ECE 695
Numerical Simulations
Lecture 31: Finite-Difference Time Domain Band Structures

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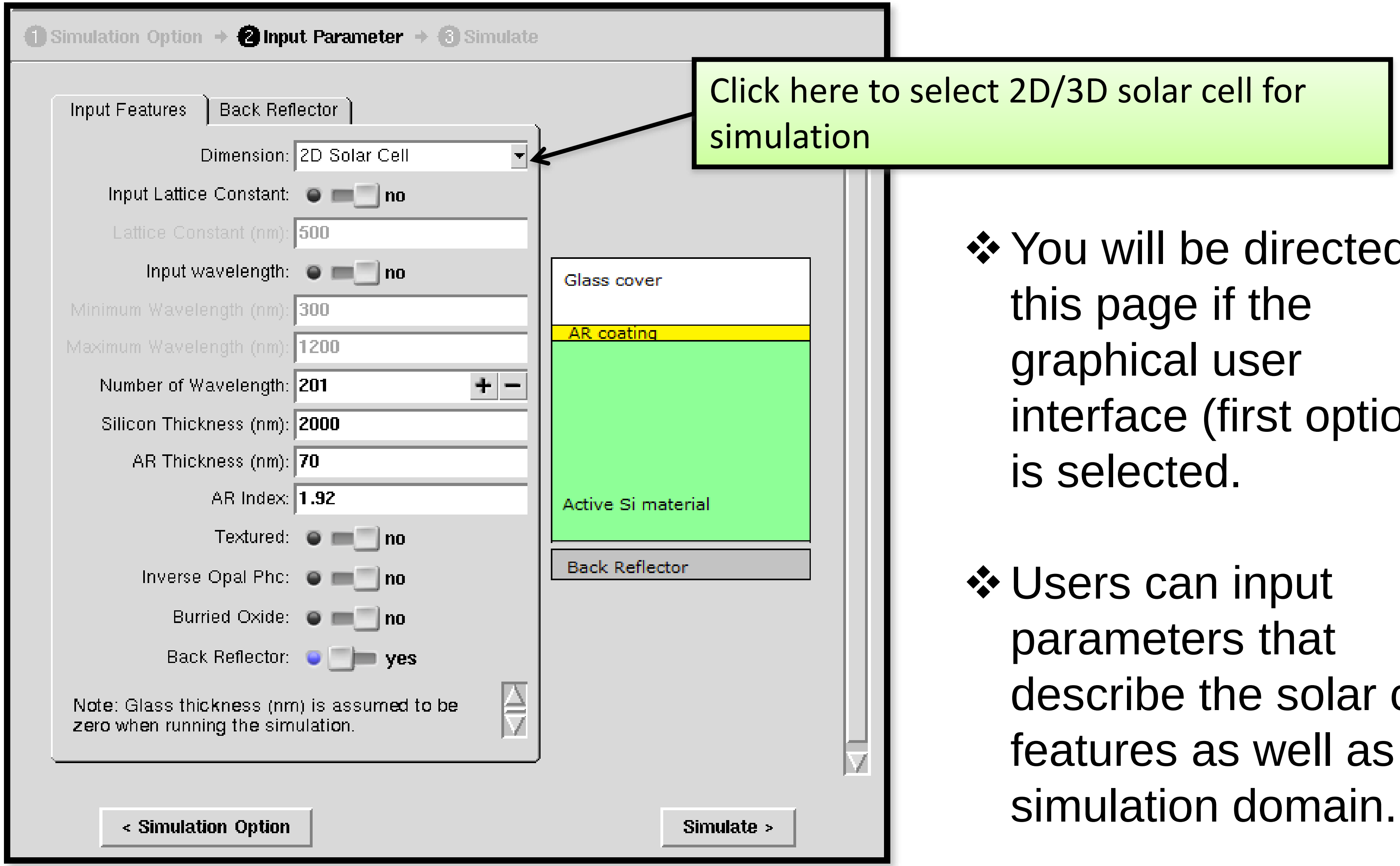
April 3, 2017

Recap from Friday: MEEPPV Graphical User Interface

https://nanohub.org/tools/meeppv



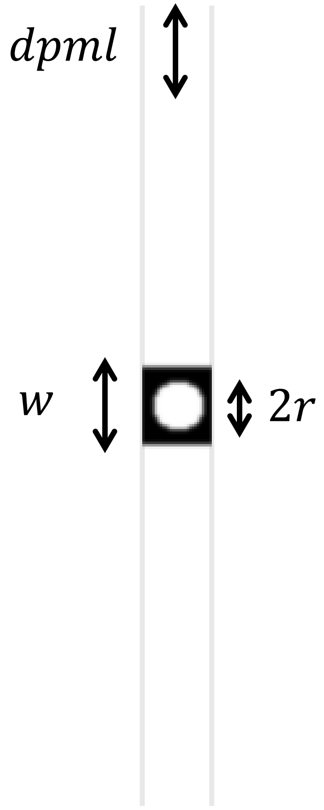
- You will be directed to this page if the graphical user interface (first option) is selected.
- Users can input parameters that describe the solar cell features as well as the simulation domain.

Outline

- Photonic Crystal Waveguides:
  - Photonic Bandstructure
  - Defect Resonant Modes
  - Waveguide Transmission
- Inverse Opal Photonic Crystals:
  - Photonic Band structures
  - Photonic Crystal Phosphors

Photonic Bandstructure

```
(define-param eps 13) ; dielectric constant of waveguide
(define-param w 1.2) ; width of waveguide
(define-param r 0.36) ; radius of holes
(define-param sy 12) ; size of cell in y direction (perp. to wvg.)
(define-param dpml 1) ; PML thickness (y direction only!)
(set! geometry-lattice (make lattice (size 1 sy no-size)))
(set! geometry (list (make block (center 0 0)
              (size infinity w infinity)
              (material (make dielectric (epsilon eps))))
             (make cylinder (center 0 0) (radius r)
              (height infinity) (material air))))
(set-param! resolution 20)
(set! pml-layers (list (make pml (direction Y) (thickness dpml))))
```

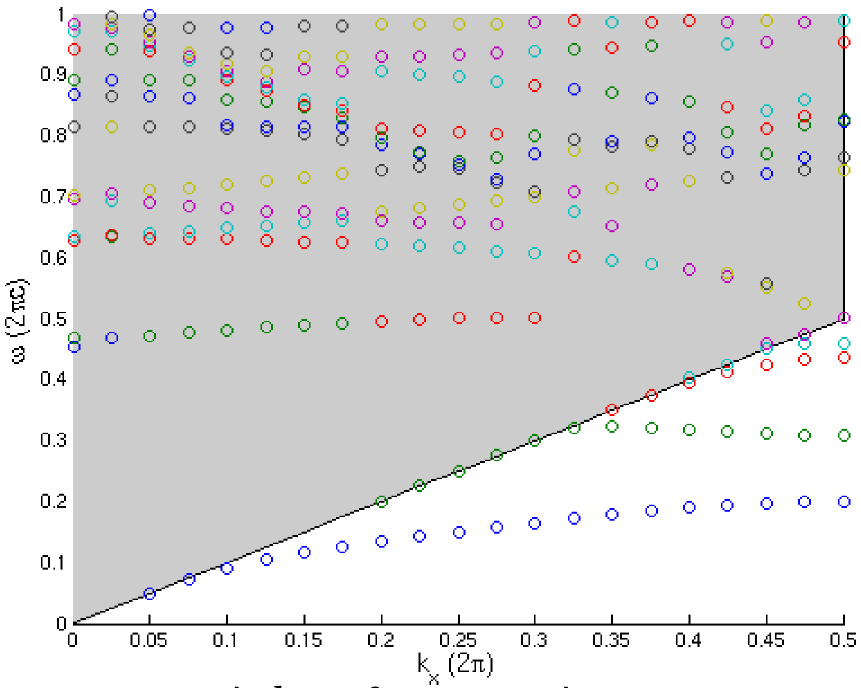


Our 1x12
unit cell

Photonic Bandstructure

```
(define-param fcen 0.25) ; pulse center frequency
(define-param df 1.5) ; pulse frequency width
(set! sources (list (make source (src
            (make gaussian-src (frequency fcen)
              (fwidth df))) (component Hz) (center 0.1234 0))))
(set! symmetries (list (make mirror-sym (direction Y) (phase -
1))))
(set-param! k-point (vector3 0.4 0))
(run-sources+ 300 (after-sources (harminv Hz (vector3 0.1234)
fcen df)))
(define-param k-interp 19)
(run-k-points 300 (interpolate k-interp (list (vector3 0)
(vector3 0.5))))
```

