Photonic Geometries for Light Trapping and Manipulation

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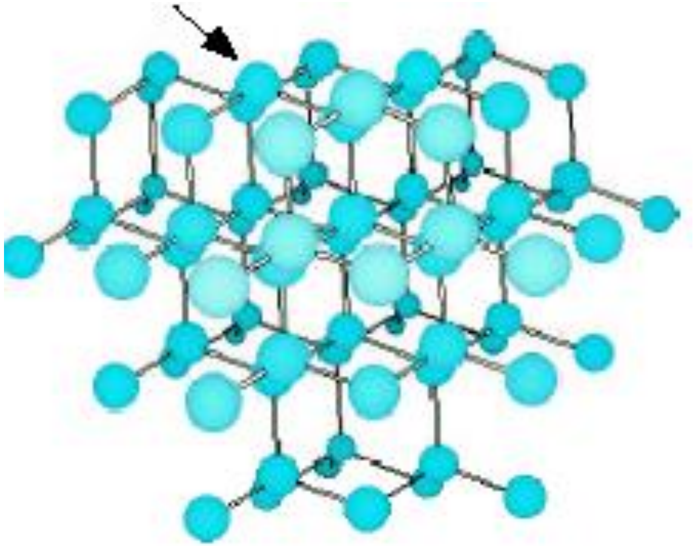
Outline

- A review of photonic crystals
  - Band structure, intentional defects and devices, disorder and robustness
- Topology optimization of nonlinear photonic cavities
  - Topology optimization, inverse design of nonlinear optical cavities

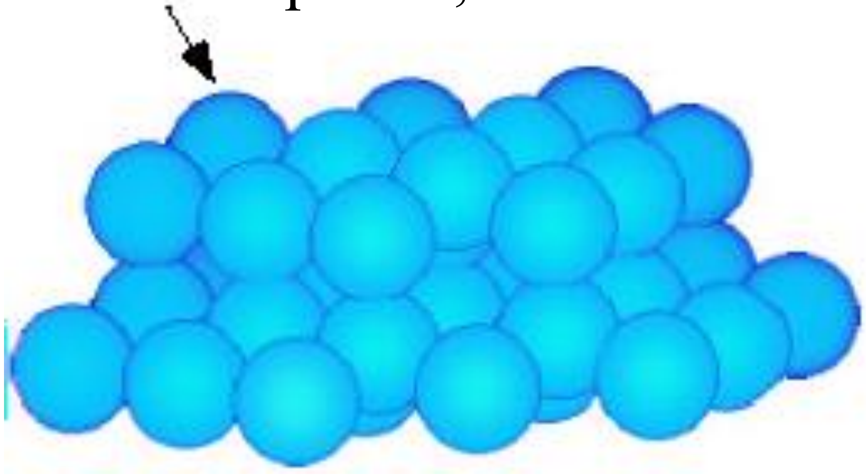
Electronic and Photonic Crystals

Periodic Medium

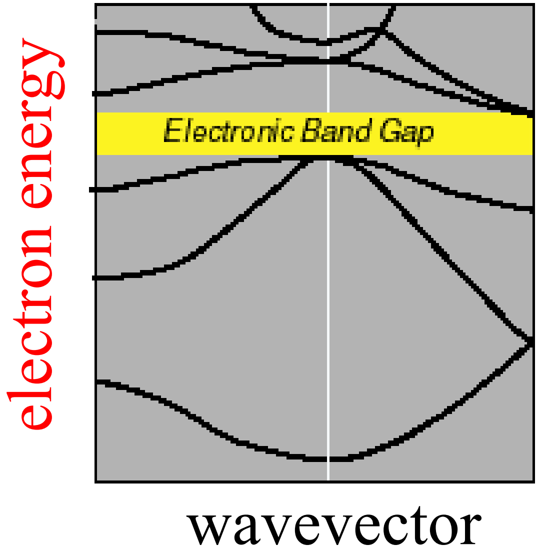
atoms in diamond structure

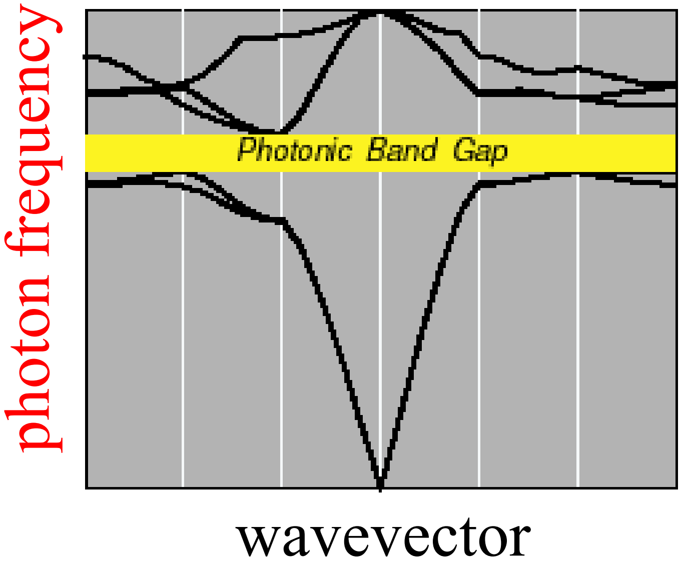


dielectric spheres, diamond lattice



Bloch waves: **Band Diagram**



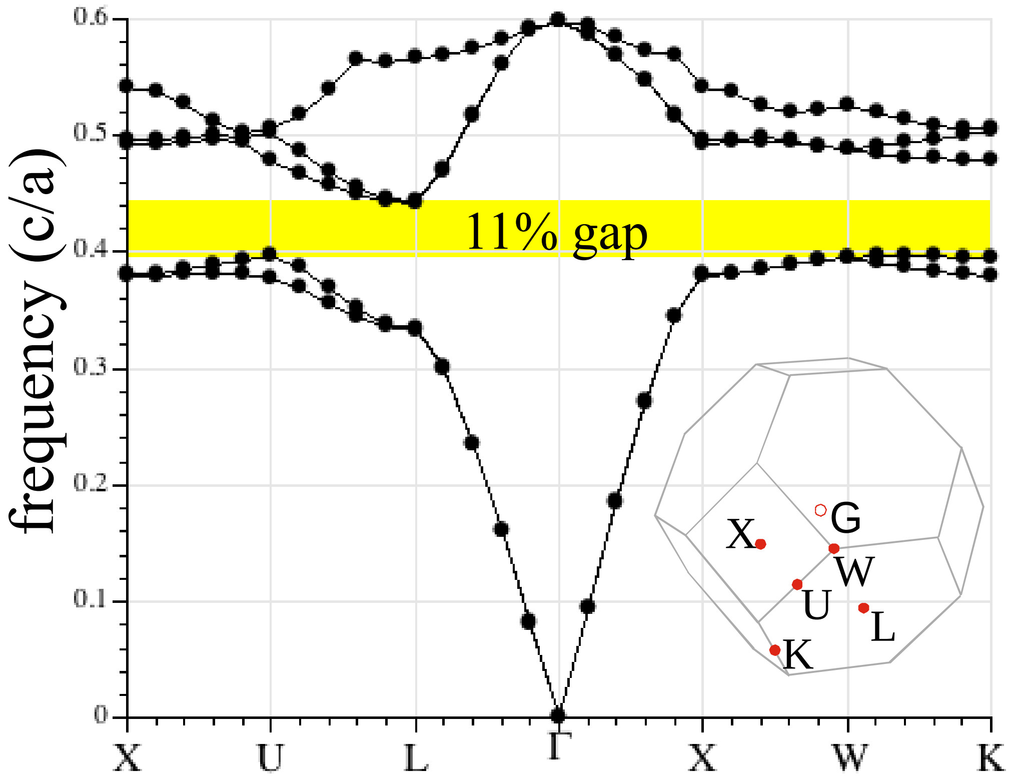


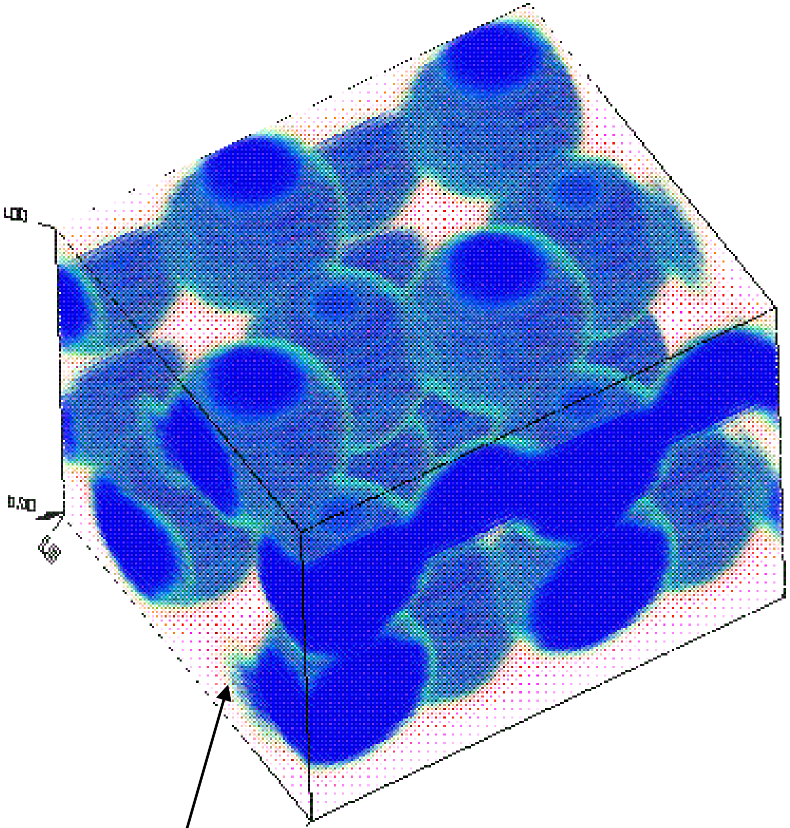
strongly interacting fermions

weakly-interacting bosons

The First 3d Bandgap Structure

K. M. Ho, C. T. Chan, and C. M. Soukoulis, *Phys. Rev. Lett.* **65**, 3152 (1990).





for gap at λ = 1.55μm,
sphere diameter ~ 330nm

overlapping Si spheres

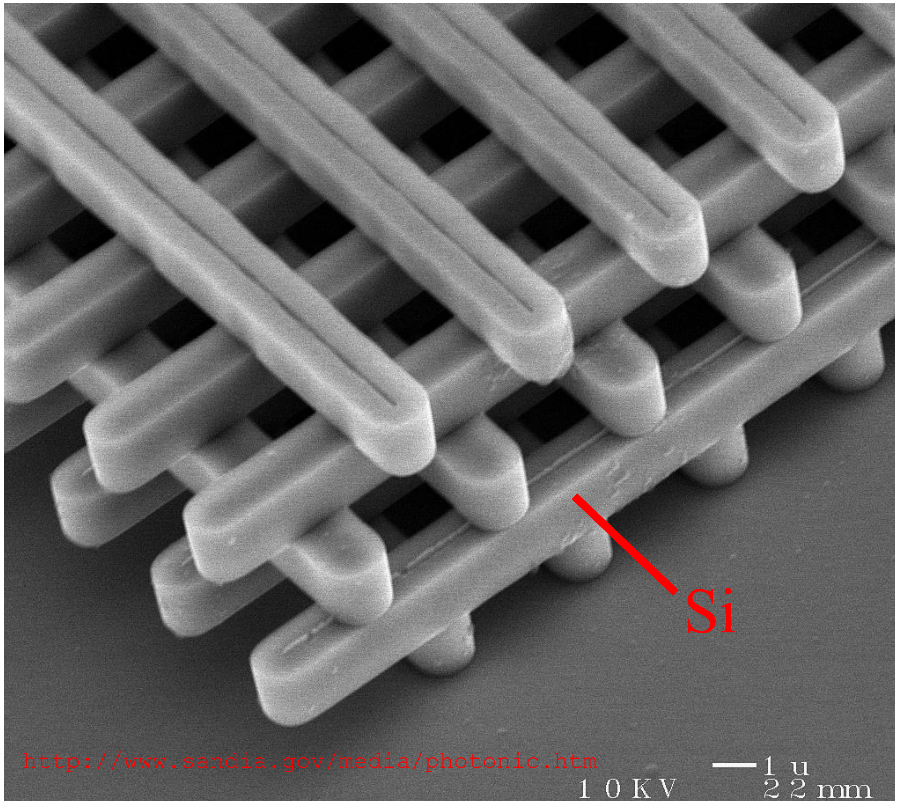
MPB tutorial, `http://ab-initio.mit.edu/mpb`

An early fabricable structure:

