Leveraging Advances in Computational Electrodynamics to Enable New Kinds of Nanophotonic Devices

From Enhanced Solar Cells to Energy-Efficient Displays and Solid-State Lighting

Ardavan Oskooi

oskooi@simpetuscloud.com

collaborators

S.G. Johnson & J.D. Joannopoulos (MIT), S. Noda (Kyoto U.), S.R. Forrest (U. Michigan)

SIMPETUS

Simulations as a Service

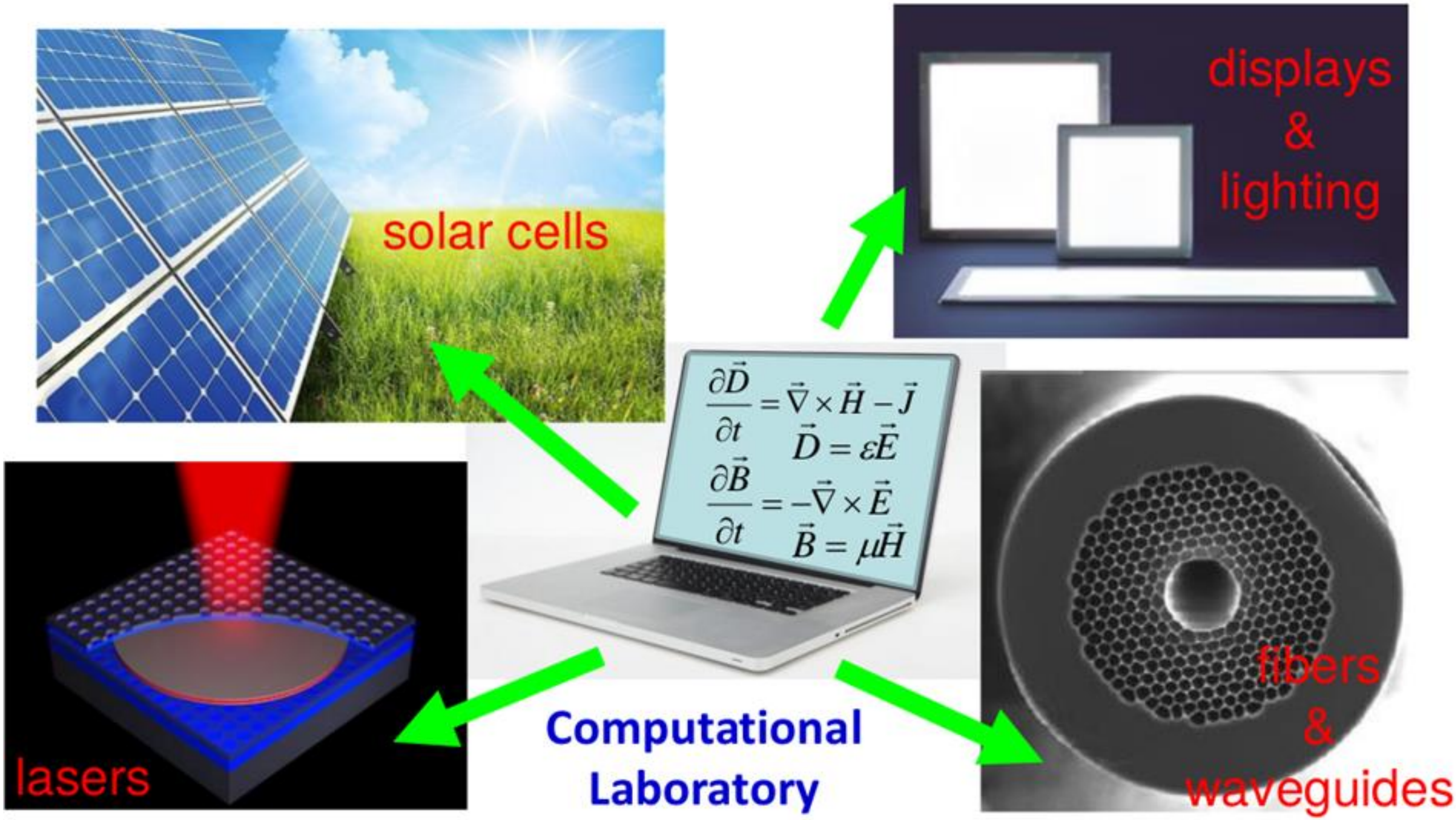
IEEE Photonics Society

Santa Clara Valley Chapter

Tuesday February 6th, 2018

Grand Vision

"To Propel Computational Simulations to the Forefront of Research and Development in Electromagnetics"



Grand Vision

“To Propel Computational Simulations to the Forefront of Research and Development in Electromagnetics”

A computational laboratory, enabled by advanced simulation tools, could make possible:

- exploration and discovery of electromagnetics
- designing and prototyping optoelectronic devices
- insights into experiments that are difficult/impossible using other means
- **taking products from lab to marketplace quickly & efficiently**

Outline

1. **Overview of the Finite-Difference Time-Domain (FDTD) Method for Computational Electromagnetics**

2. **Enhancements to Core Capabilities of FDTD**
   - *Sub-pixel Smoothing of Dielectric Surfaces*
   - *Absorbing Boundary Layers for Inhomogeneous Media*

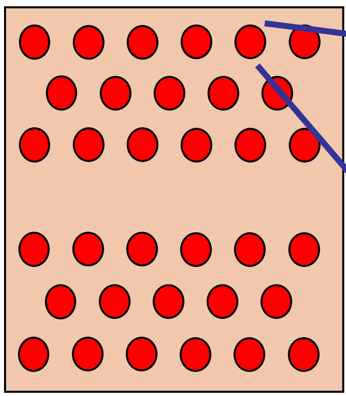
3. **MEEP: A Flexible Free-Software Package for Electromagnetic Simulations by the FDTD method**

