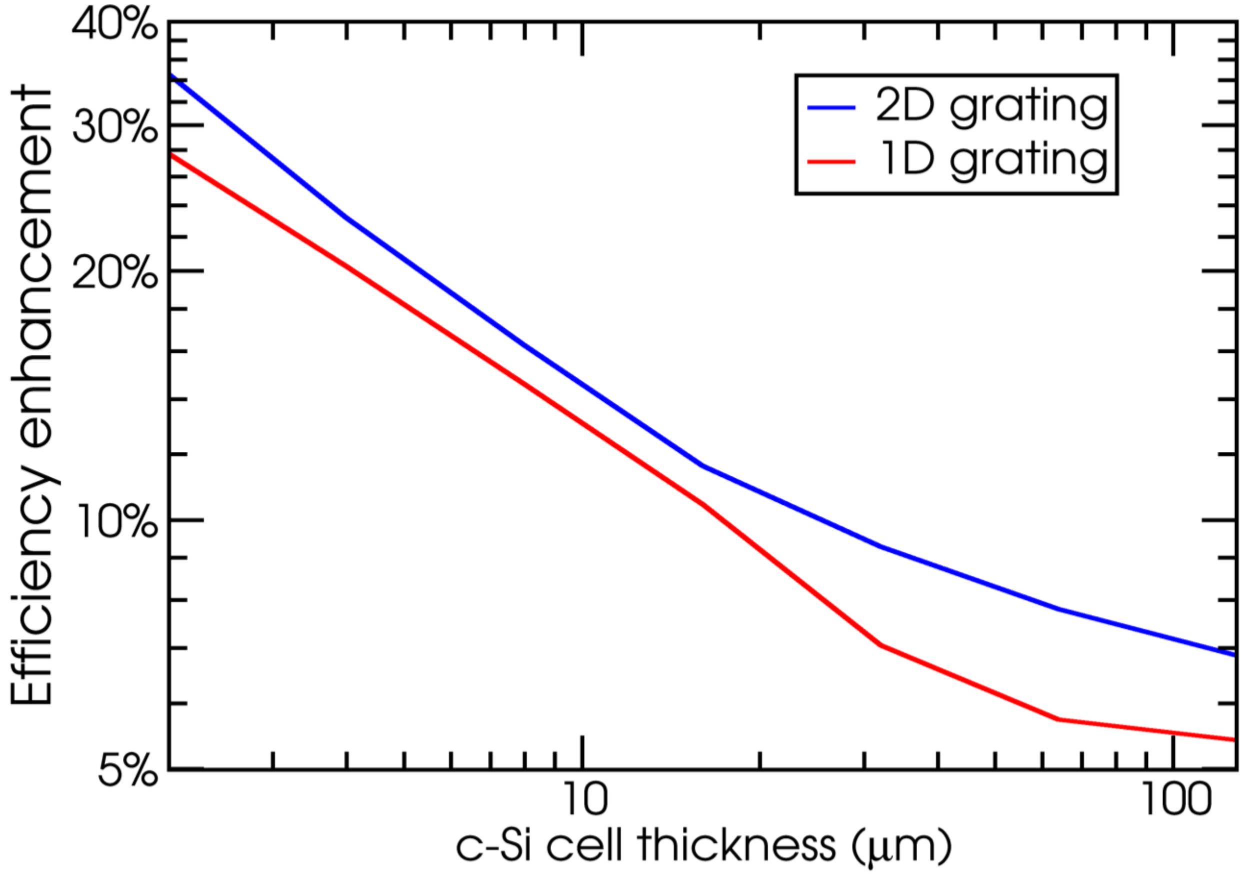


Calculated Absorption Spectrum for 2 μm μc-Si



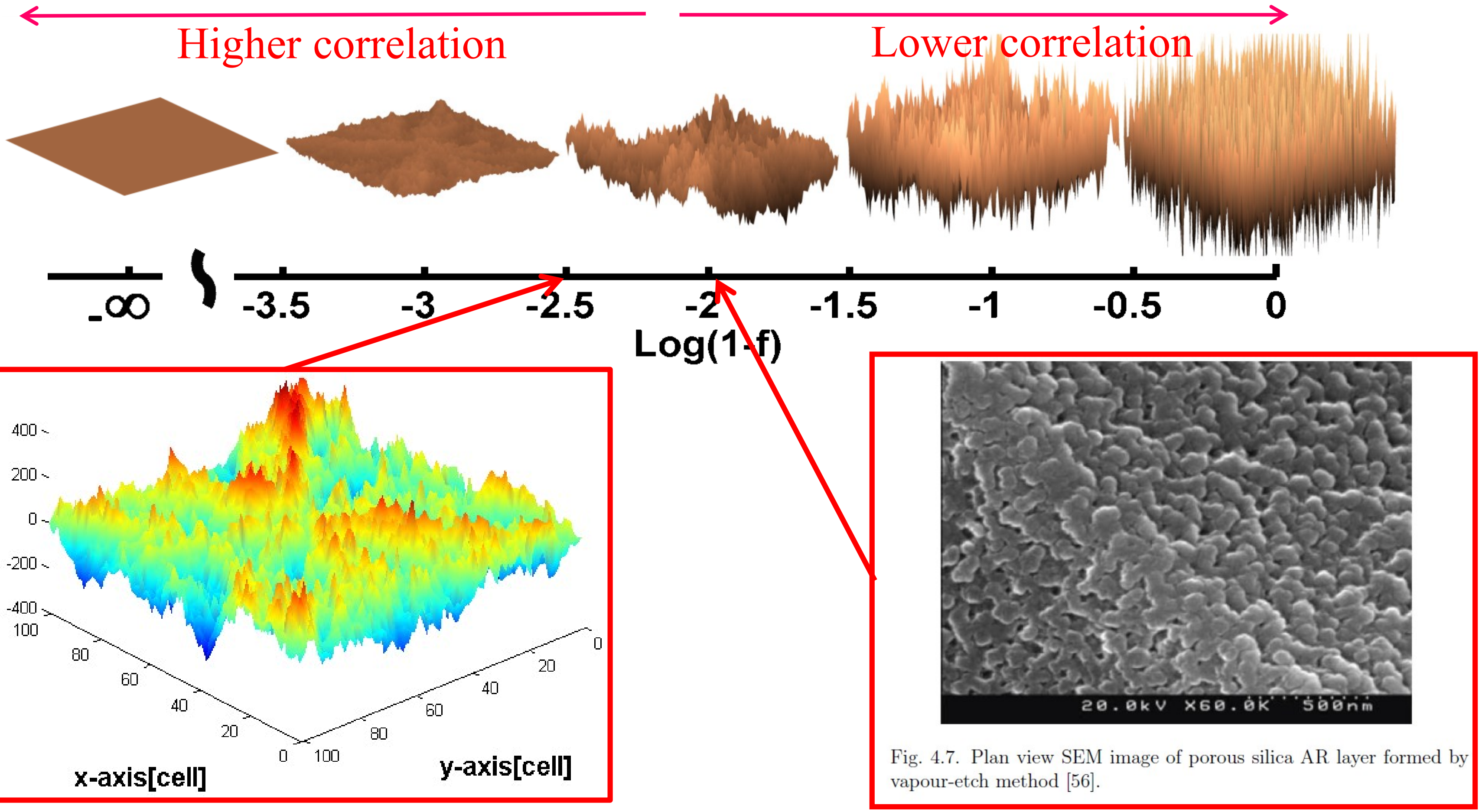
P. Bermel *et al.*, *Opt. Express* **15**, 16986 (2007)

Efficiency Enhancement of Period Structures



For optimized parameters, 2D grating efficiency enhancement ranges from 7% at 128 μm up to 35% at 2 μm