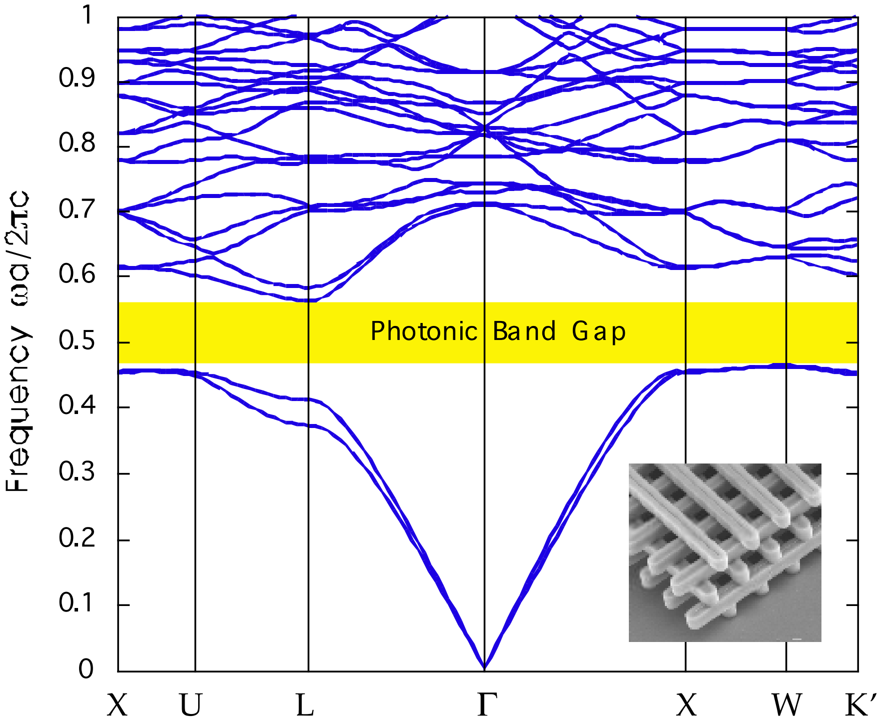
The Woodpile Crystal

[K. Ho *et al.*, *Solid State Comm.* **89**, 413 (1994)] [H. S. Sözüer *et al.*, *J. Mod. Opt.* **41**, 231 (1994)]

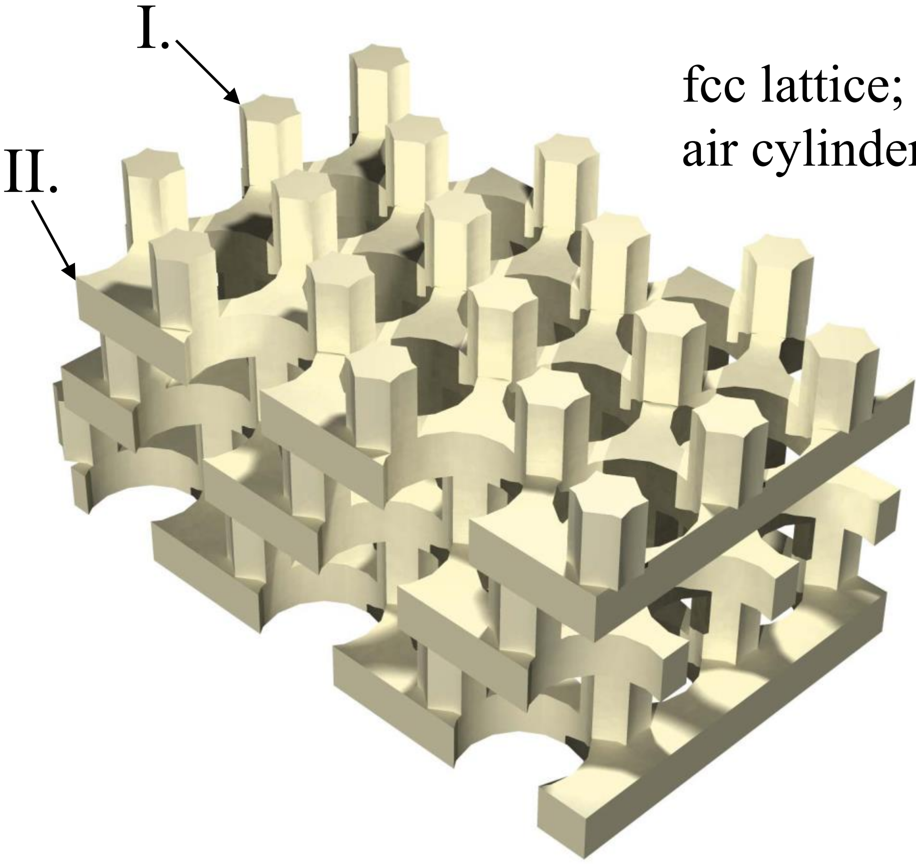
(4 “log” layers = 1 period)



[S. Y. Lin *et al.*, *Nature* **394**, 251 (1998)]

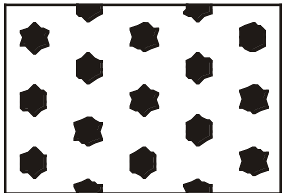


3d photonic crystal: complete gap , ε=12:1

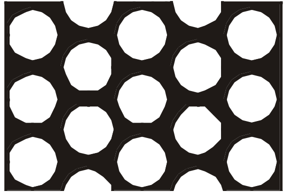


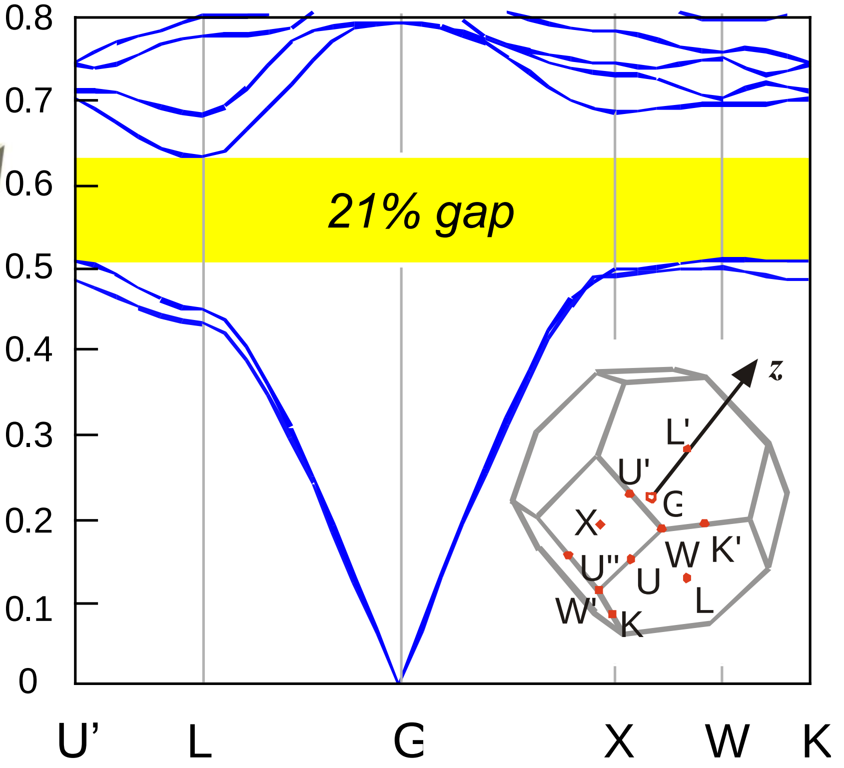
fcc lattice;
air cylinders in 111 direction

I: rod layer



II: hole layer

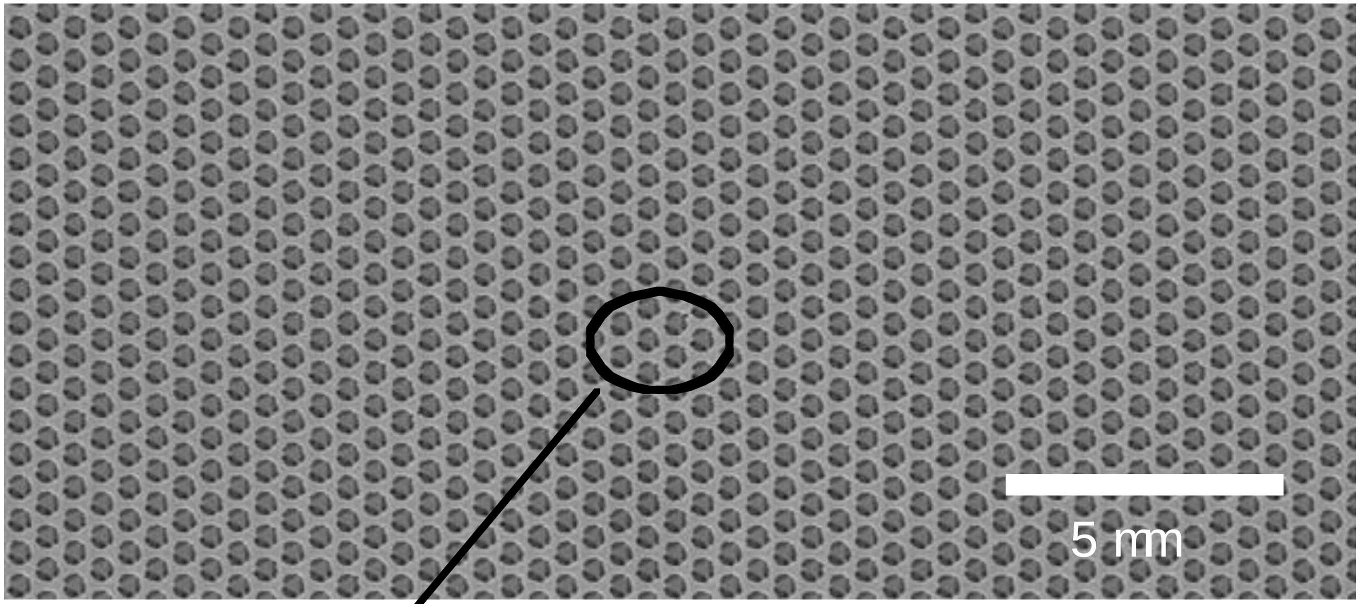


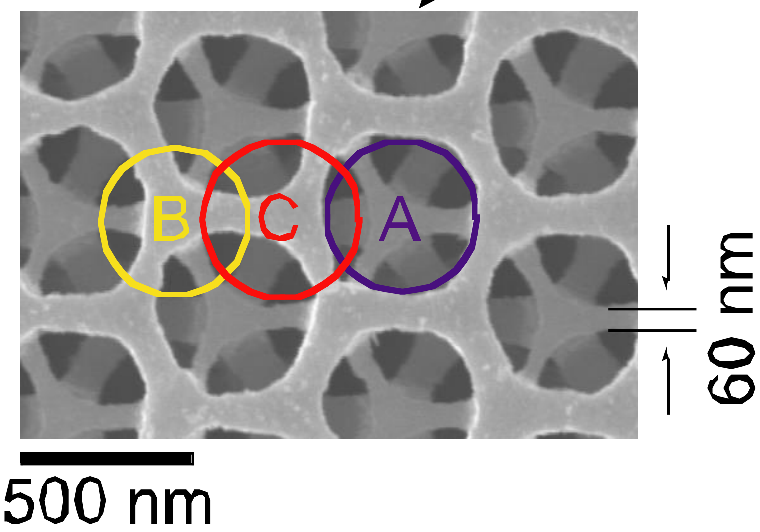


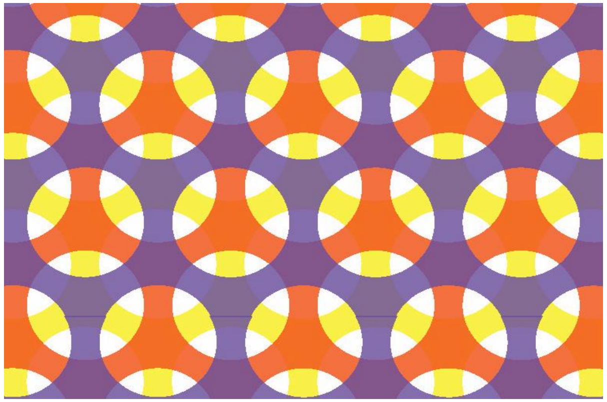
gap for n > ~2:1

[S. G. Johnson *et al.*, *Appl. Phys. Lett.* **77**, 3490 (2000)]

7-layer E-Beam Fabrication



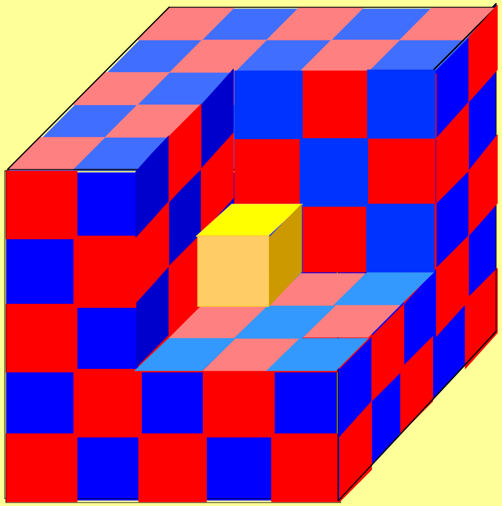




[M. Qi, *et al.*, *Nature* **429**, 538 (2004)]