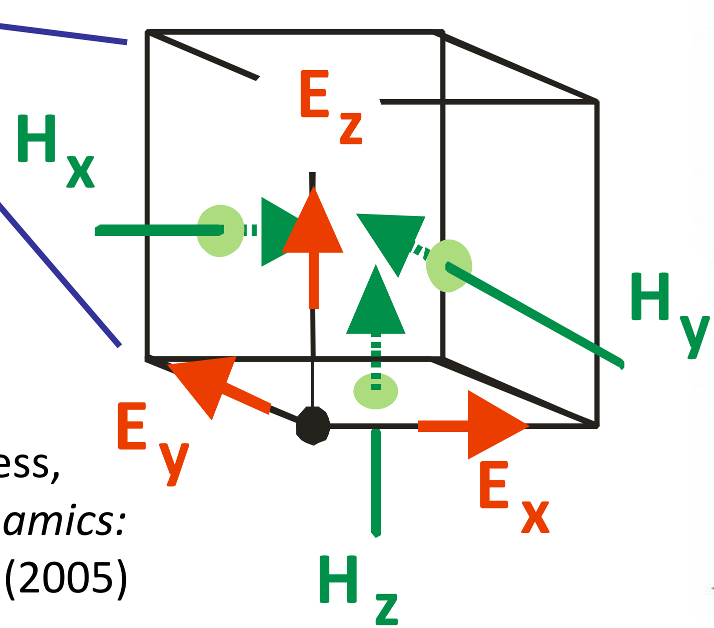
4. **New Kinds of Nanophotonic Devices**
   - *Light Trapping in Silicon Thin Films for Enhanced Solar Cells*
   - *Light Extraction from Organic Light-Emitting Diodes (OLEDs) for Energy-Efficient Displays and Solid-State Lighting*

5. **New Opportunities for Large-Scale Device Design using High-Performance Computing (HPC) in the Public Cloud**

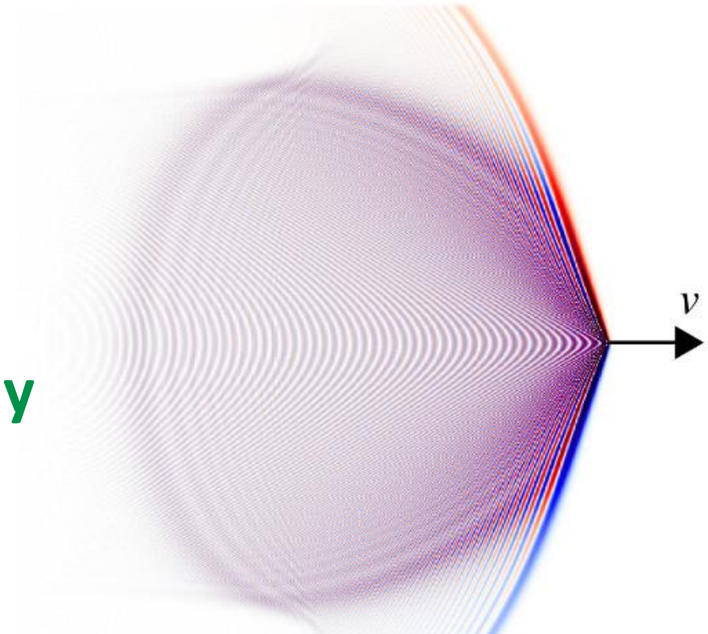
Finite Difference Time Domain (FDTD)

FDTD is a method used in computational electromagnetics to model Maxwell's eqns. on a **discrete time** and **space grid** using finite, centered differences