From flat to totally random structures via correlated random textures



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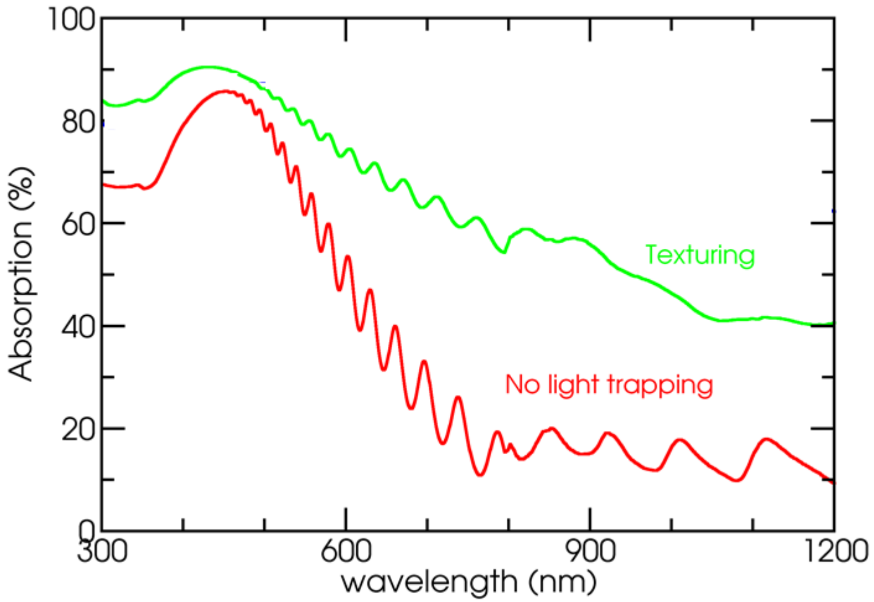
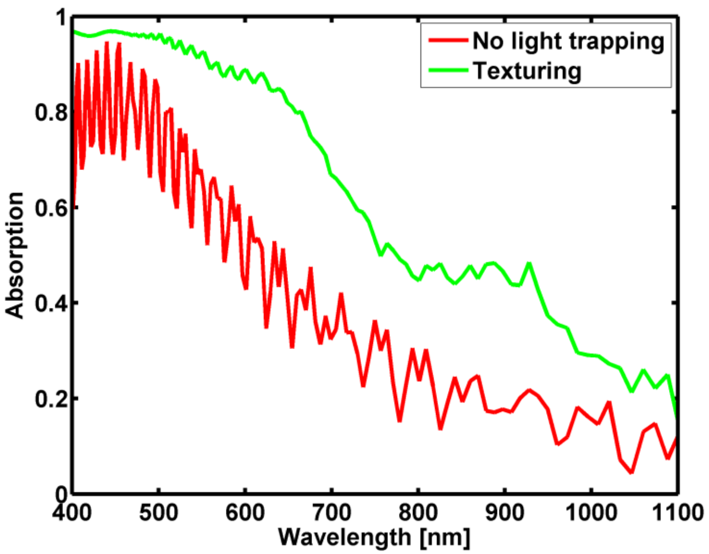
Experimental absorption versus simulated absorption

Experiment



Simulation (3D QCRF-FDTD)



L. T. Varghese, Y. Xuan, B. Niu, L. Fan, P. Bermel, and M. Qi, "Enhanced photon management of thin-film silicon solar cells using inverse opal photonic crystals with 3d photonic bandgaps," *Advanced Optical Materials* **1**, 692–698 (2013).

H. Chung, K-Y. Jung, X. T. Tee, and P. Bermel, "Time domain simulation of tandem silicon solar cells with optimal textured light trapping enabled by the quadratic complex rational function," *Opt. Express* **22**, A818-A832 (2014).

Next Class

- Next time: we will continue finite-difference time domain techniques
- Suggested reference: S. Obayya's book, Chapter 5, Sections 4-6