Intentional “defects” are good

microcavities



Resonance

an oscillating mode trapped for a long time in some volume

(of light, sound, …)

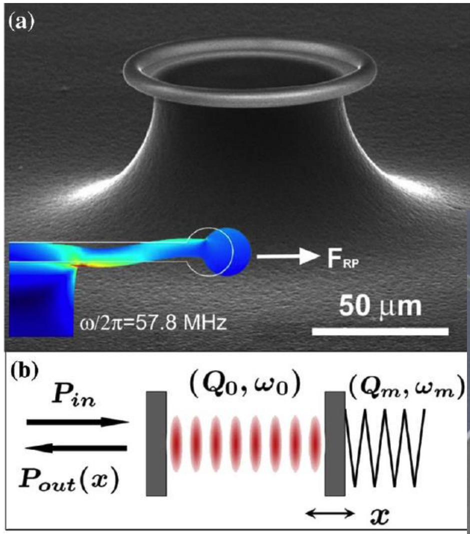
lifetime $\tau >> 2\pi/\omega_0$

frequency ω_0

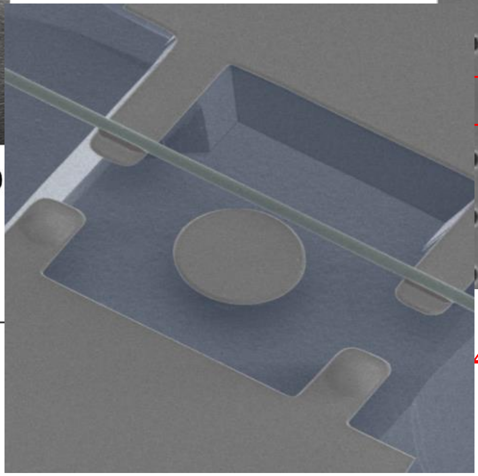
quality factor $Q = \omega_0\tau/2$

energy $\sim e^{-\omega_0 t/Q}$

modal
volume V

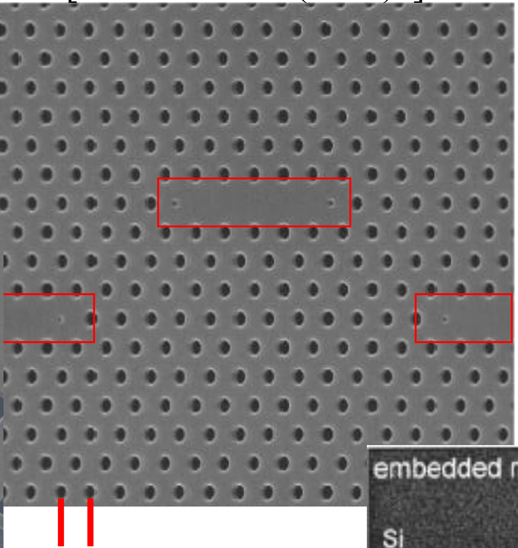


[Schliesser et al.,
PRL **97**, 243905 (2006)]

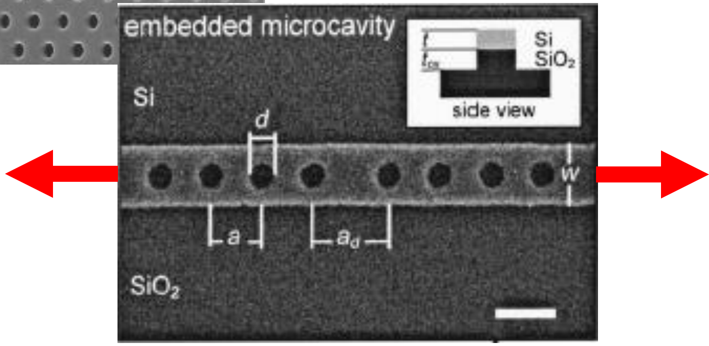


[Eichenfield et al. *Nature Photonics* **1**, 416 (2007)]

[Notomi *et al.* (2005).]

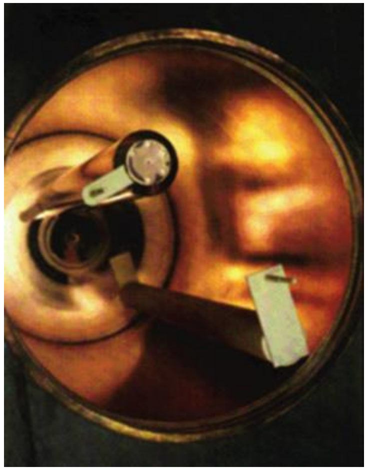


[C.-W. Wong,
APL **84**, 1242 (2004).]



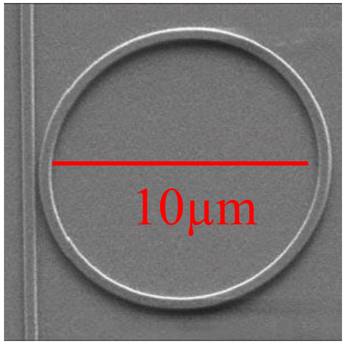
How Resonance?

need mechanism to trap light for long time



[llnl.gov]

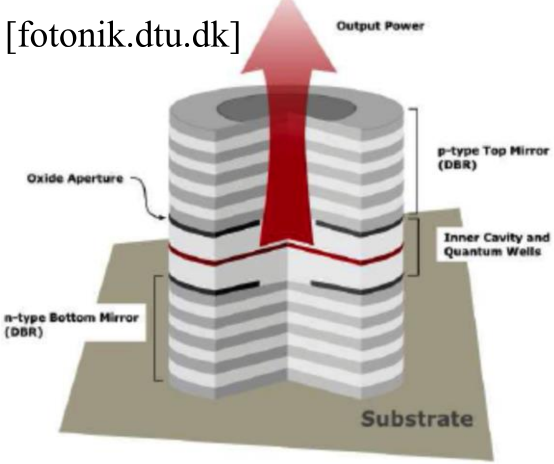
metallic cavities:
good for microwave,
dissipative for infrared

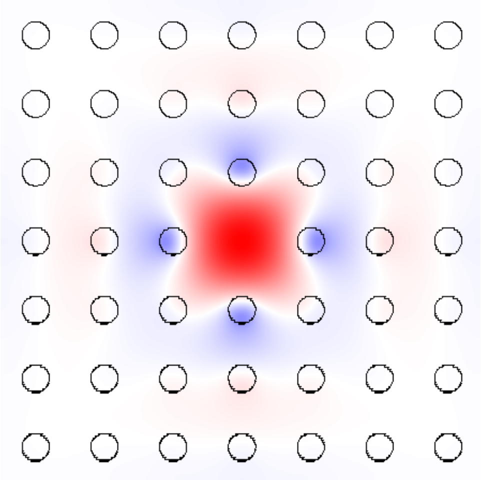


[Xu & Lipson (2005)]

ring/disc/sphere resonators:
a waveguide bent in circle,
bending loss ~ exp(–radius)

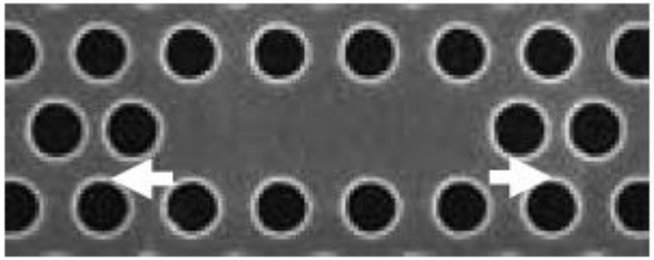
VCSEL
[fotonik.dtu.dk]





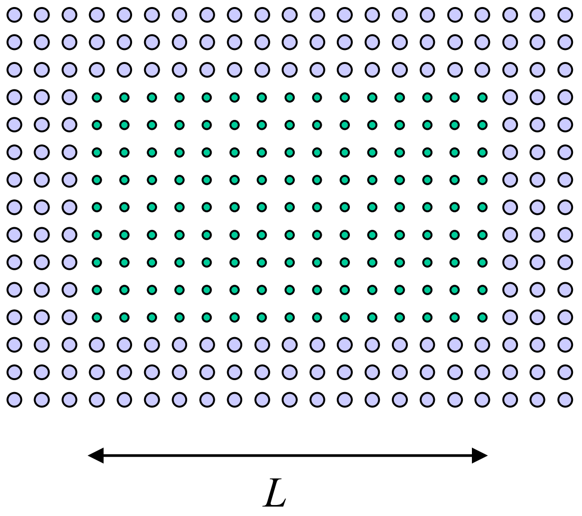
photonic bandgaps
(complete or partial
+ index-guiding)

[Akahane, *Nature* **425**, 944 (2003)]

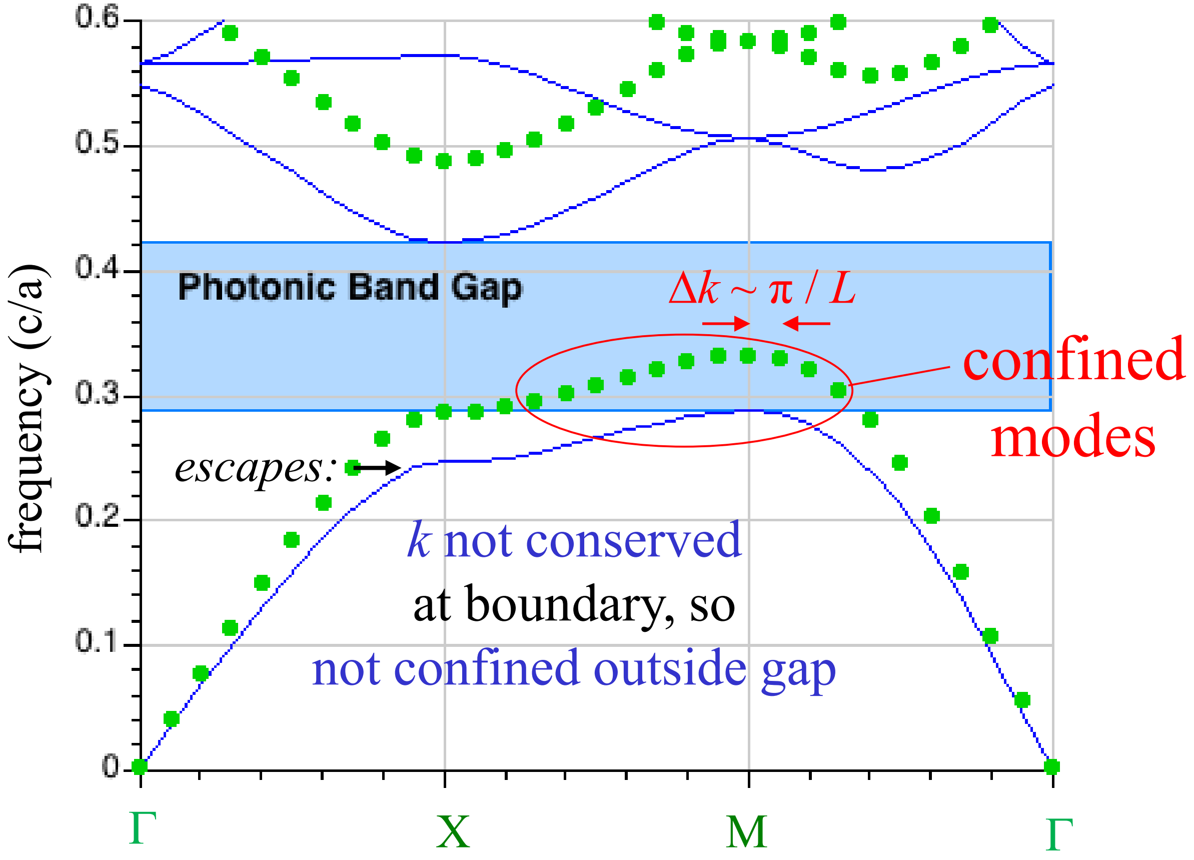


(planar Si slab)