Photonic Bandstructure



- Output frequencies at each k_x – for example:

freqs:, 14, 0.325, 0.0, 0.0, 0.171671252741341, 0.319717964514696, 0.323470450791478

freqs-im:, 14, 0.325, 0.0, 0.0, -8.74808991364674e-8, 1.82230861728163e-4, 0.00144227925408331

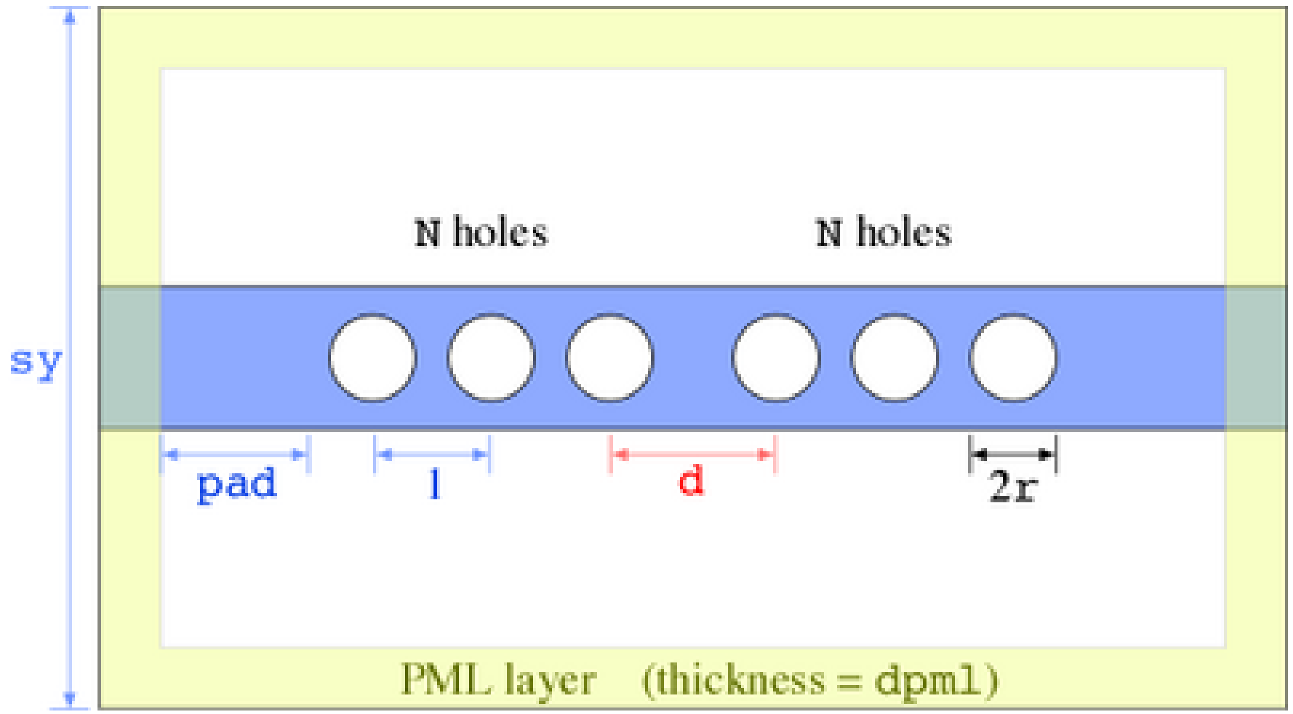
- Extract frequency lines via grep:

unix% meep holey-wvg-bands.ctl | tee holey-wvg-bands.out

unix% grep freqs: holey-wvg-bands.out > fre.dat

unix% grep freqs-im: holey-wvg-bands.out > fim.dat

Defect Resonant Modes



N holes on each side surround a defect cavity of size *d* (in units of *a*)

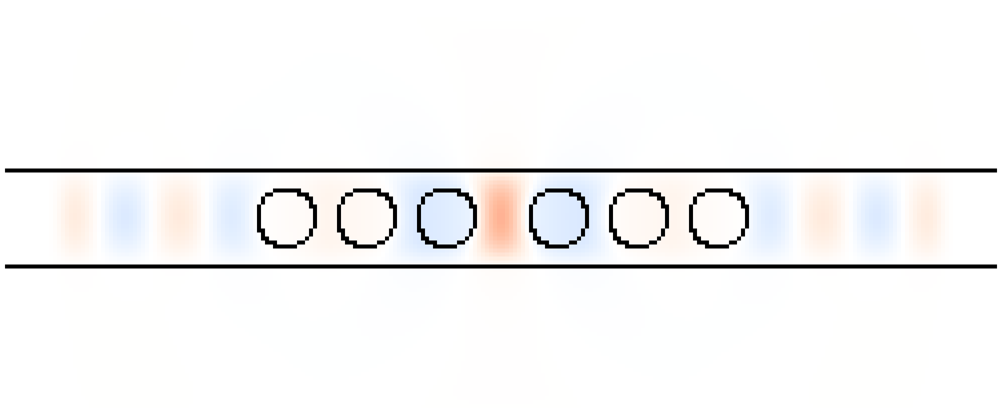
Defect Resonant Modes

```
(define-param eps 13) ; dielectric constant of waveguide
(define-param w 1.2) ; width of waveguide
(define-param r 0.36) ; radius of holes
(define-param d 1.4) ; defect spacing (ordinary spacing = 1)
(define-param N 3) ; number of holes on either side of defect
(define-param sy 6) ; size of cell in y direction (perpendicular to wvg.)
(define-param pad 2) ; padding between last hole and PML edge
(define-param dpml 1) ; PML thickness
(define sx (+ (* 2 (+ pad dpml N)) d -1)) ; size of cell in x direction
(set! geometry-lattice (make lattice (size sx sy no-size)))
(set! geometry (append ; combine lists of objects:
        (list (make block (center 0 0) (size infinity w infinity)
          (material (make dielectric (epsilon eps)))))
        (geometric-object-duplicates (vector3 1 0) 0 (- N 1) (make cylinder
          (center (/ d 2) 0) (radius r) (height infinity) (material air)))
        (geometric-object-duplicates (vector3 -1 0) 0 (- N 1) (make cylinder
          (center (/ d -2) 0) (radius r) (height infinity) (material air)))))
```

Defect Resonant Modes

```
(set! pml-layers (list (make pml (thickness dpml))))
(set-param! resolution 20)
(define-param fcen 0.25) ; pulse center frequency
(define-param df 0.2)  ; pulse width (in frequency)
(set! sources (list (make source (src (make gaussian-src (frequency fcen)
(fwidth df))) (component Hz) (center 0 0))))
(set! symmetries (list (make mirror-sym (direction Y) (phase -1)) (make
mirror-sym (direction X) (phase -1))))
(run-sources+ 400 (at-beginning output-epsilon) (after-sources (harminv Hz
(vector3 0) fcen df)))
(run-until (/ 1 fcen) (at-every (/ 1 fcen 20) output-hfield-z))
```