A. Taflove & S.C. Hagness, *Computational Electrodynamics: The FDTD Method*, 3rd ed. (2005)

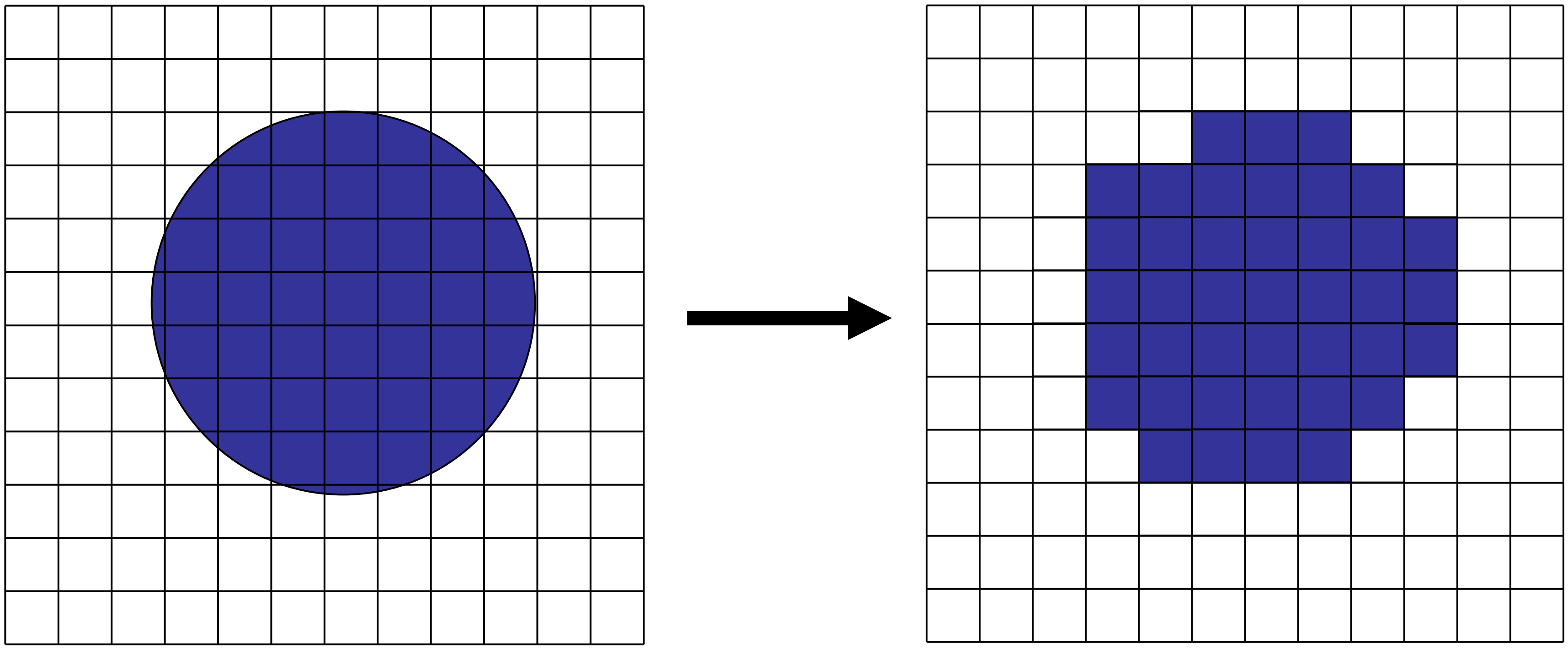


v=1.05 c/n (0.35 pixels/Δt)

- FDTD is rigorous and flexible enough to model a large variety of effects involving different materials and geometries
- FDTD has Two Key Attributes for Device Design:
    - short pulse produces *broadband* spectral response in a single simulation
    - explicit parallelization enables simulating *large computational volumes*

Staircasing and "Pixellization" in FDTD

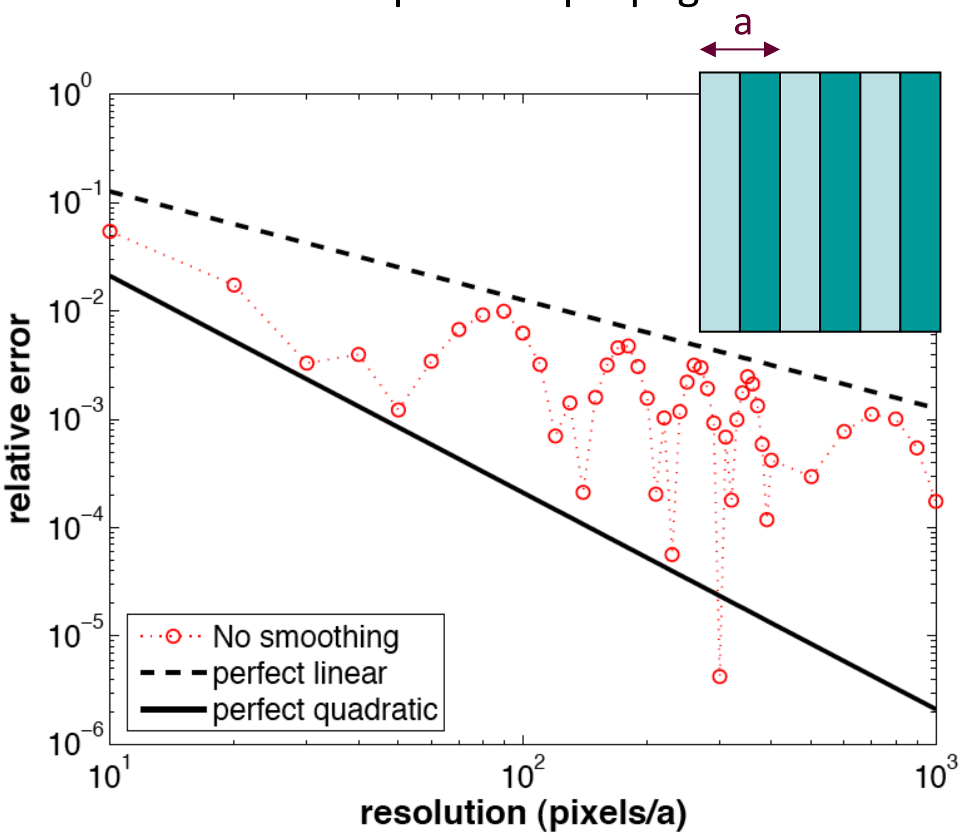
How to discretize a *discontinuous* dielectric surface?