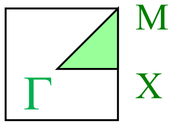
Cavity Modes



Defect Crystal Band Diagram



Bulk Crystal Band Diagram



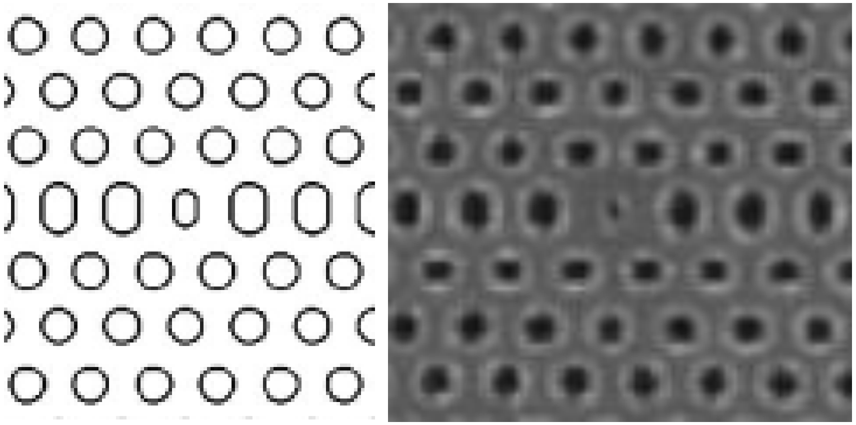
Defect bands are shifted *up* (less ε)

with *discrete k*

$$\# \times \frac{\lambda}{2} \sim L \qquad (k \sim 2\pi/\lambda)$$

2D PhC slab cavities: Q vs. V

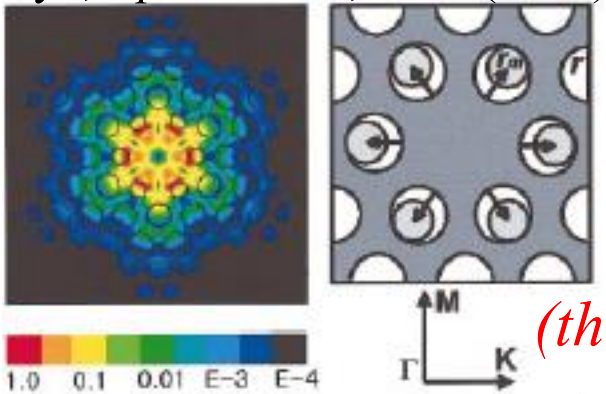
[Loncar, *APL* **81**, 2680 (2002)]



$Q \sim 10{,}000$ ($V \sim 4 \times$ optimum)

$= (\lambda/2n)^3$

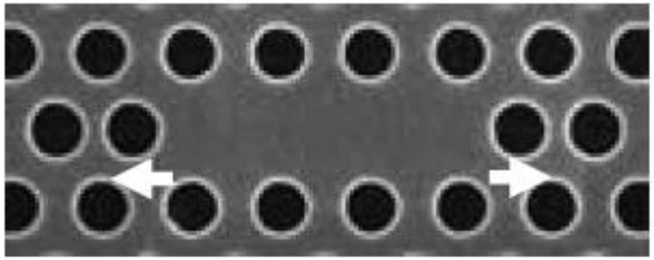
[Ryu, *Opt. Lett.* **28**, 2390 (2003)]



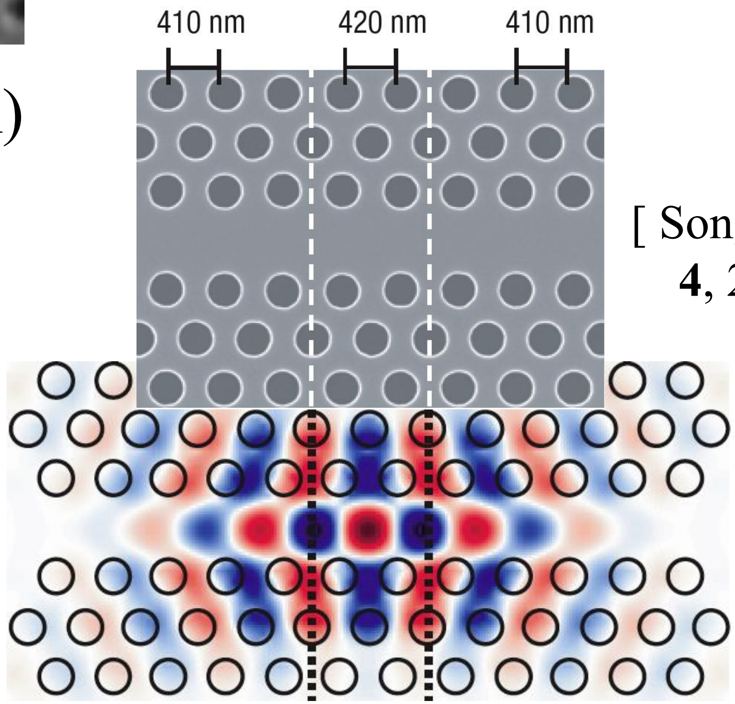
(theory only)

$Q \sim 10^6$ ($V \sim 11 \times$ optimum)

[Akahane, *Nature* **425**, 944 (2003)]



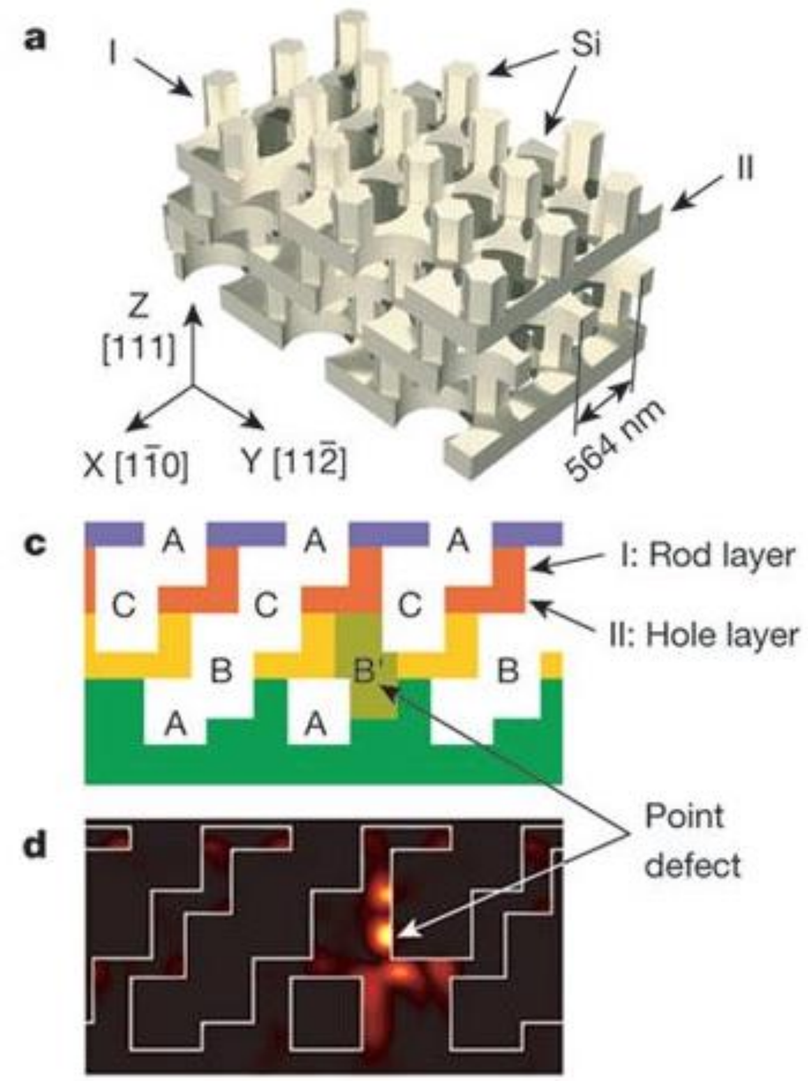
$Q \sim 45{,}000$ ($V \sim 6 \times$ optimum)

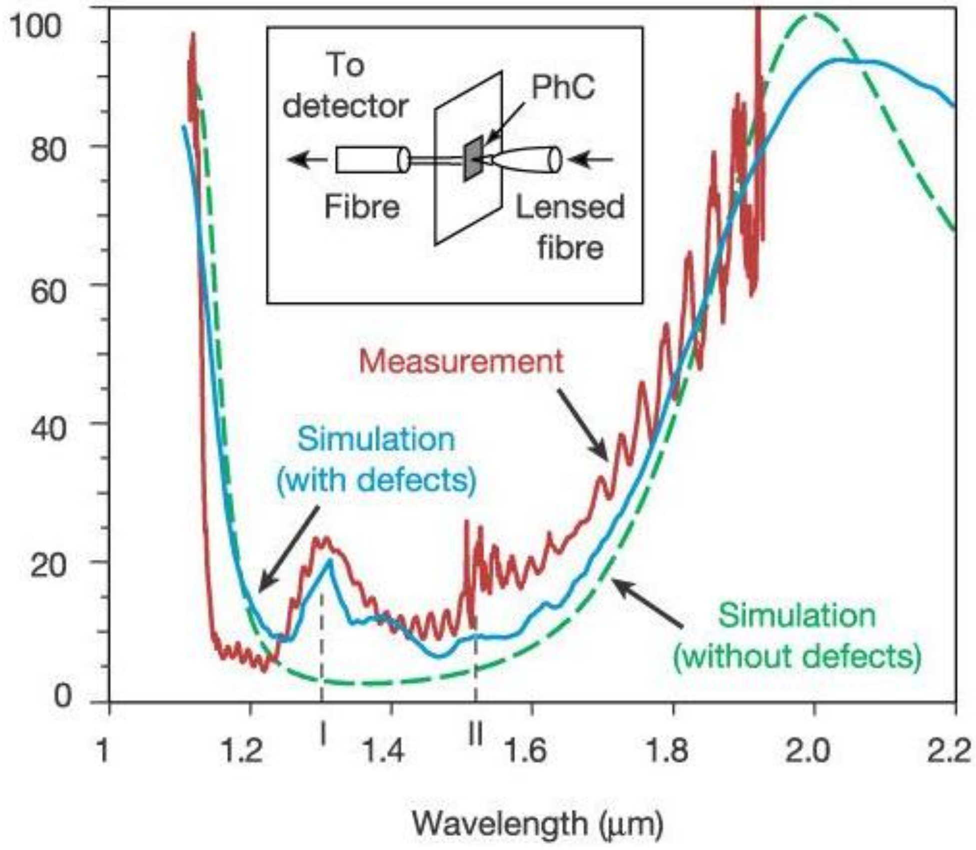


[Song, *Nature Mat.*
4, 207 (2005)]

$Q \sim 600{,}000$ ($V \sim 10 \times$ optimum)

3D Photonic Bandgap Mode





[M. Qi, *et al.*, *Nature* **429**, 538 (2004)]

Surface roughness disorder?

[http://www.physik.uni-wuerzburg.de/TEP/Website/groups/opto/etching.htm]

conventional

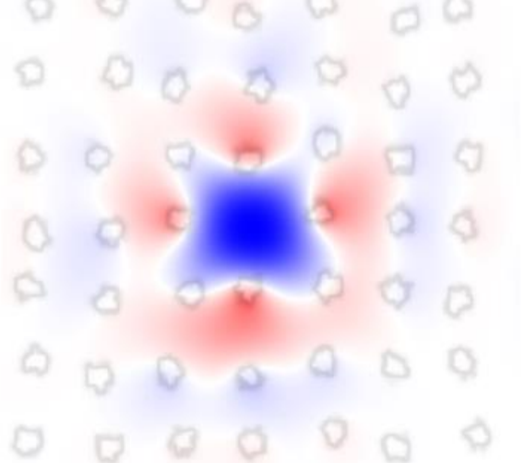
ring resonator

loss limited by disorder

(in addition to bending)