Defect Resonant Modes

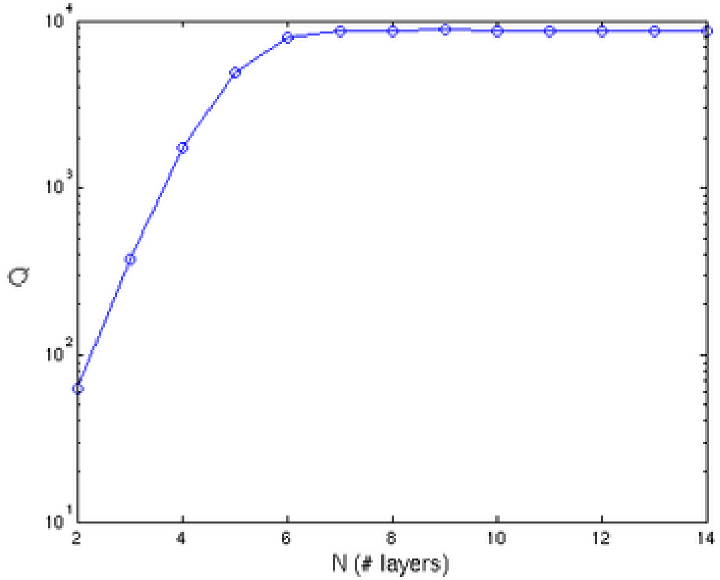


- Create a movie of defect mode over time:

unix% h5topng -RZc dkbluered -C holey-wvg-cavity-eps-000000.00.h5 holey-wvg-cavity-hz-*.h5

unix% convert holey-wvg-cavity-hz-*.png holey-wvg-cavity-hz.gif

Defect Resonant Modes



- Determine quality factor versus number of holes:

unix% meep N=4 compute-mode?=true holey-wvg-cavity.ctl |grep harminv

unix% meep N=5 compute-mode?=true holey-wvg-cavity.ctl |grep harminv

...

Defect Resonant Modes

- For large *N*, a second mode is observed…

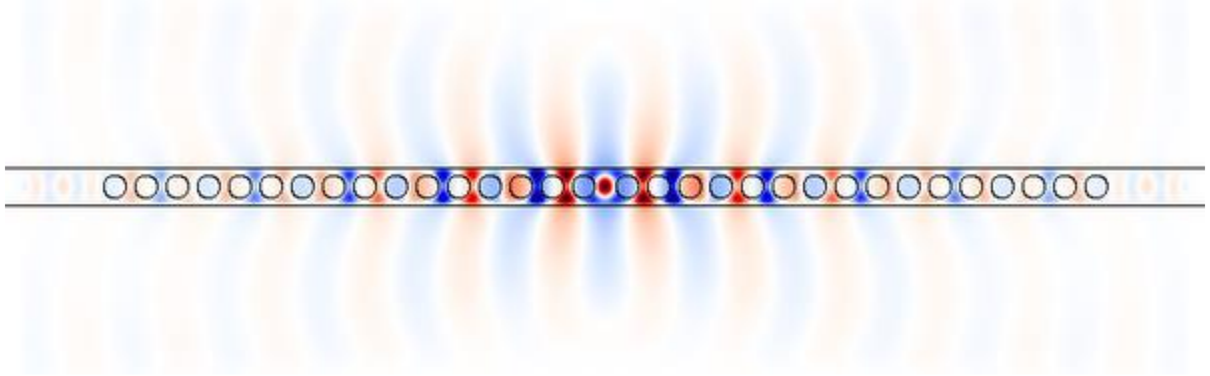
harminv0:, frequency, imag. freq., Q, |amp|, amplitude, error

harminv0:, 0.235201161007777, -1.34327185513047e-5, 8754.78631184943, 9.83220617825986, 6.83285024080876-7.06996717944934i, 3.03237056700397e-9

harminv0:, 0.328227374843021, -4.6405752015136e-4, 353.649451404175, 0.134284355228178, -0.131856646632894-0.0254187489419837i, 4.11557526694386e-7

- Generate field profile in time for extended mode at band edge:

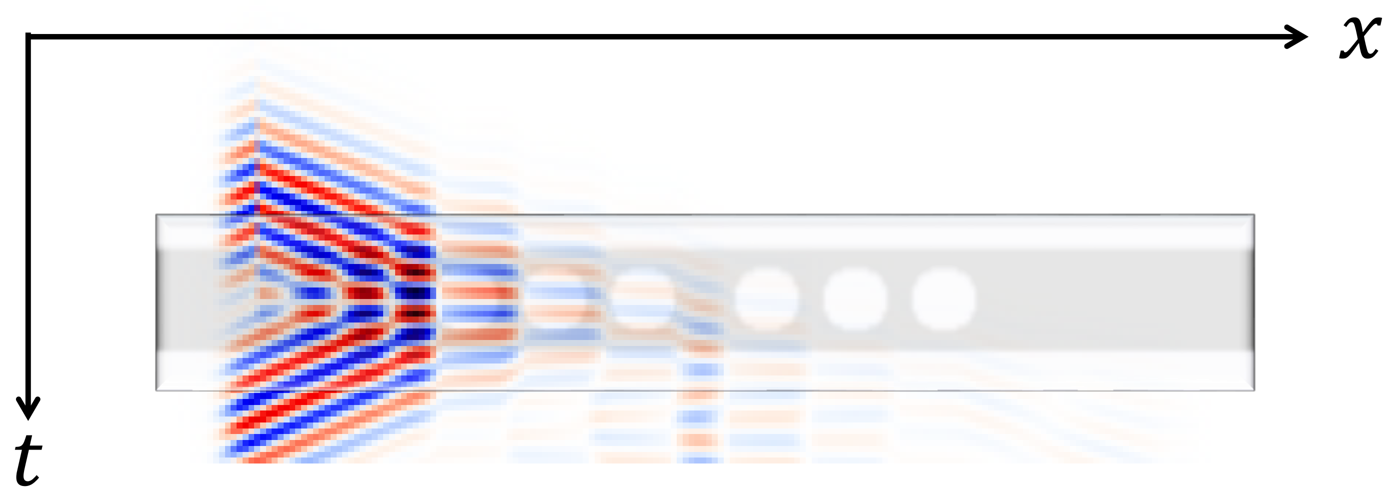
unix% meep sy=12 fcen=0.3282 df=0.01 N=16 holey-wvg-cavity.ctl



Waveguide Transmission

```
(define-param nfreq 500) ; num. frequencies at which to compute flux
(set! sources (list (make source (src (make gaussian-src
            (frequency fcen) (fwidth df))) (component Ey)
            (center (+ dpml (* -0.5 sx)) 0) (size 0 w))))
(set! symmetries (list (make mirror-sym (direction Y) (phase -1))))
(define trans ; transmitted flux
            (add-flux fcen df nfreq
            (make flux-region (center (- (* 0.5 sx) dpml 0.5) 0) (size 0 (* w 2)))))
(run-sources+ (stop-when-fields-decayed 50 Ey (vector3 (- (* 0.5 sx) dpml 0.5) 0) 1e-3)
            (at-beginning output-epsilon)
            (during-sources (in-volume (volume (center 0 0) (size sx 0)) (to-appended "hz-slice" (at-
every 0.4 output-hfield-z)))))
(display-fluxes trans) ; print out the flux spectrum
```