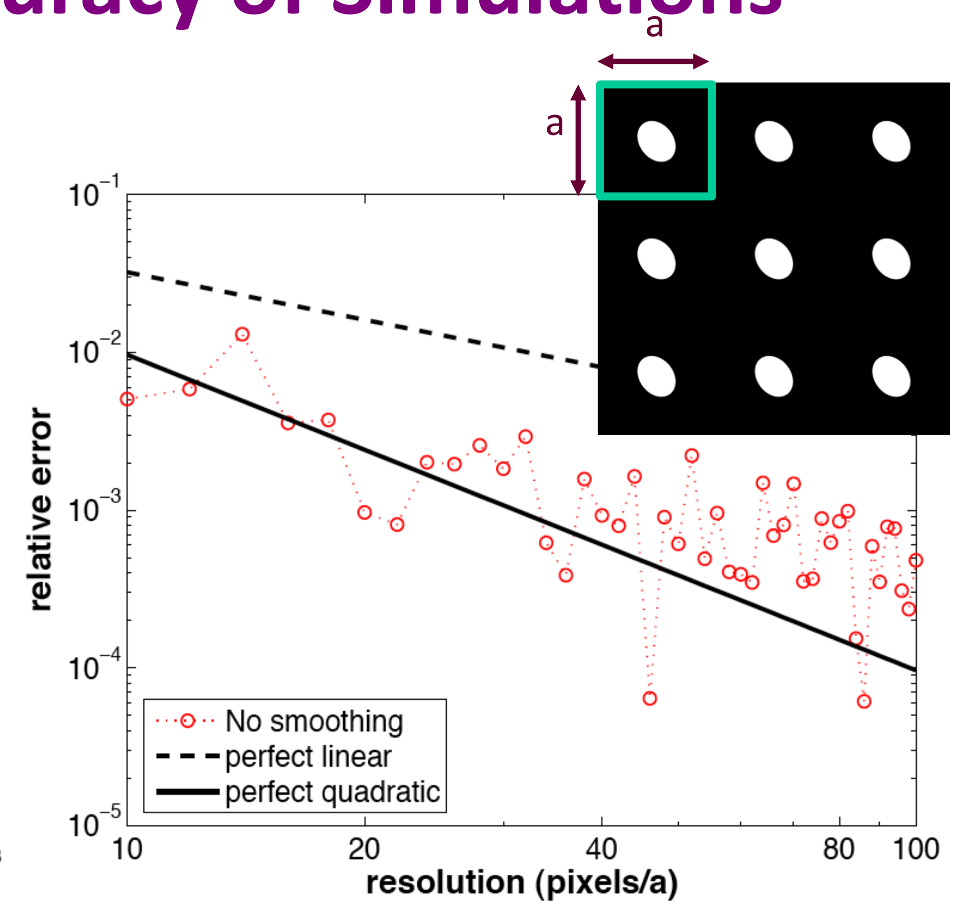


simplest scheme: just take ε at grid point (here, ε at *center* of "pixel")

Problem: Field Discontinuity at Dielectric Surface Degrades Accuracy of Simulations

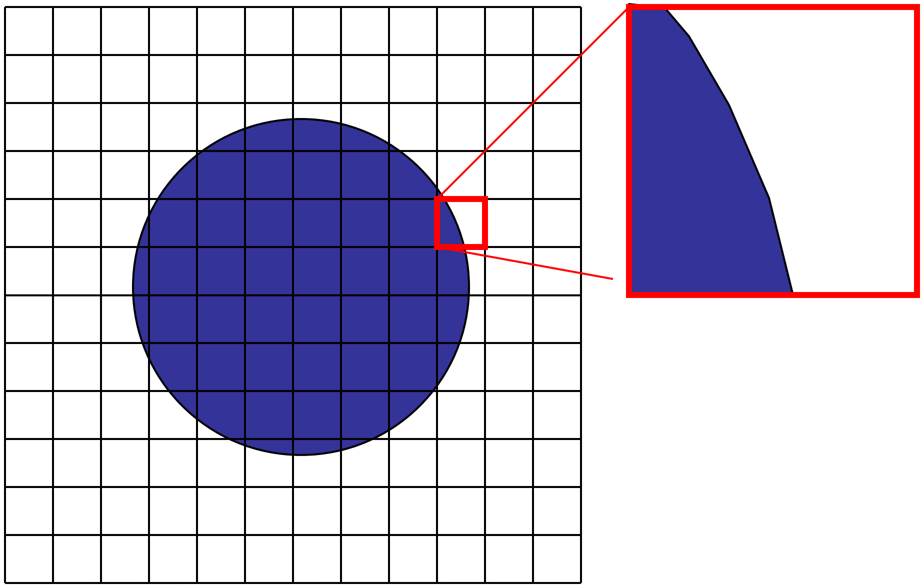
electric field in the plane of propagation

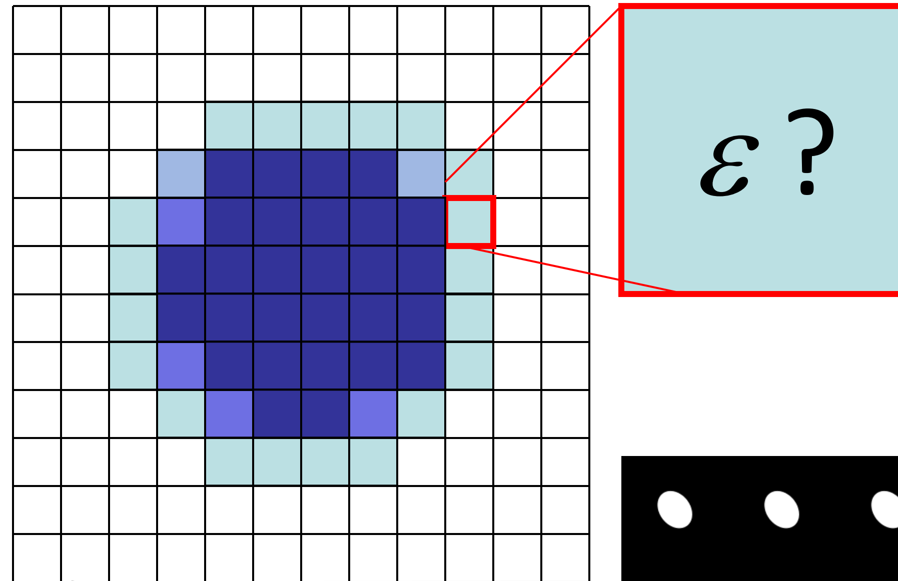




even though the finite differences used in the discretization of MEs have second-order accuracy with respect to resolution, the error is converging only linearly due to the field discontinuities at dielectric interfaces
(similar to Gibbs Phenomenon in signal processing)