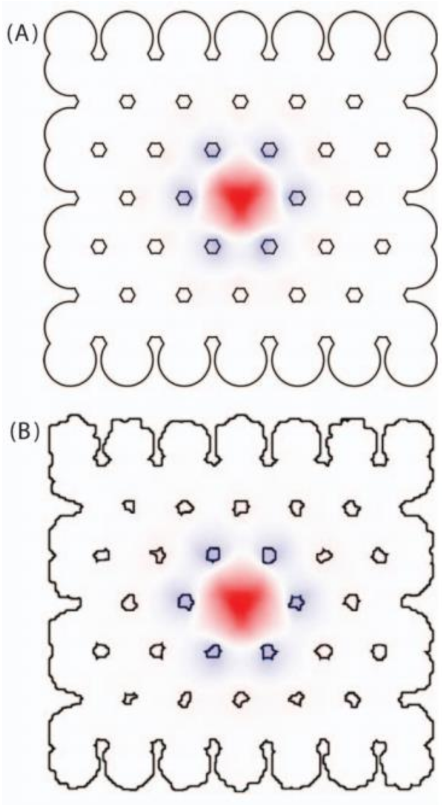
disordered

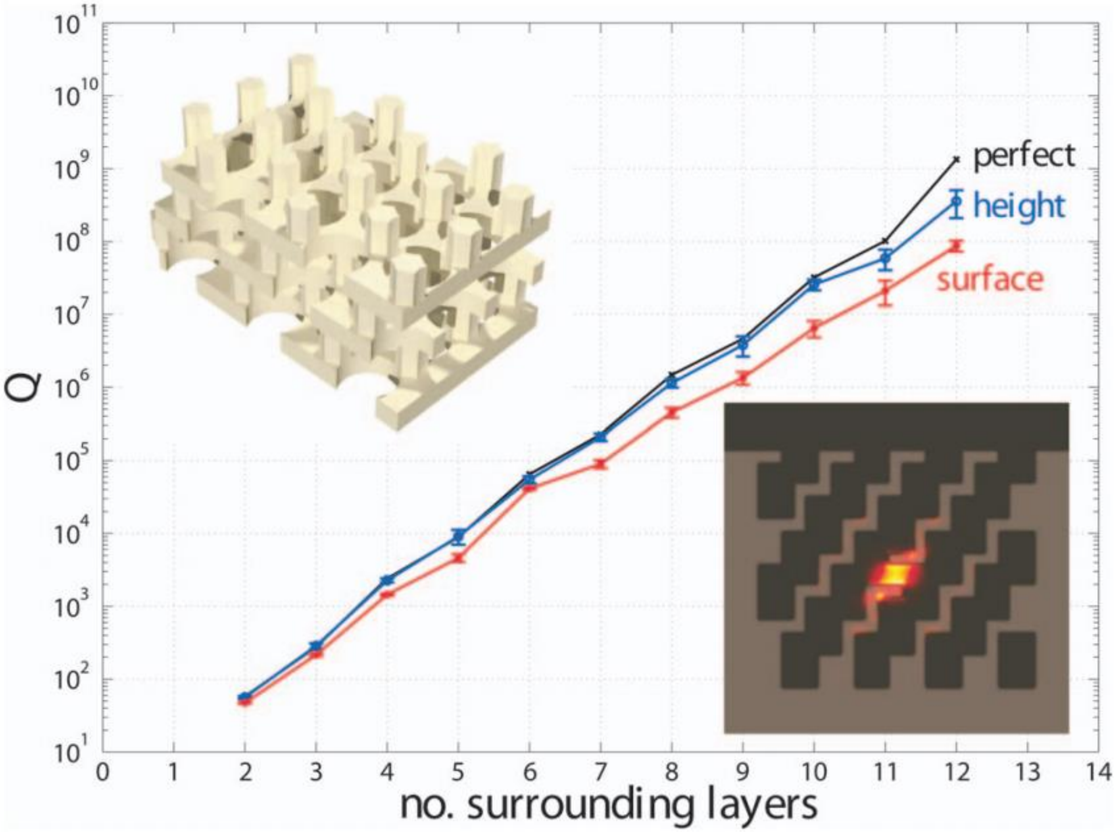
photonic crystal



[A. Rodriguez, MIT]

Surface roughness disorder?





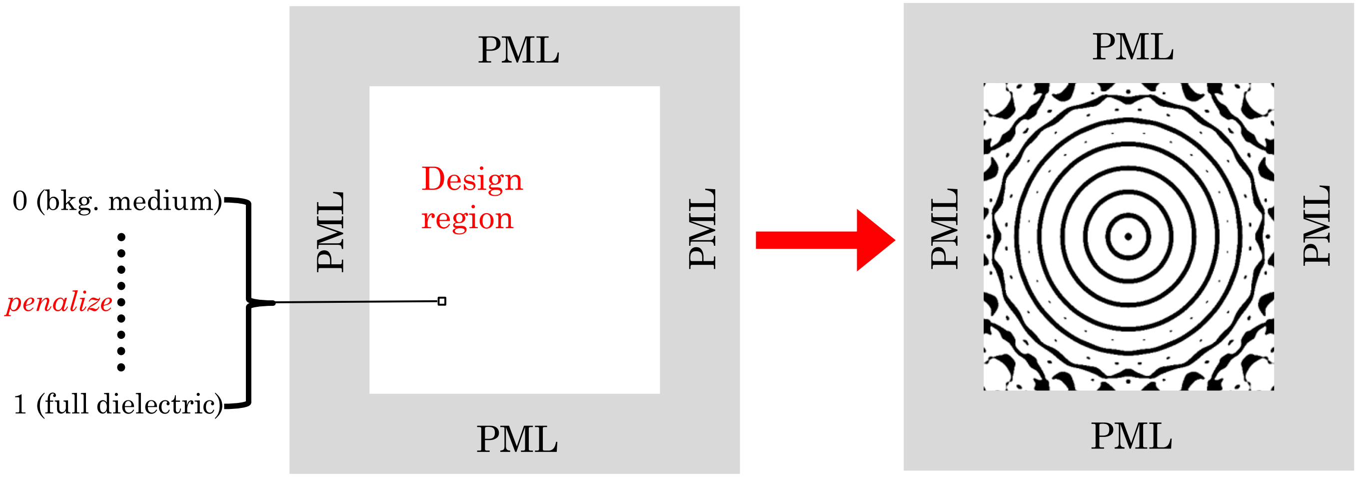
small (bounded) disorder does not destroy the bandgap

[A. Rodriguez *et. al.*, *Opt. Lett.* **30**, 3192 (2005).]

Q limited only by crystal size (for a 3d complete gap) …

Why should we stick to regular shapes?

Topology optimization: *all pixels count*



0 (bkg. medium)

penalize

1 (full dielectric)

PML

Design region

PML

PML

PML

PML

PML

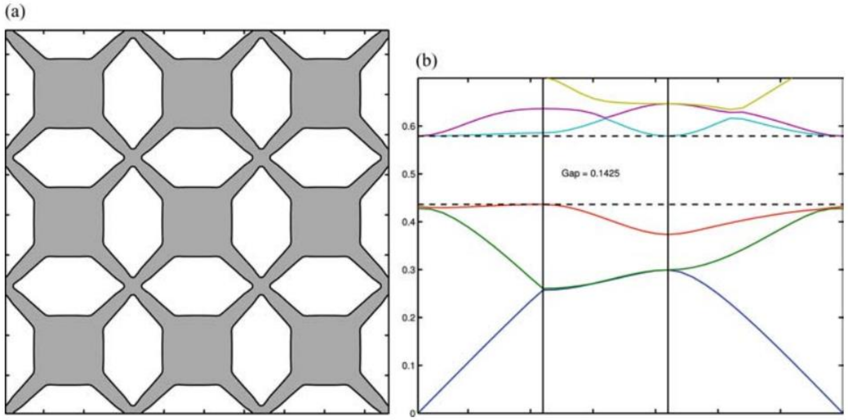
PML

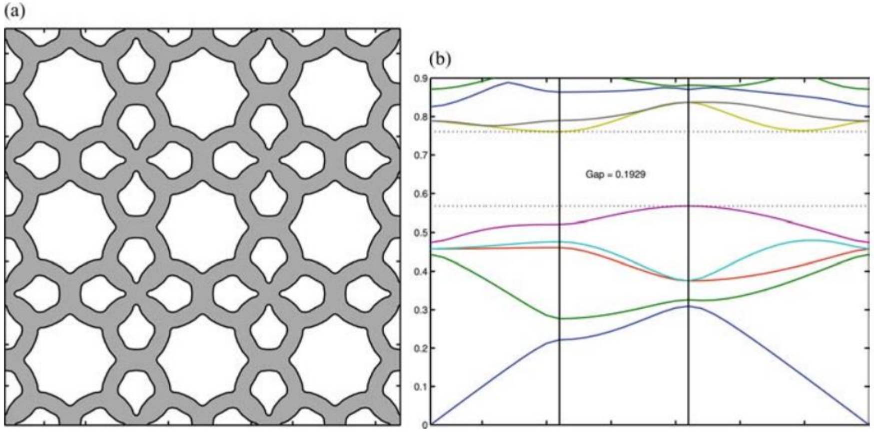
PML

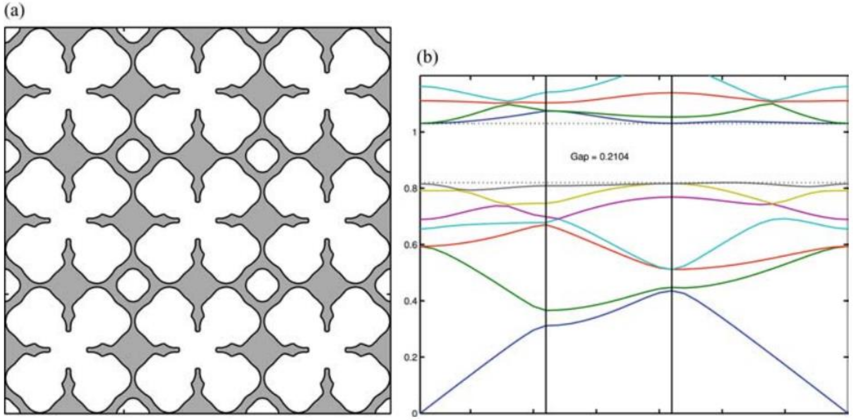
- Arbitrary shapes and topologies
- Every pixel is a *continuous* DOF
- *Key*: differentiability → adjoint algorithms
- Manufacturability (binarity) achieved via regularization filters

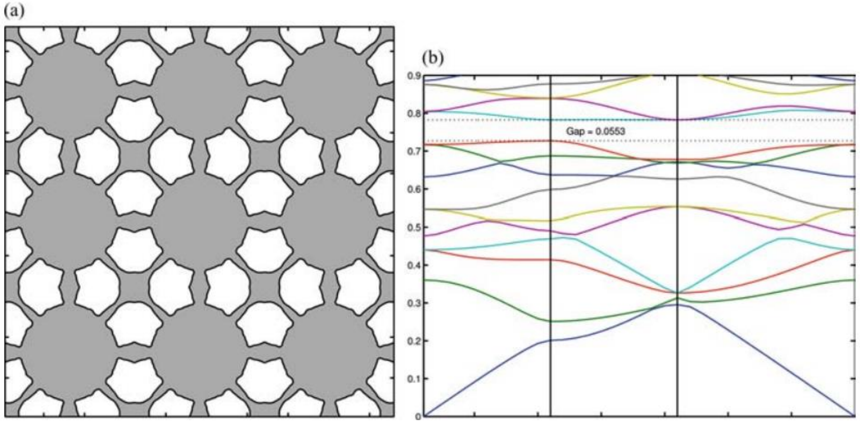
$$\begin{aligned} \max_{\epsilon(\mathbf{r})} \quad & f(\mathbf{E};\epsilon) \\ \text{subject to} \quad & g(\mathbf{E};\epsilon) \leq 0 \\ & \epsilon_{\text{min}} \leq \epsilon(\mathbf{r}) \leq \epsilon_{\text{max}} \\ \text{given} \quad & \frac{\partial f}{\partial \epsilon(\mathbf{r})}, \ \frac{\partial g}{\partial \epsilon(\mathbf{r})} \end{aligned}$$

Bandgap optimization (2D)





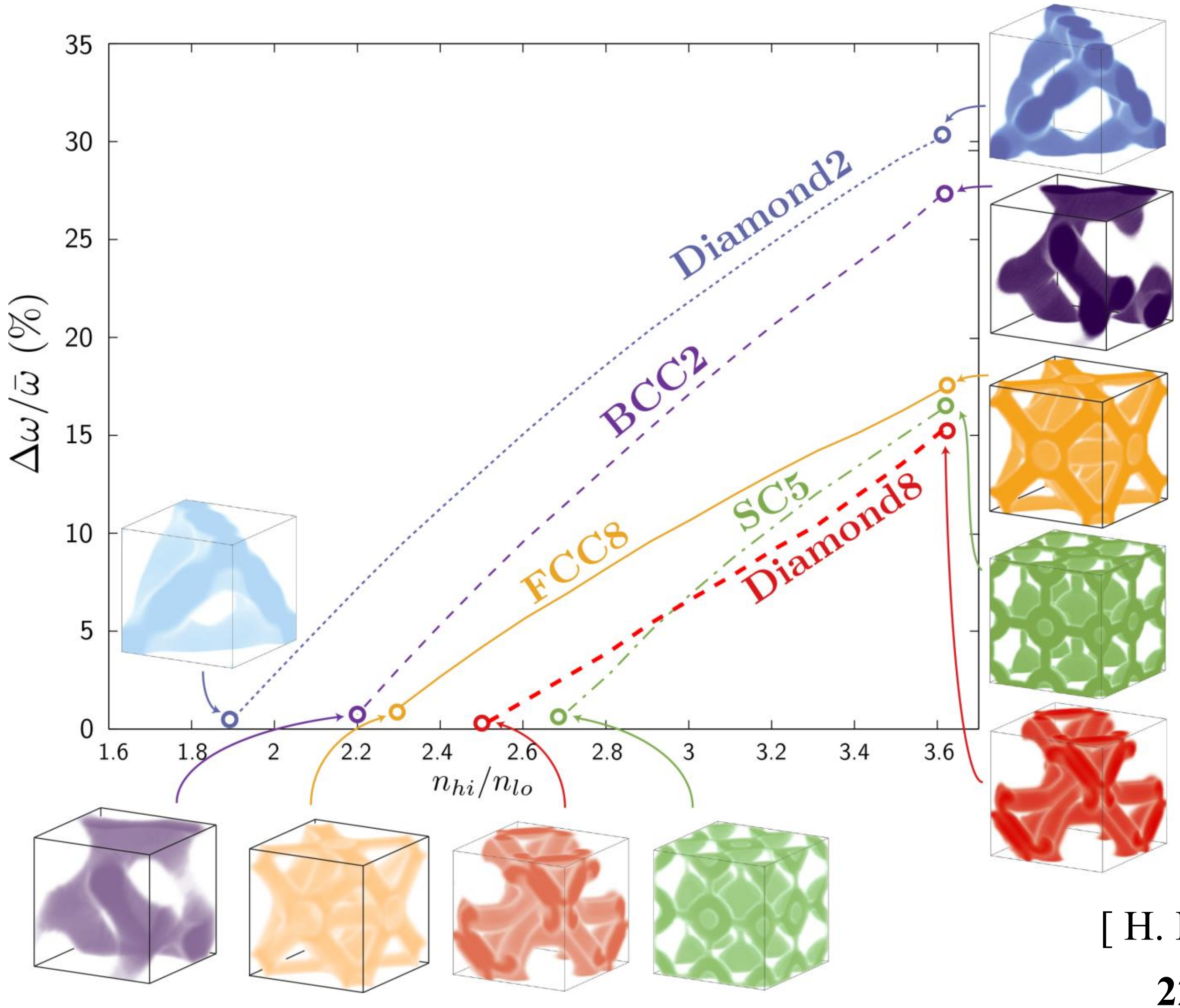




Opening a gap between any 2 bands

[Kao *et. al.*, *Appl. Phy. B* **81**, 235 (2005).]