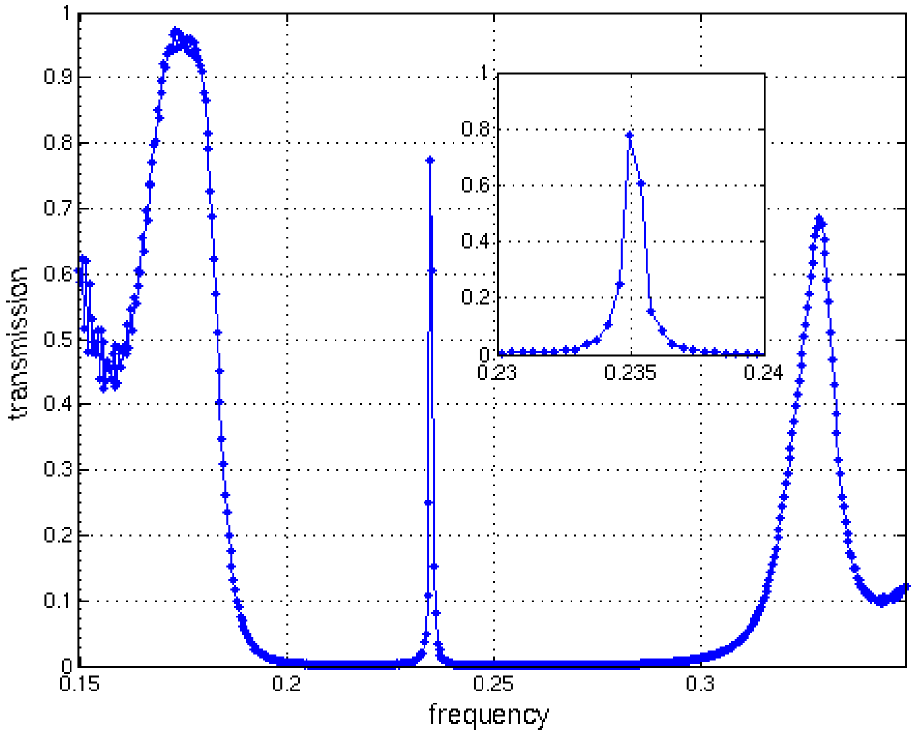
Waveguide Transmission



- View H_z field over space and time:

unix% meep holey-wvg-cavity.ctl | tee holey-wvg-cavity.out
unix% h5topng holey-wvg-cavity-eps-000000.00.h5
unix% h5topng -Zc dkbluered holey-wvg-cavity-hz-slice.h5

Waveguide Transmission

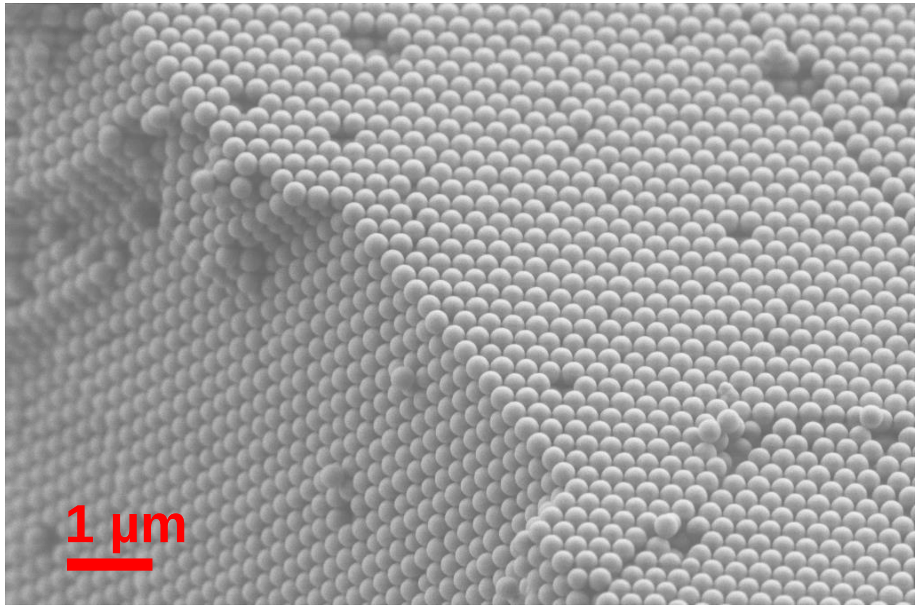


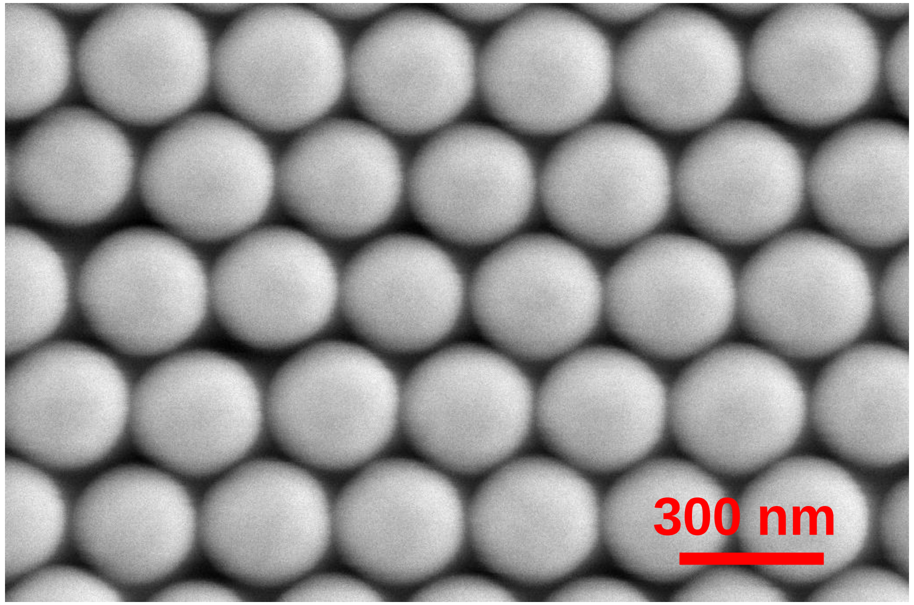
- Transmission spectrum computed as ratio:

unix% meep N=0 holey-wvg-cavity.ctl | tee holey-wvg-cavity.out0
unix% grep flux1: holey-wvg-cavity.out > flux.dat
unix% grep flux1: holey-wvg-cavity.out0 > flux0.dat
unix% divide2.pl flux0.dat flux.dat > flux-q.dat

SiO_2 Opal Films

- Opal films are polycrystalline, 10 μm thick, FCC films with the (111) planes oriented parallel to the surface.
- For visible spectrum, lattice constant ~ 140 – 500 nm.



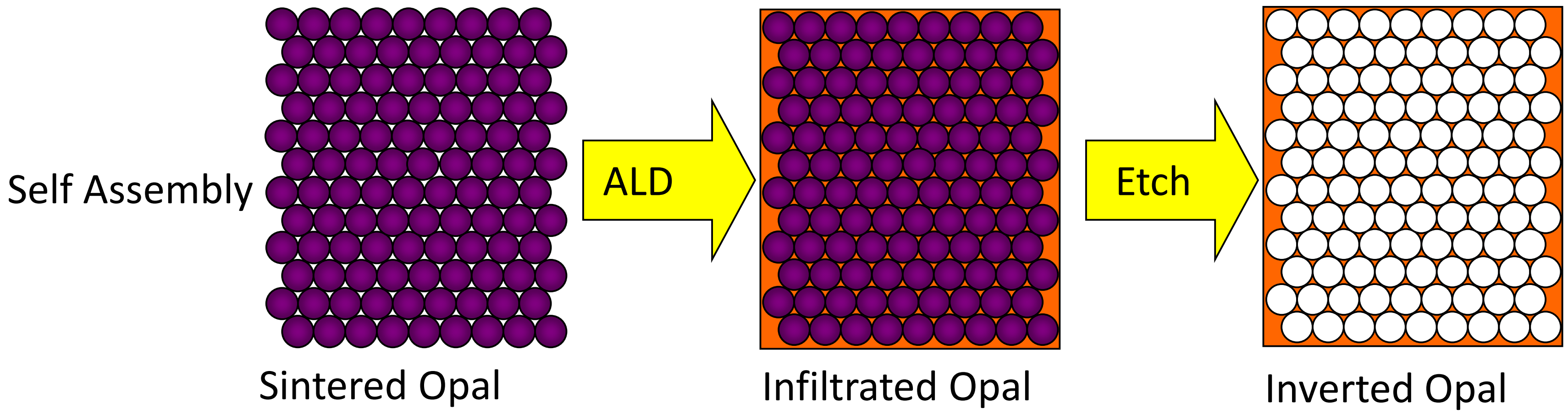


E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

Inverse Opal:

Fabrication

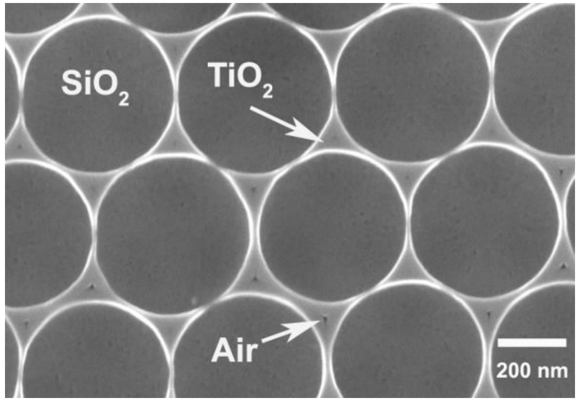
- Self-assembled silica opal template
  - 10 µm thick FCC polycrystalline film, (111) oriented.
- Infiltration of opal with high index materials
  - ZnS:Mn n~2.5 @ 425 nm (directional PBG)
  - TiO_2 (rutile) n_{avg}~ 3.08 @ 425 nm (omni-directional PBG)



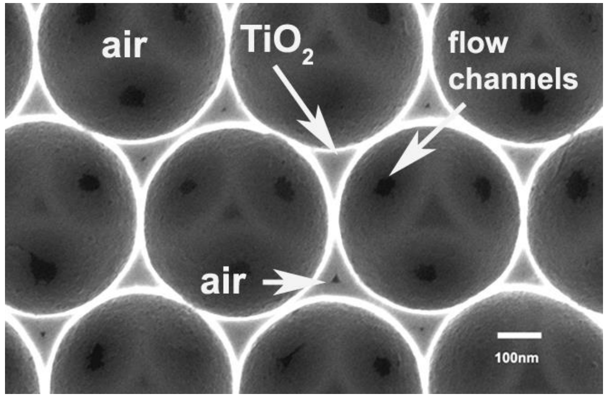
E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

ALD of TiO_2 at 100ºC

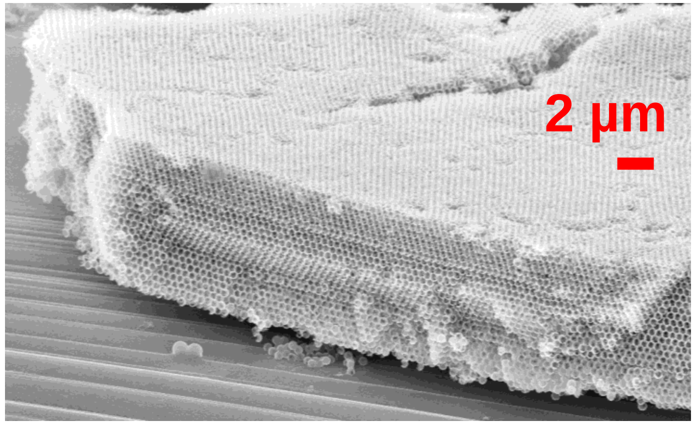
(111) ⊙ **Cross-sections**



433 nm opal infiltrated with TiO_2



433 nm TiO_2 inverse opal



433 nm TiO_2 inverse opal

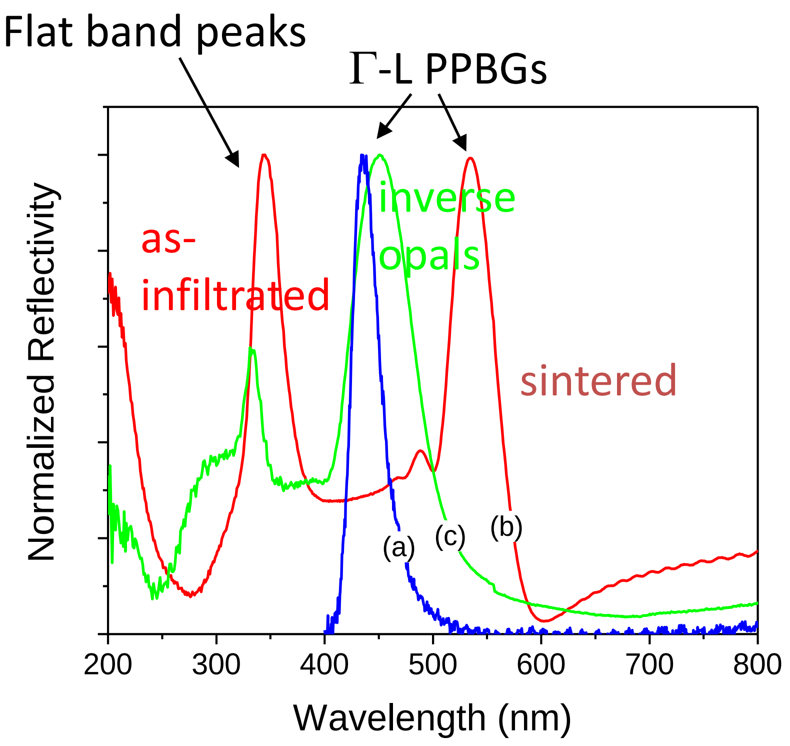
- TiO_2 infiltration at 100°C produces very smooth and conformal surface coatings with rms roughness ~2Å.
- Heat treatment (400C, 2 hrs.) of infiltrated opal converts it to anatase TiO_2, increasing the refractive index from 2.35 to 2.65, with only a 2Å increase in the rms surface roughness.

E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

Specular Reflectivity

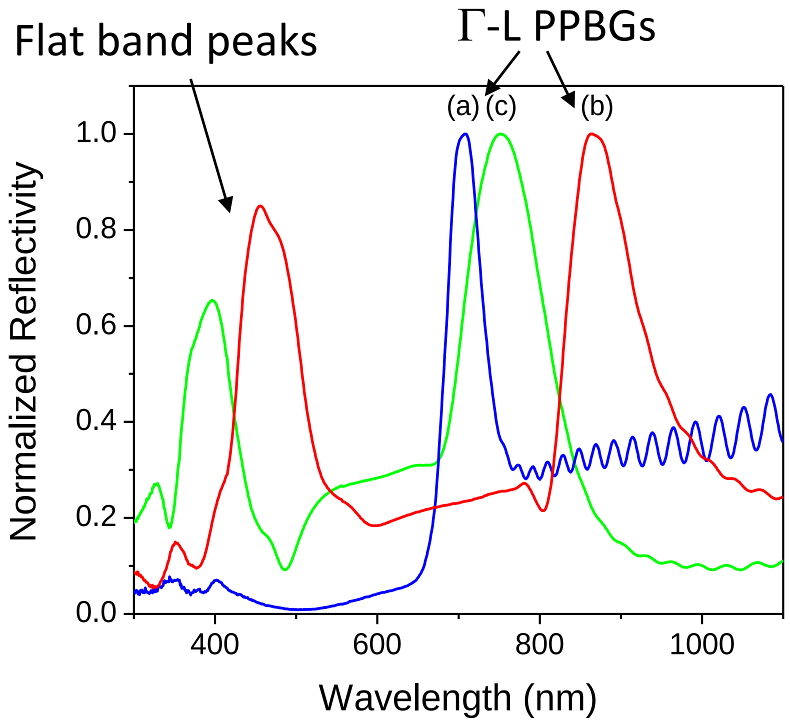
- Measurements: 15° from normal
- Probes changes in Γ-L photonic band structure (111)