Sub-Pixel Smoothing of Dielectric Surfaces



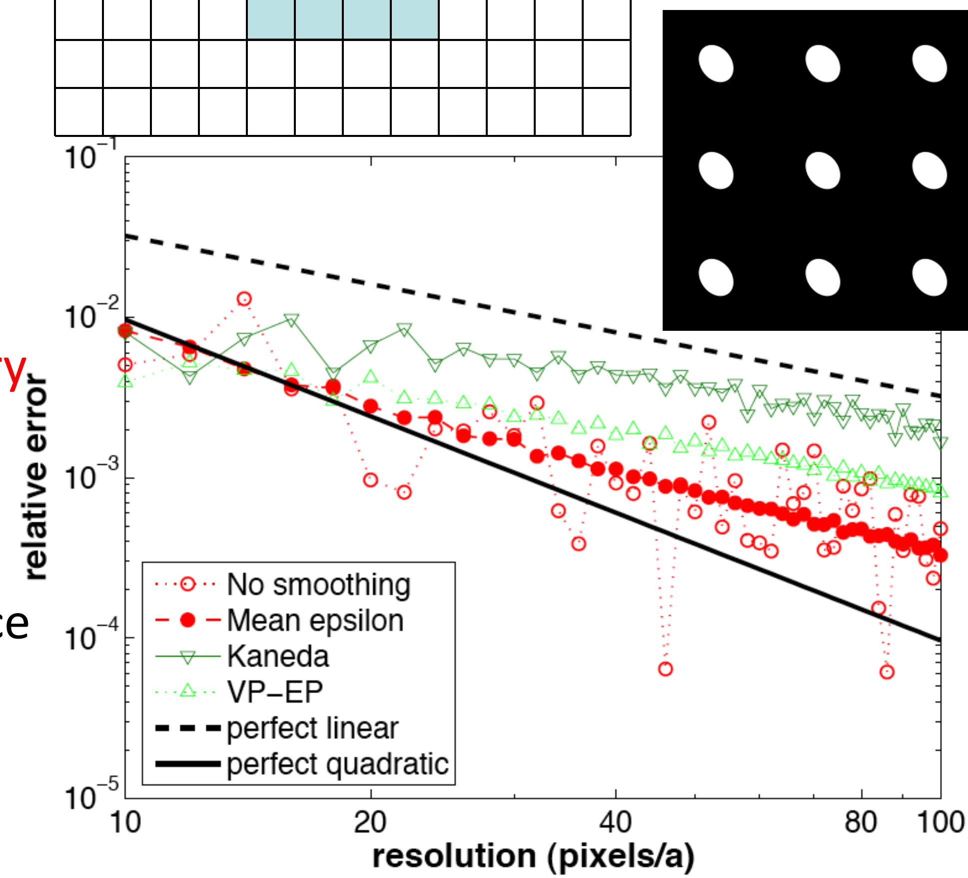


- can eliminate discontinuities by "gray scaling": assigning an **averaged** ε to each pixel. But how?
- any kind of smoothing changes geometry and may actually increase the error (even *before* the discretization)
- prior smoothing methods made error worse than no smoothing and convergence with resolution was still only linear

Kaneda et al., IEEE MTT 45 (1997)

Dey et al., IEEE MTT 47 (1999)

Mohammadi et al., Optics Express 13 (2005)



An Analytic Criterion for Accurate Smoothing

- to ensure small errors and second-order accuracy, *first-order* effect of smoothing in changing the geometry should be <u>zero</u>
- this requires correct perturbation theory near sharp boundaries with large index contrast

first-order errors from $\Delta\varepsilon$ perturbation

$$\Delta\omega \approx \int \left(\Delta\varepsilon \left| E_{\|} \right|^2 - \Delta\left(\varepsilon^{-1}\right) \left| D_{\perp} \right|^2 \right)$$

continuous field components

use a tensor ε :

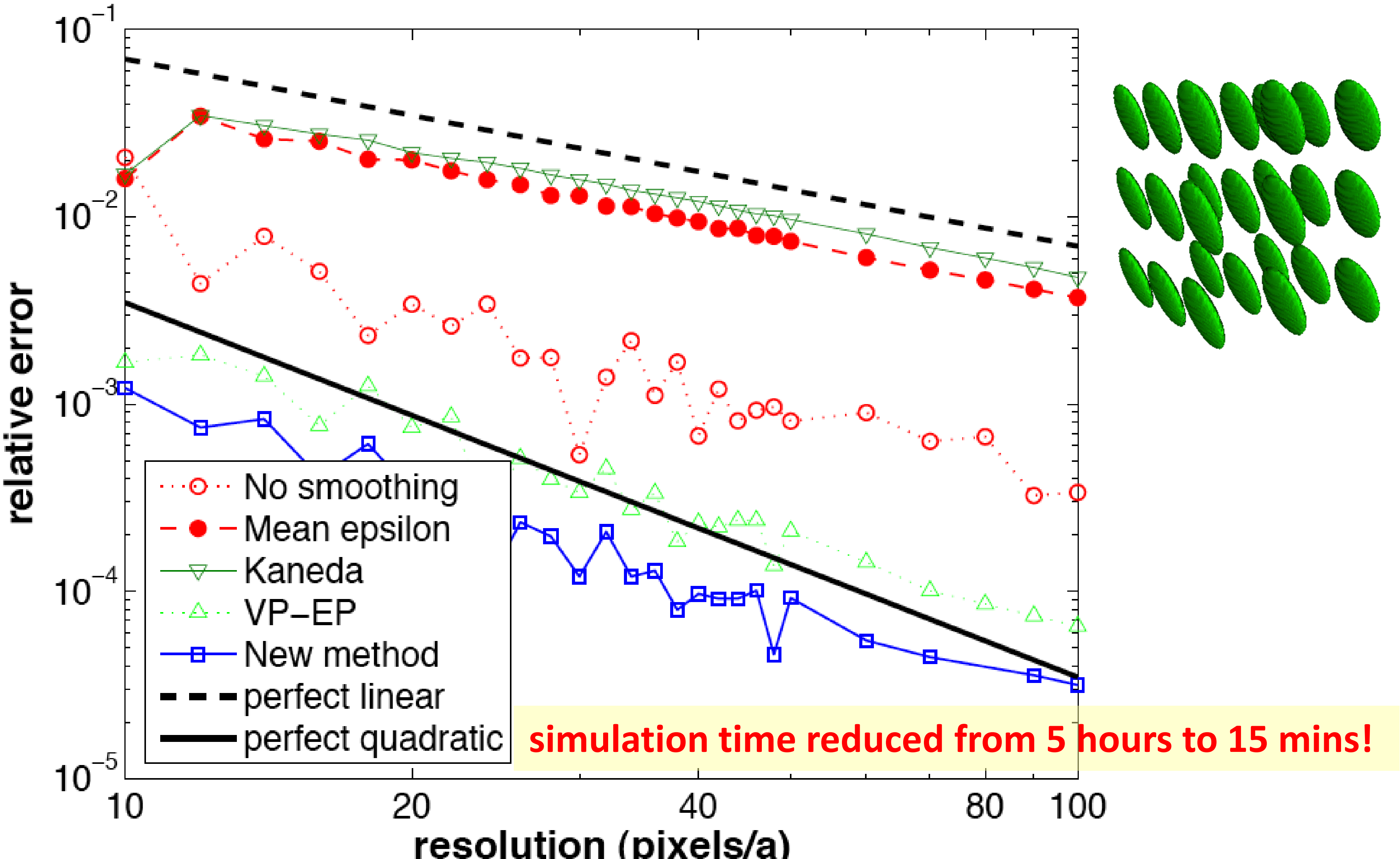
$$\begin{array}{cc} \begin{pmatrix} \langle\varepsilon\rangle & & \\ & \langle\varepsilon\rangle & \\ & & \langle\varepsilon^{-1}\rangle^{-1} \end{pmatrix} & \begin{array}{l} \mathbf{E}_{\|} \\ \\ \mathbf{E}_{\perp} \end{array} \end{array}$$