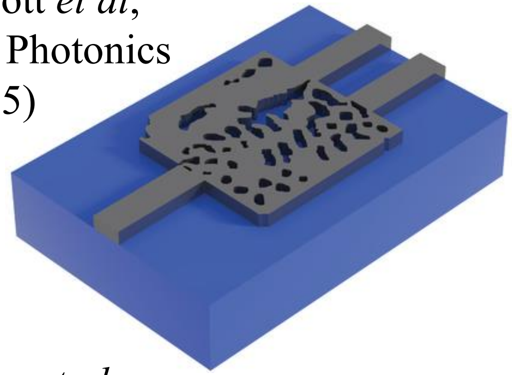
Bandgap optimization (3D)

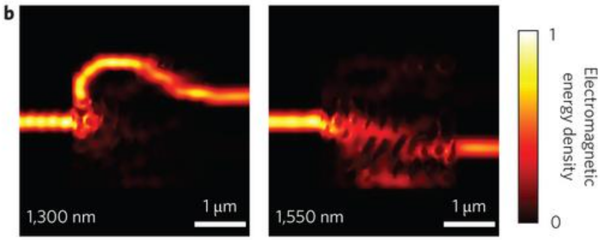


[H. Men *et. al.*, *Opt. Exp.* **22**, 22632 (2014).]

More recent works (marketed as "inverse design")…

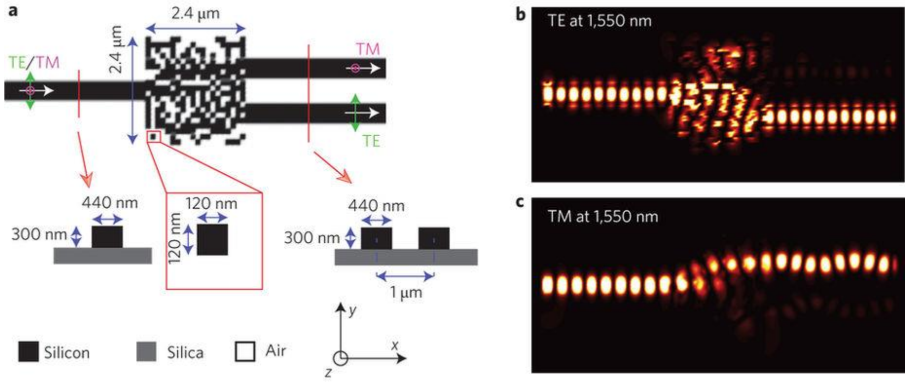
Piggott *et al*, Nat. Photonics (2015)





Compact, on-chip photonic WDMs that function with high efficiency over multiple, discrete frequency bands

Shen *et al*, Nat. Photonics (2015)

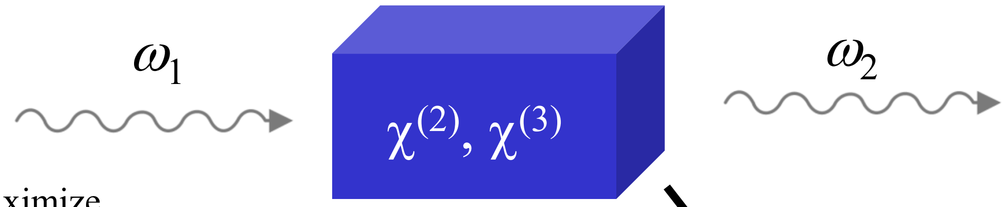


Compact, on-chip polarization beam splitters

Beyond bandgaps, mode splitters and converters …

- Nonlinear frequency conversion
- Singular spectral features (Dirac cones and Exceptional points)
- Multi-layered meta-optical devices
- Many more …

Nonlinear Frequency Conversion



How do we maximize the conversion? Pattern the material such that …

Confined mode at ω_1 with large Q_1

Concentrate (squeeze) and overlap the two modes as much as possible → β

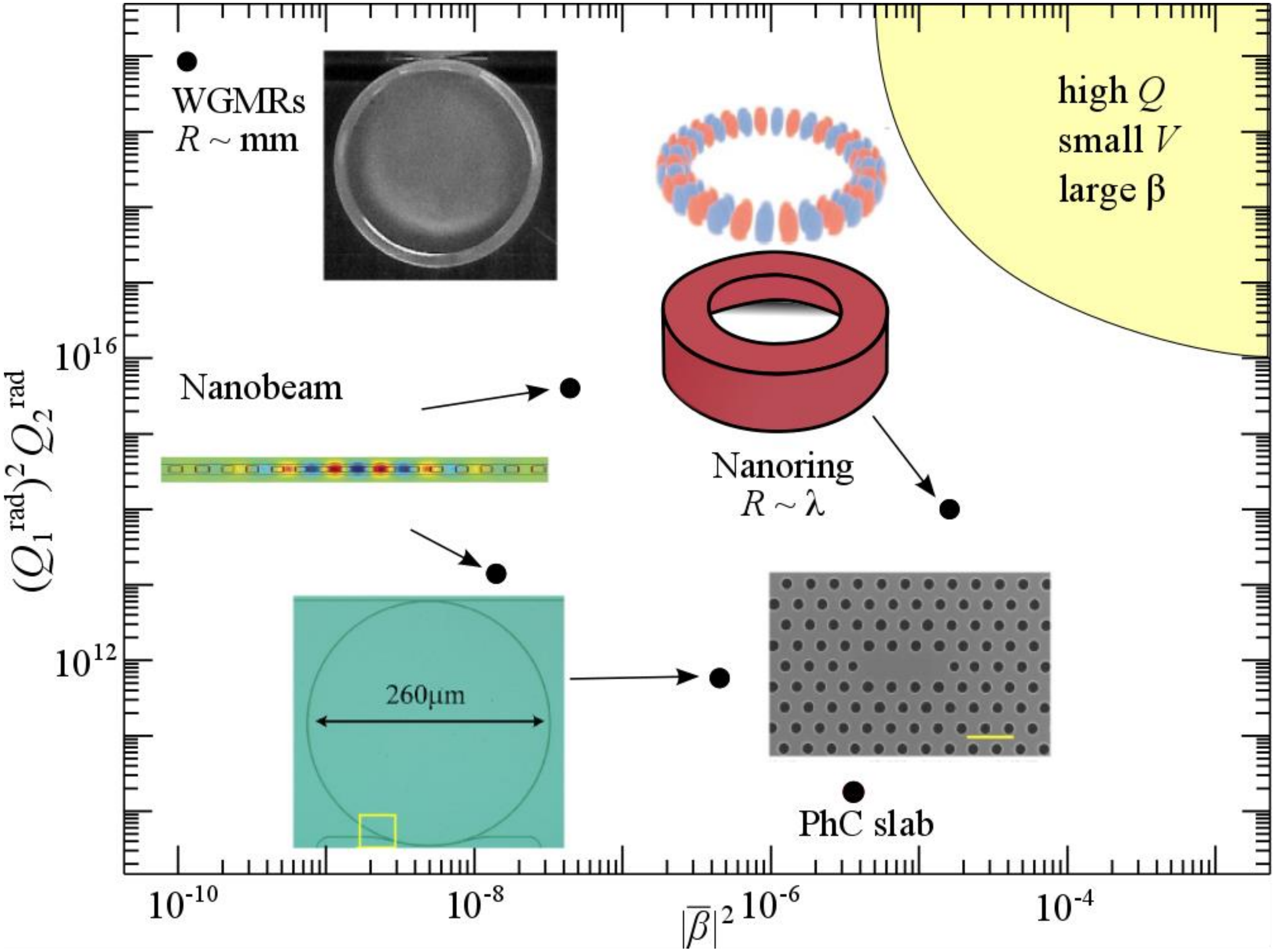
Confined mode at ω_2 with large Q_2

Example: Second Harmonic Generation

$$\omega_2 = 2\omega_1$$

$$\frac{P_{\text{out}}(\omega_2)}{\left(P_{\text{in}}(\omega_1)\right)^2} = \frac{\chi^{(2)}_{\text{eff}}}{8\omega_1\sqrt{\epsilon_0\lambda_1^3}} \boxed{\left(Q_1^{\text{rad}}\right)^2 Q_2^{\text{rad}} |\bar{\beta}|^2}$$

$$\bar{\beta} = \frac{\int_{\text{NL}} E_2^* E_1^2 \; d\mathbf{r}}{\left(\int \epsilon_1 |\mathbf{E}_1|^2 \; d\mathbf{r}\right) \sqrt{\int \epsilon_2 |\mathbf{E}_2|^2 \; d\mathbf{r}}} \sqrt{\lambda_1^3}$$


WGMRs
$R \sim$ mm
high Q
small V
large β
Nanobeam
Nanoring
$R \sim \lambda$
260μm
PhC slab
10^{16}
10^{12}
$(Q_1^{\mathrm{rad}})^2 Q_2^{\mathrm{rad}}$
10^{-10}
10^{-8}
10^{-6}
10^{-4}
$|\overline{\beta}|^2$

Topology optimization for nonlinear photonics

Design a cavity with multiple resonances at *exactly "matched" frequencies, high quality factors and largest nonlinear overlap between the modes*

Example: Second Harmonic Generation

$$\begin{aligned} \mathbf{J}_1 &= \hat{\mathbf{e}}_j \delta(x - x'), \\ \Rightarrow \mathcal{M}(\bar{\epsilon}_i, \omega_1)\mathbf{E}_1 &= i\omega_1 \mathbf{J}_1, \\ \Rightarrow \mathbf{J}_2 &= \bar{\epsilon} E_{1j}^2 \hat{\mathbf{e}}_k, \\ \Rightarrow \mathcal{M}(\bar{\epsilon}_i, \omega_2)\mathbf{E}_2 &= i\omega_2 \mathbf{J}_2 \end{aligned}$$

Basically, the physics of SHG at non-depletion limit!