ZnS:Mn



200 nm opal

TiO_2

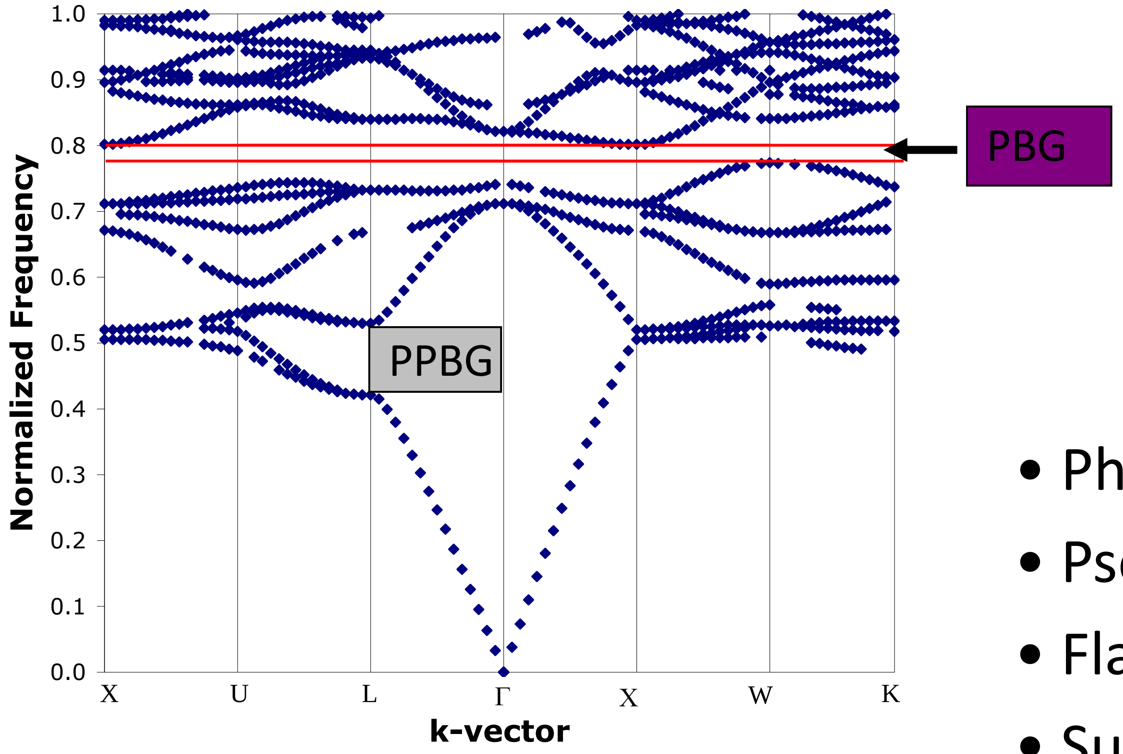


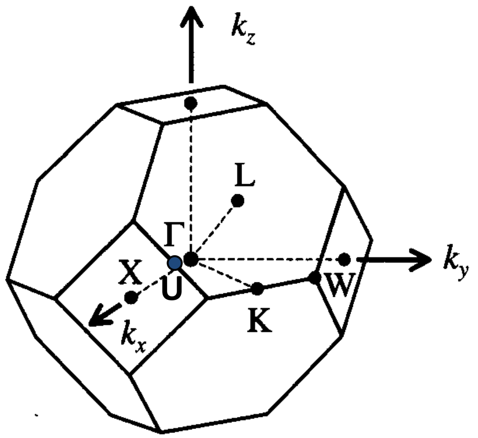
330 nm opal

E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

Photonic Crystal Band Diagram

ω vs. *k* as calculated from Finite-difference time domain (FDTD)



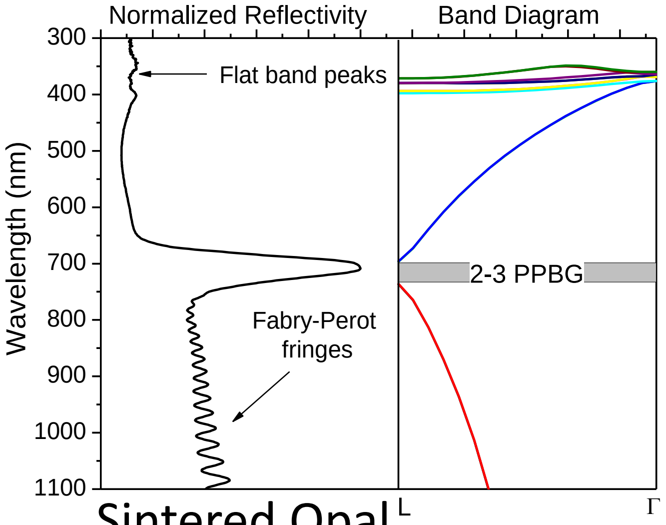


FCC Brillouin zone

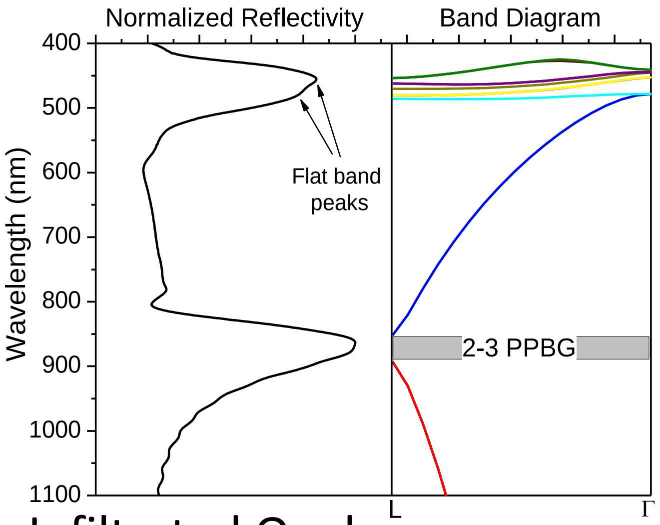
- Photonic band gaps (PBG)
- Pseudo-photonic band gaps (PPBG)
- Flat bands, low group velocity
- Superprism and giant refraction

Inverse Opal Reflectivity

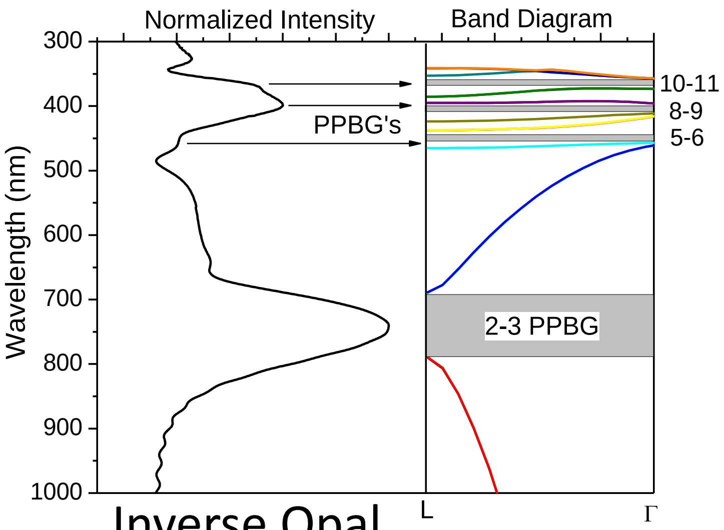
- TiO_2 infiltration of 330 nm opal.
- ~88% filling fraction
- 2.65 Refractive Index
- Agreement: full index attained!