$$\boxed{\tilde{\varepsilon}^{-1} = P\langle\varepsilon^{-1}\rangle + (1-P)\langle\varepsilon\rangle^{-1}}$$

P: projection matrix onto normal of interface

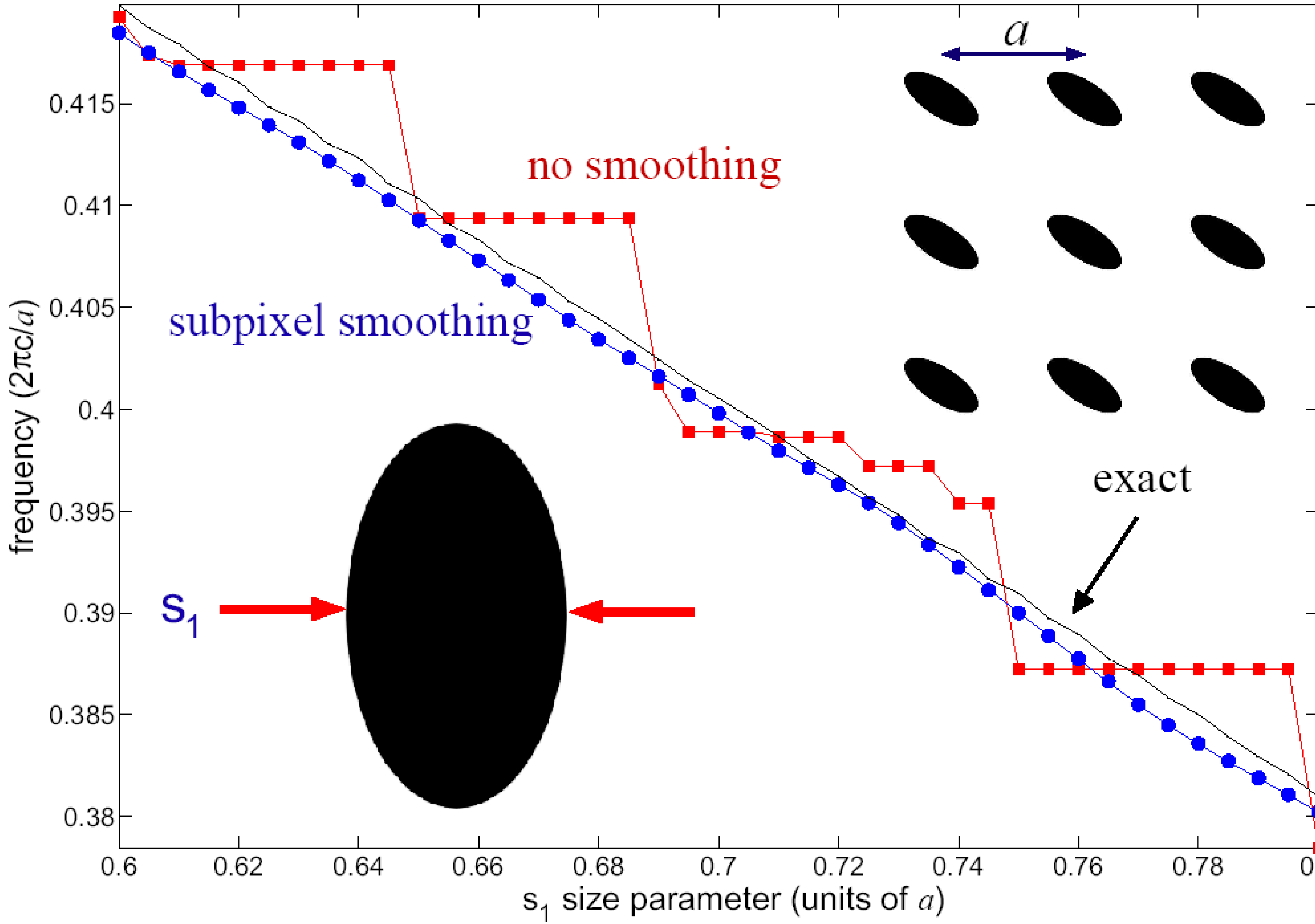
A. Oskooi et al., *Optics Letters*, **31**, pp. 2972-4 (2006)