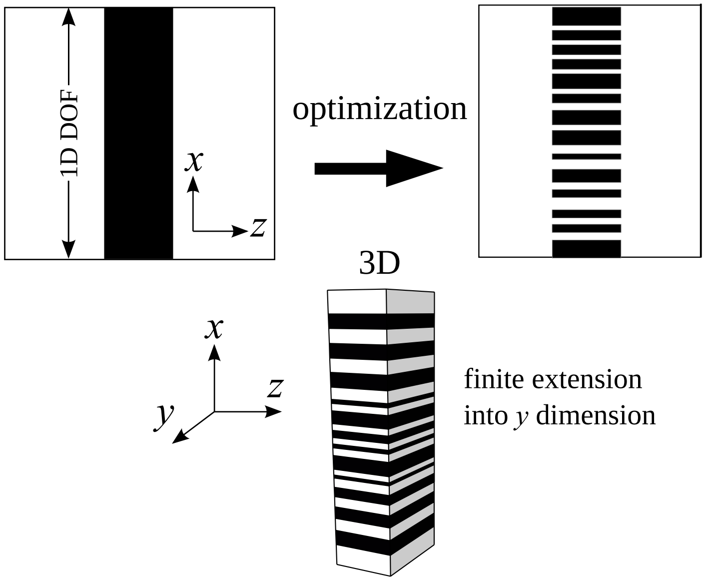
$$\max_{\bar{\epsilon}_i} \; f\Big(\bar{\epsilon_i}, \mathbf{E}; \omega_1, \omega_2 = 2\omega_1\Big) = -\mathrm{Re}\Big[\int \mathbf{J}_2^* \cdot \mathbf{E}_2 \, dx\Big]$$

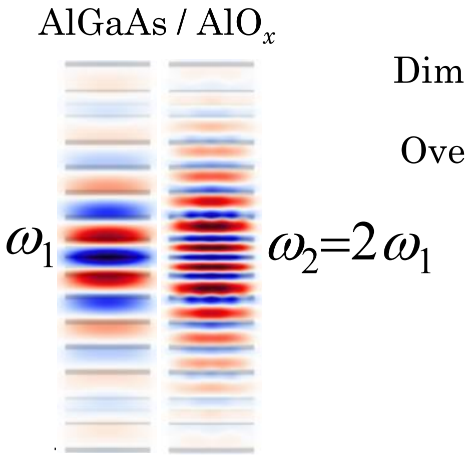
$$\mathcal{M}\;\mathbf{E} = \nabla \times \mu^{-1} \nabla \times \mathbf{E} - \omega^2 \epsilon(\mathbf{r})\mathbf{E}$$

*****Similar straightforward formulations can be written for any other process, e.g THG, SFG, etc.*****

Lin *et al*, Optica Vol. 3, 233 (2016)

Multi-layer stack cavity





Dimensions: $8.4 \times 3.5 \times 0.84 \ (\lambda_1^3)$

Overlap and quality factors:

$$\beta \approx 0.018 \frac{\chi^{(2)}}{\sqrt{\epsilon_0 \lambda_1^3}}$$

$$Q_1^{\text{rad}} = 1.4 \times 10^5$$

$$Q_2^{\text{rad}} = 1.3 \times 10^5$$

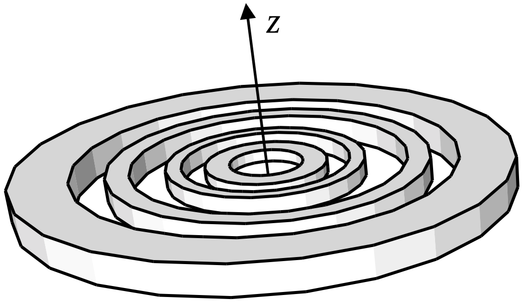
- Orders of magnitude improvement in mode overlap while still maintaining very high *radiative* Q's and perfect frequency matching

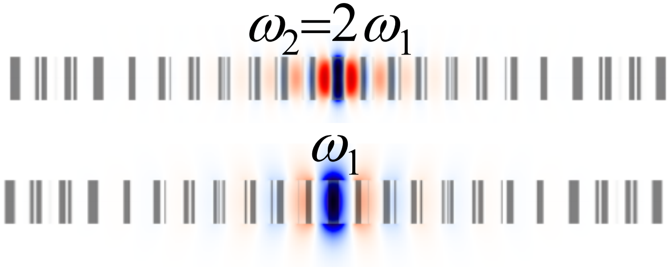
- At critical coupling, conversion efficiency $P_2 / P_1^2 \sim 10^4$ / Watt

- In over-coupled regime with *loaded* Q's ~ 1000, $P_2 / P_1^2 \sim 10$ / Watt (gain in bandwidth, tolerate frequency mismatch due to fab errors)

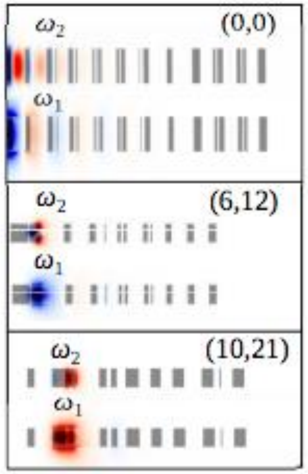
Lin *et al*, Optica Vol. 3, 233 (2016)

Rotationally symmetric cavities





$$\bar{\beta} = 0.04$$
$$Q_1^{\text{rad}} = 10^5$$
$$Q_2^{\text{rad}} = 3 \times 10^4$$

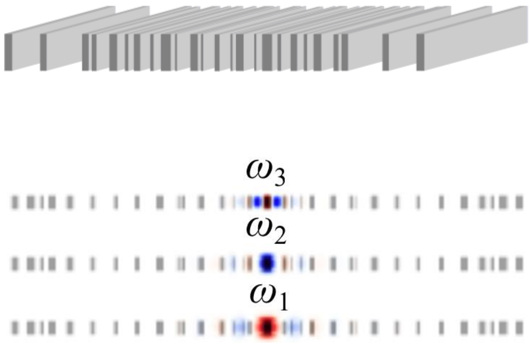


(m_1, m_2)	Polarization	Q_1	Q_2	$\bar{\beta}\left(\frac{\chi^{(2)}}{4\sqrt{(\varepsilon_0 \lambda^3)}}\right)$	Thickness (λ_1)
(0, 0)	(E_z, E_z)	10^5	3×10^4	0.041	0.39
(4, 8)	(E_z, E_z)	3.1×10^4	3×10^3	0.009	0.30
(5, 10)	(E_z, E_r)	8×10^3	3.7×10^4	0.008	0.18
(6, 12)	(E_z, E_z)	9.5×10^4	2.7×10^4	0.008	0.18
(10, 20)	(E_z, E_z)	10^6	1.2×10^4	0.004	0.22
(10, 21)	(E_z, E_r)	1.6×10^6	7.4×10^4	0.004	0.24

Lin *et al*, Optics Letters (2017)

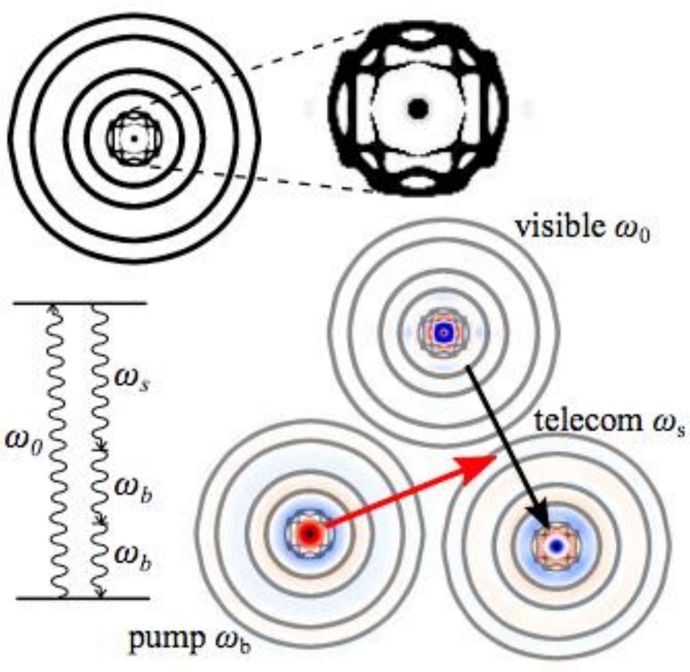
Of course, we can generalize to other processes …

$\chi^{(2)}$ Difference Frequency Generation in a gratings cavity



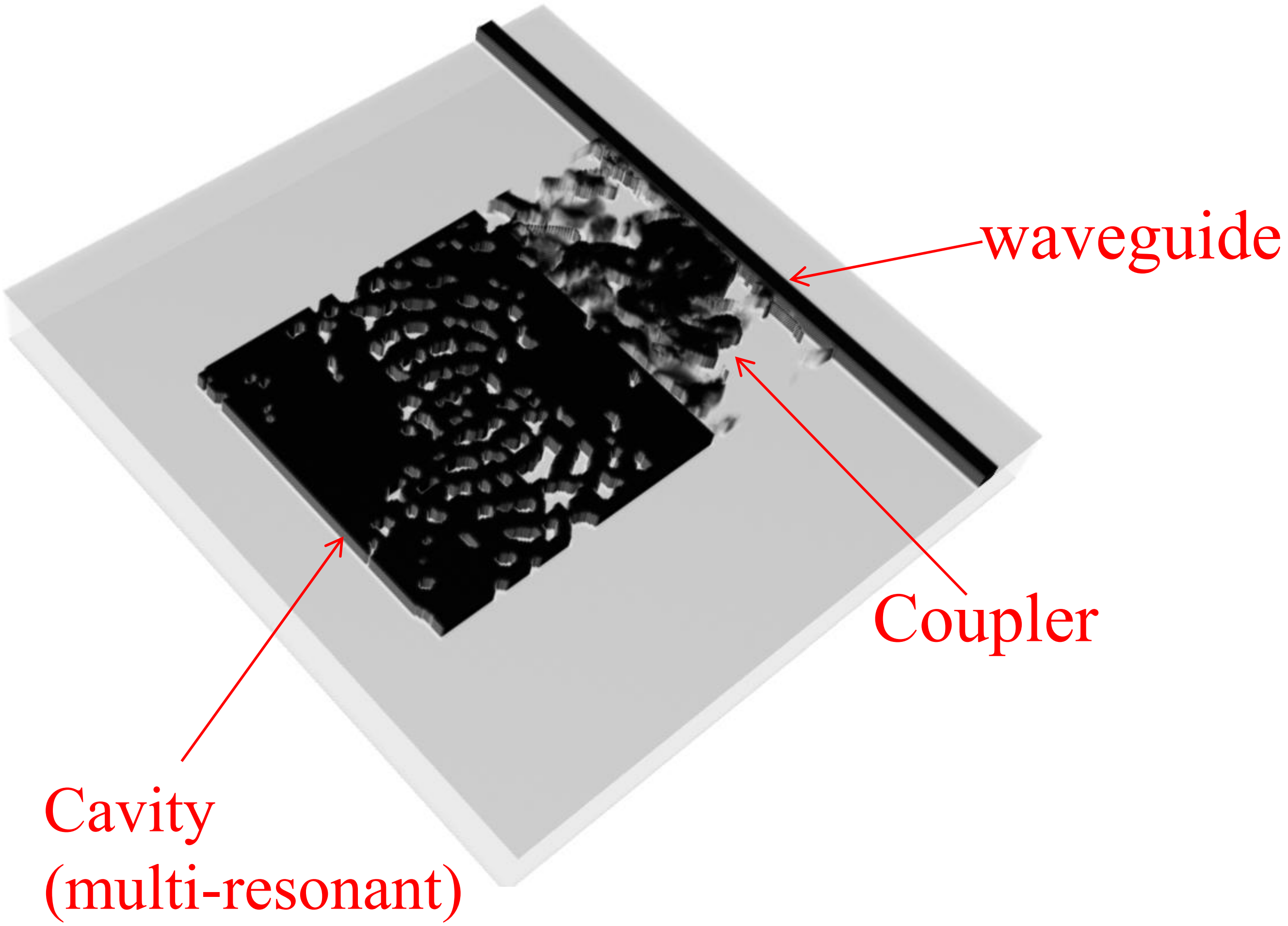
$$637\ \text{nm} \rightarrow 1550\ \text{nm}$$
$$\bar{\beta} \sim 0.03$$
$$Q^{\text{rad}} \sim 10^5$$