Sintered Opal



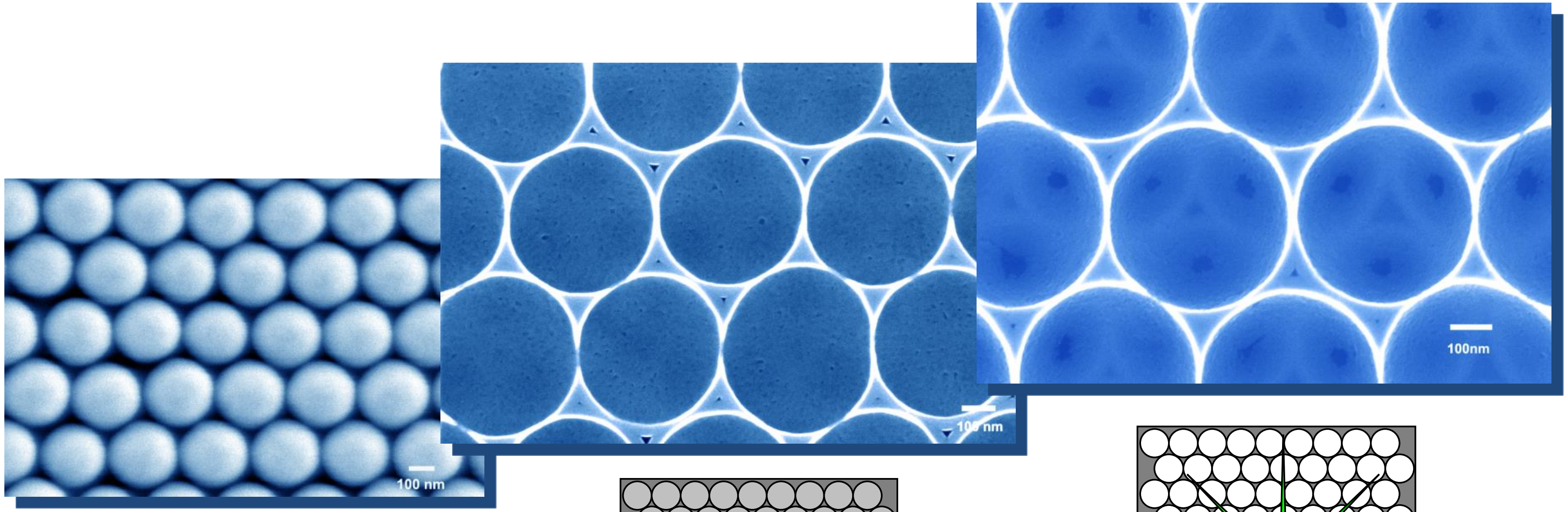
Infiltrated Opal

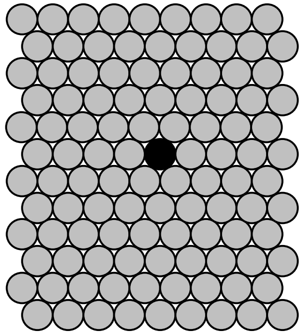


Inverse Opal

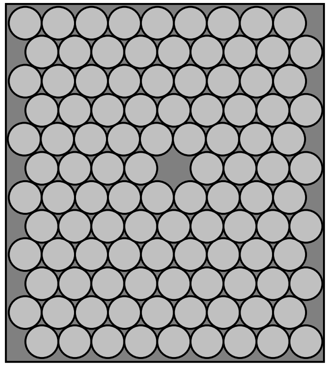
E. Graugnard et al., Photonic Crystals at Georgia Tech, www.nanophotonics.gatech.edu/PCs_at_GaTech.ppt

Opal Defect Engineering

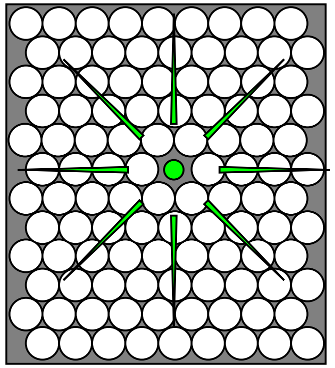




Silica Opal with Defect



Infiltrated Opal

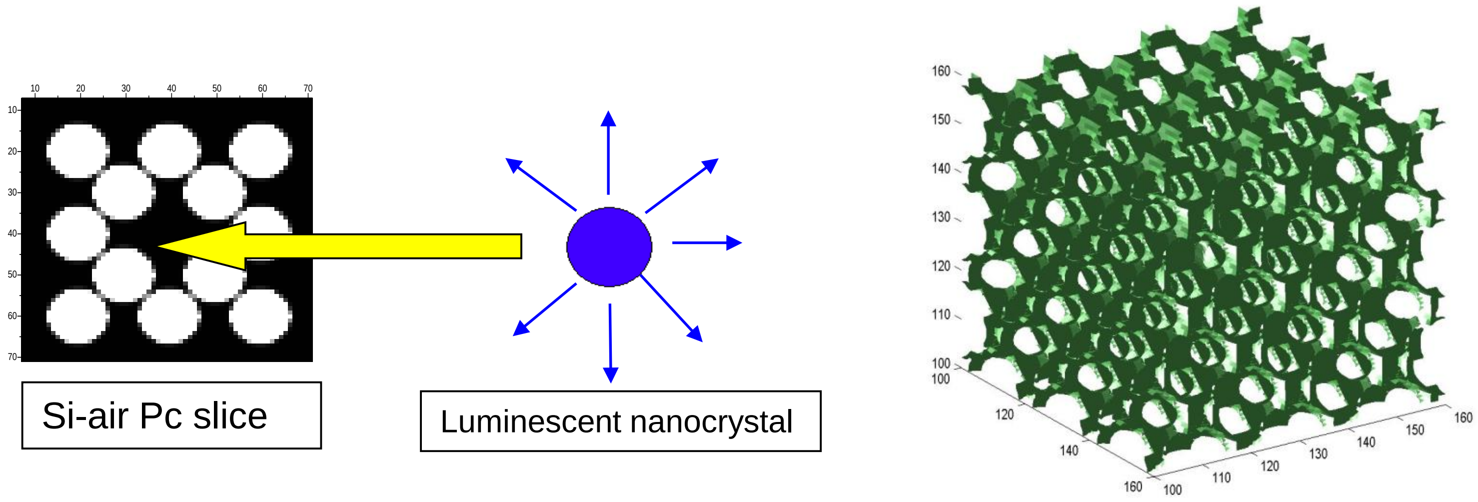


Inverted Opal Structure

(With Defect – soon!)