Improved Sub-Pixel Smoothing has Lowest Error and Restores Second-Order Accuracy



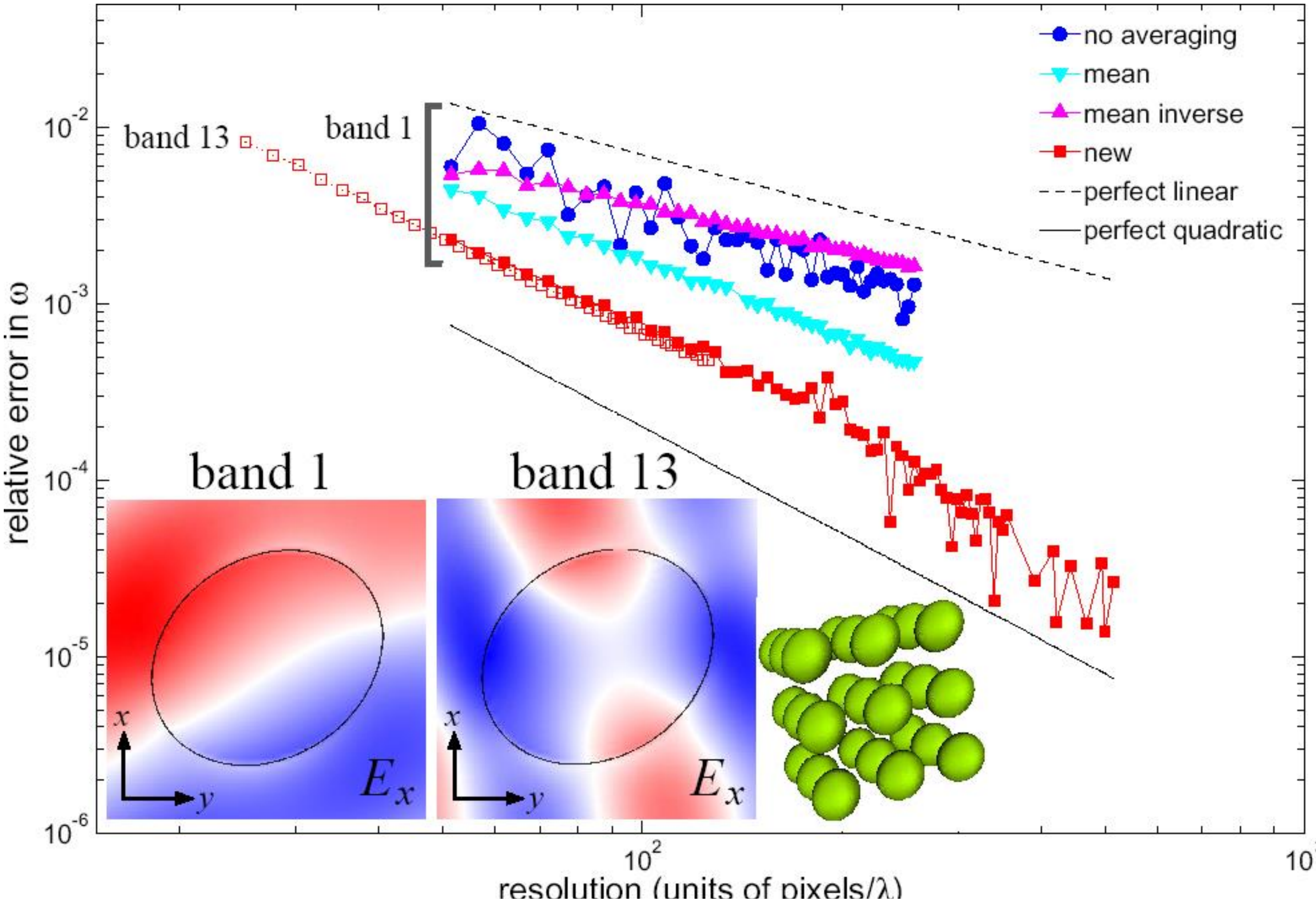
A. Oskooi et al., *Optics Letters*, **31**, pp. 2972-4 (2006)