$\chi^{(3)}$ Difference Frequency Generation in a 2D microcavity

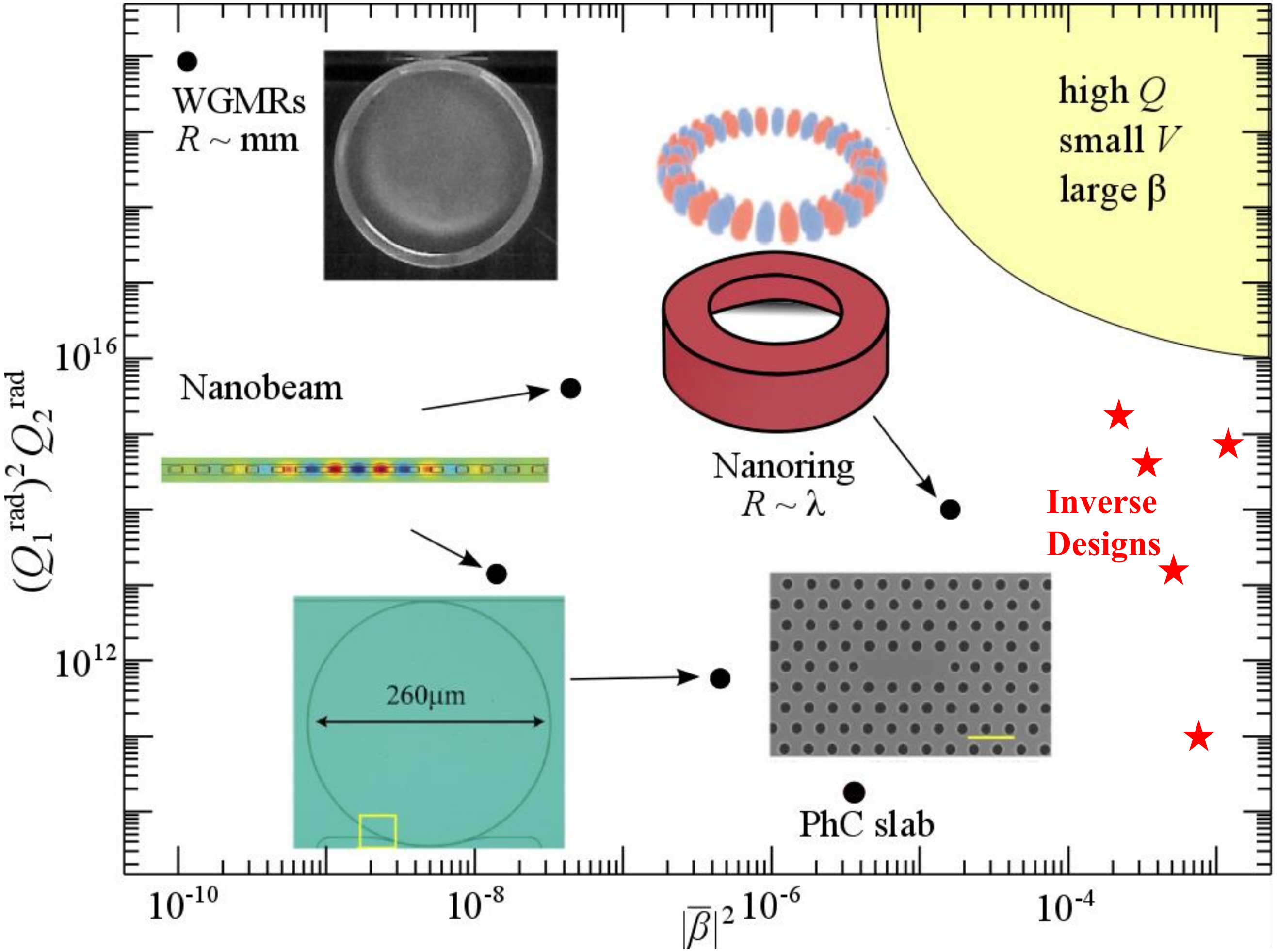


Lin *et al*, Optics Letters (2017)

A recent result (3D slab cavity with coupler) …

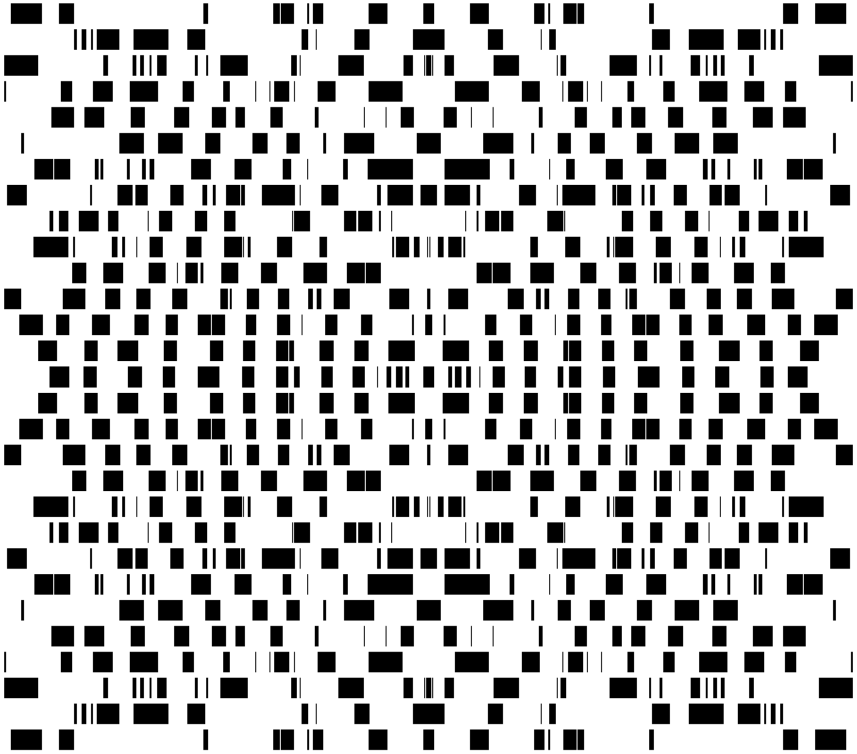


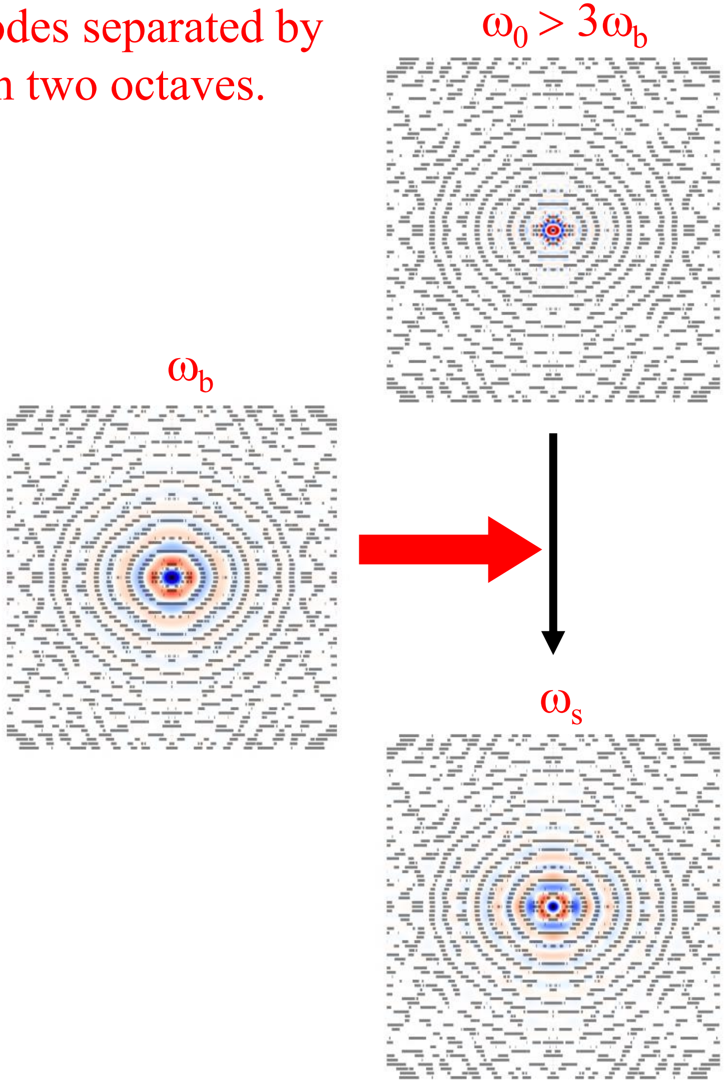
Credit: W. Jin, Rodriguez group (Princeton)


WGMRs
$R \sim$ mm
high Q
small V
large β
10^{16}
10^{12}
Nanobeam
Nanoring
$R \sim \lambda$
Inverse Designs
260μm
PhC slab
$(Q_1^{\text{rad}})^2 Q_2^{\text{rad}}$
10^{-10}
10^{-8}
$|\overline{\beta}|^2$
10^{-6}
10^{-4}

3D Multi-layered Nonlinear Cavity?

Three modes separated by more than two octaves.





A complementary list of free software

- Finite Difference Time Domain: MEEP (some unique features such as epsilon averaging and harmonic inversion)
  - https://meep.readthedocs.io/en/latest/Introduction/

- Photonic Band Structure Calculation for Hermitian Systems: MPB (plane wave expansion methods)
  - https://mpb.readthedocs.io/en/latest/

- Periodic in xy, layered in z? → Rigorous Coupled Wave Analysis: S4 (Stanford); can be orders of magnitude faster than FD methods for certain 3D problems
  - https://web.stanford.edu/group/fan/S4/

- Nonlinear optimization package: Nlopt
  - https://nlopt.readthedocs.io/en/latest/

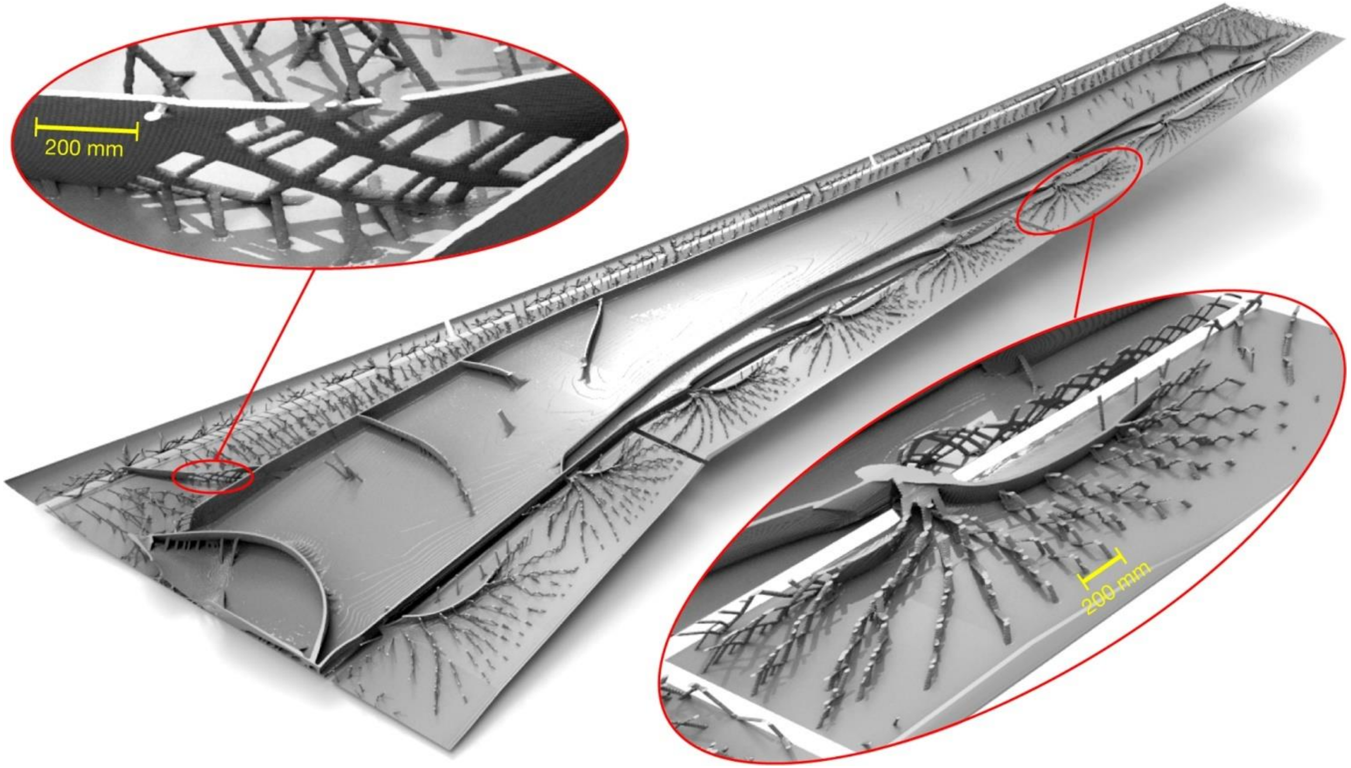
- Boundary Element Method: scuff-em
  - http://homerreid.github.io/scuff-em-documentation/

- Flexible FEM software (one that could be developed into a customized EM solver): FEniCS
  - https://fenicsproject.org/

- Ultimately very high frequency structures? → domain decomposition methods
  - M.-F. Xue, Y. M. Kang, A. Arbabi, S. J. McKeown, L. L. Goddard, and J. M. Jin, "Fast and accurate finite element analysis of large-scale three-dimensional photonic devices with a robust domain decomposition method," Optics Exp., vol. 22, no. 4, pp. 4437-4452, Feb. 2014. (~ 60 λ diameter ring resonator with a waveguide, 300 cpus, 1.2 hrs)

A billion voxels optimization

Aage, N., Andreassen, E., Lazarov, B. S., & Sigmund, O. (2017). Giga-voxel computational morphogenesis for structural design. Nature, 550(7674), 84.



8000 cpus over 1 million cpu hours

Outlook

- three-dimensional topology optimization for photonics has been barely explored.

- Theory: solving 3D Maxwell's equations is very expensive.

- Experiment: fabricating 3D photonic structures (even layer-by-layer) is very challenging.

But …

New computational techniques
+ super-computing resources
+ new fabrication techniques
(e.g. nanoscribes)
→ novel 3D geometries

→ new physics + functionalities

Check out our review:
An Outlook for Inverse Design in Nanophotonics, arXiv:1801.06715