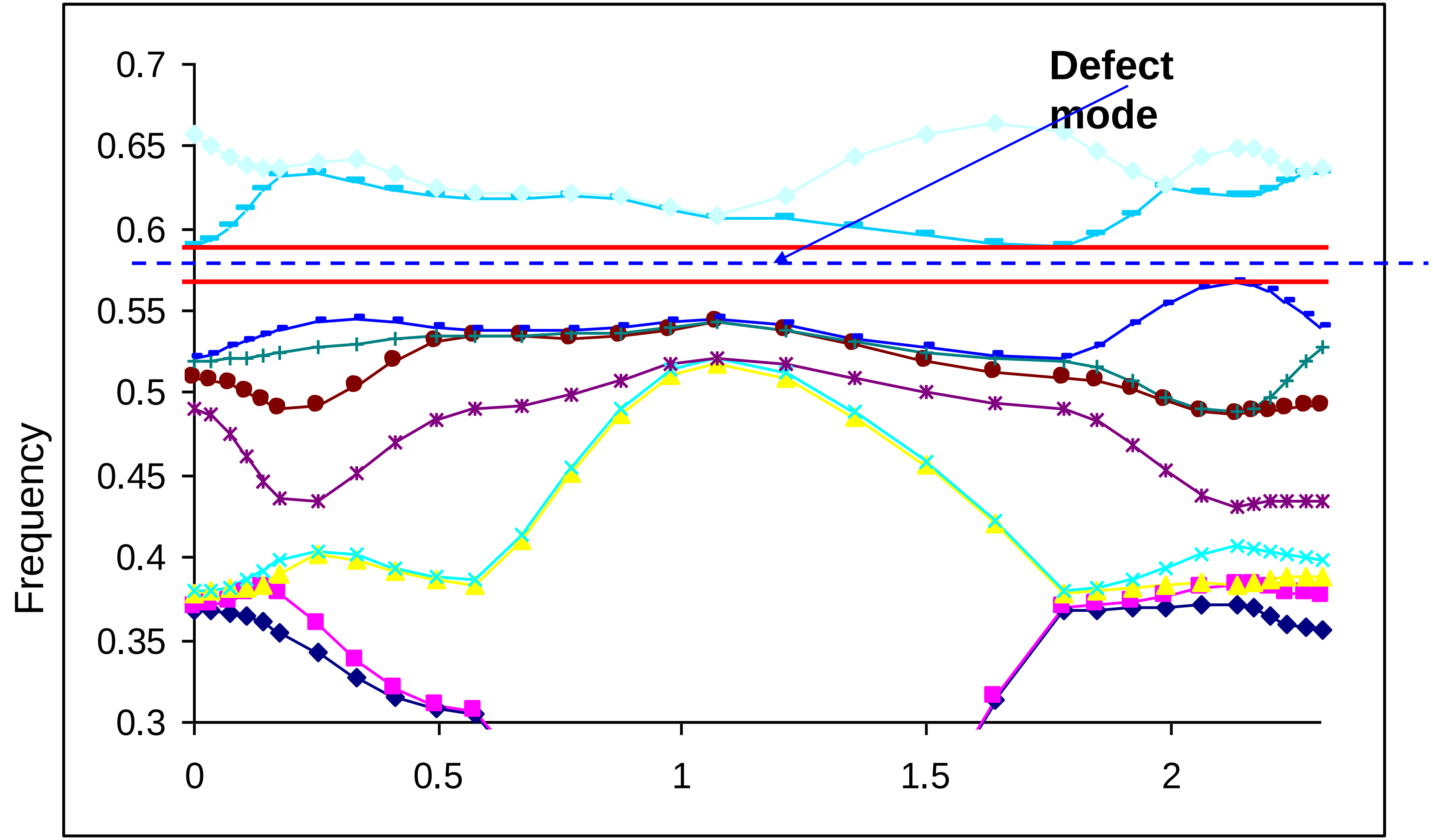
Inverse Opal Defect Mode Calculations for PhCPs

- What is the main idea behind Photonic Crystal Phosphor (PhCP)?
  - Combining a 3D inverse opal with nanophosphors as a local defect in the PhC lattice



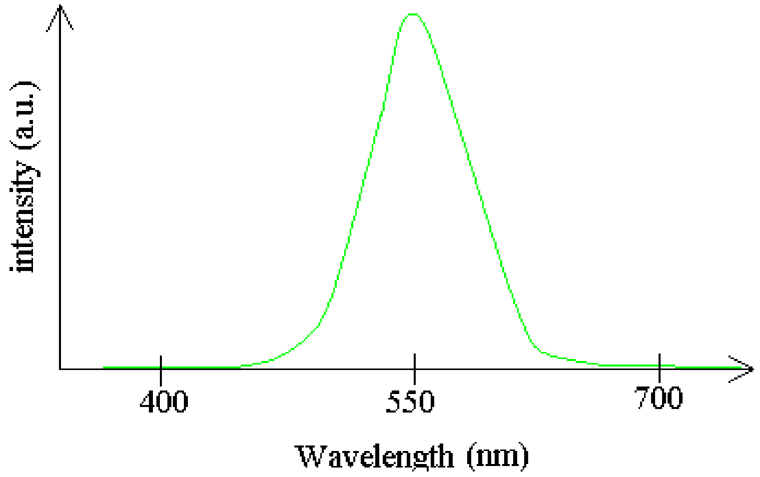
- Specific frequencies in the Photonic Band-Gap of the inverse structure are inhibited except for the defect modes
- A broad luminescent material spectrum within this band-gap would be filtered by the resonant frequency and therefore tuned up

Photonic Band-Gap Analysis

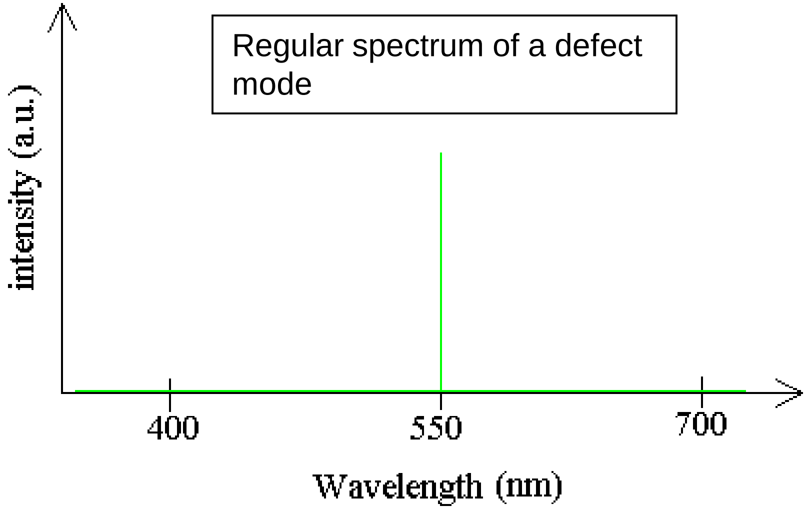


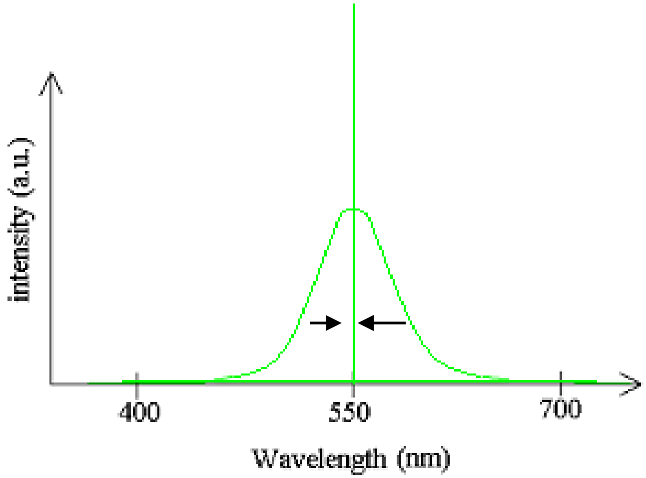
Spectrum analysis for PhCPs

Regular spectrum of a green phosphor



Regular spectrum of a defect mode





Both spectrum combine and

Emission Energy of phosphor is totally quenched into the defect mode

Main Characteristics of PhcPs

- The cavity mode emission spectrum lies within the phosphor emission spectrum
- The position and peak cavity spectrum from the host statically controls the color, luminous intensity and decay time
- Ultimate tunability would be achieved by tunable materials like liquid-crystal, PLZT, etc. to change both the position and peak of cavity mode

PhCPs are candidates for High-Definition Display devices

Next Class

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