Elimination of Numerical Artifacts



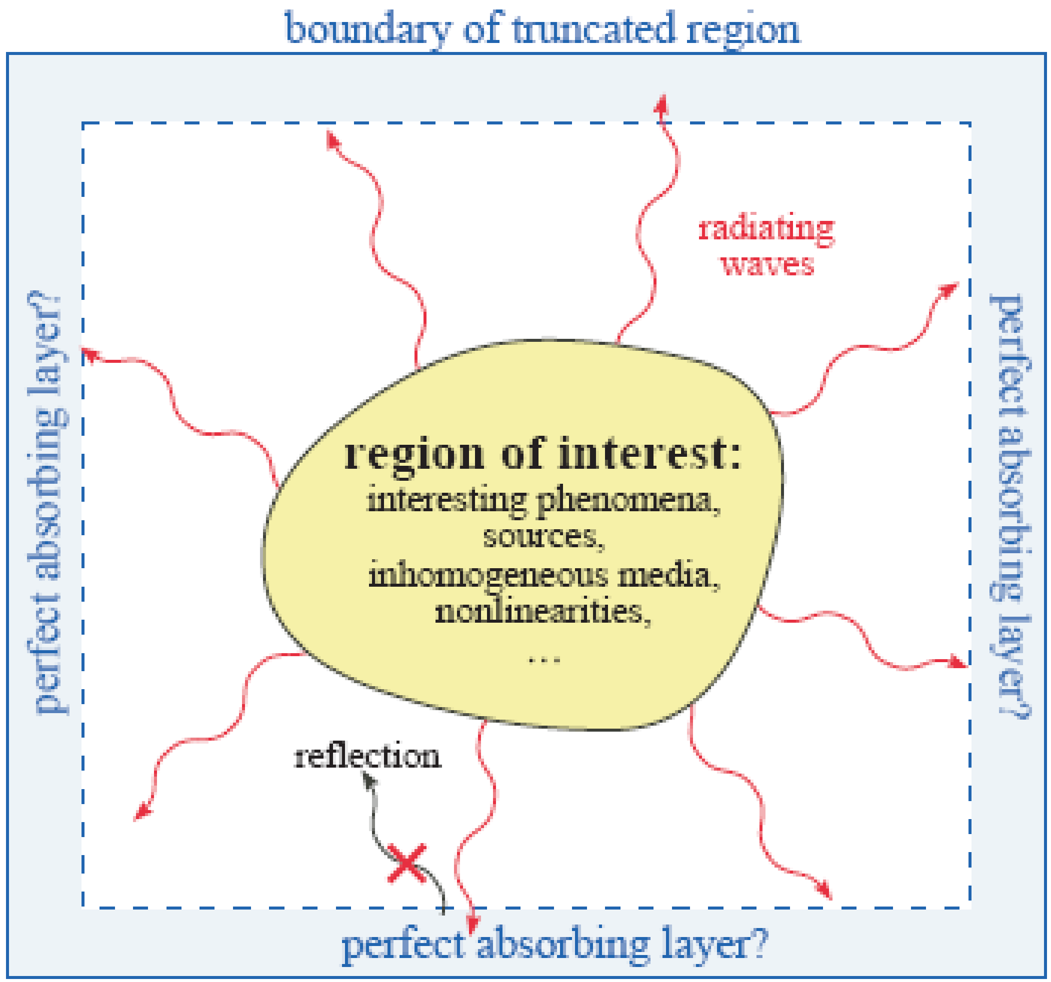
A. Oskooi et al., *Comp. Phys. Comm.*, **181**, pp. 687-702 (2010)

Extension of Sub-Pixel Smoothing to Anisotropic ε



A. Oskooi et al., *Optics Letters*, **34**, pp. 2778-80 (2009)

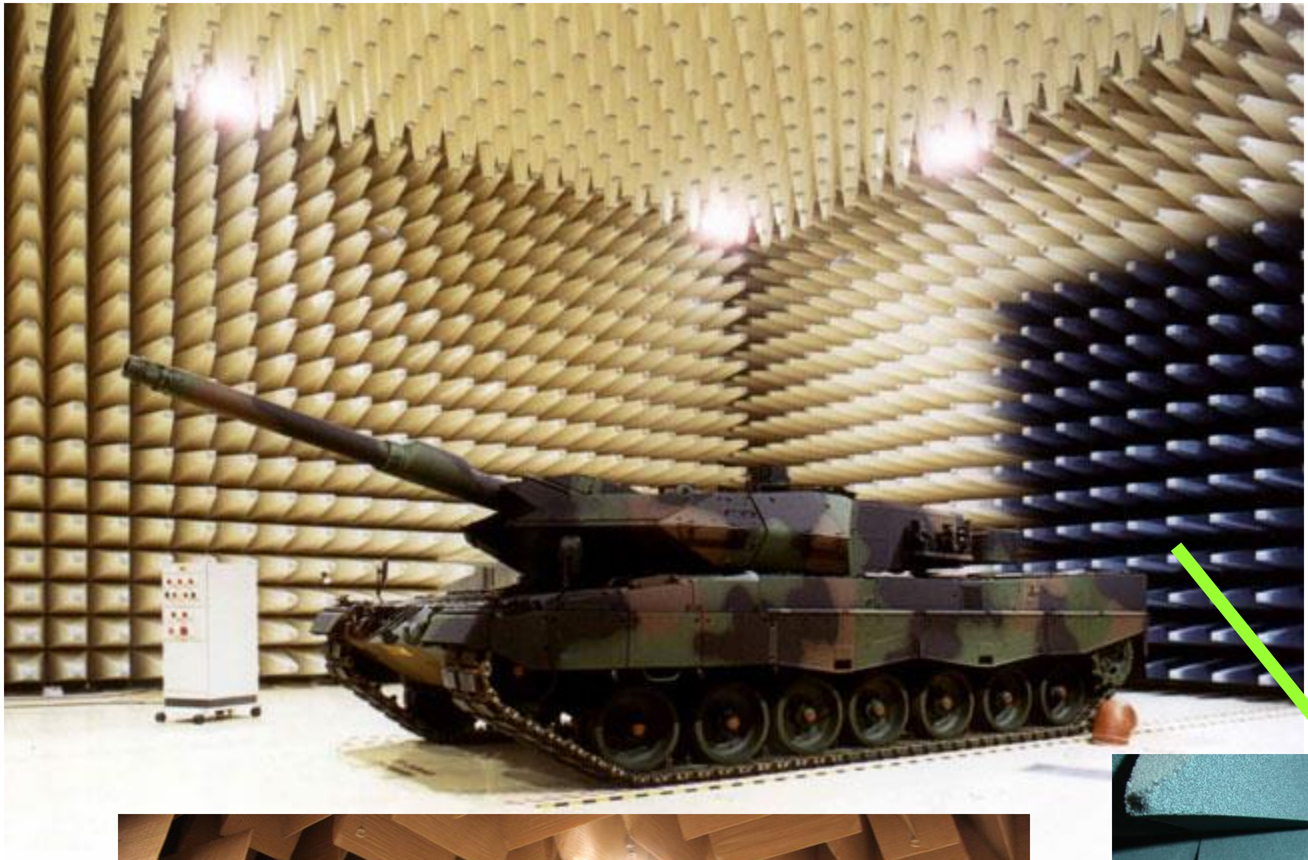
Simulating Open Boundaries in Computational Electromagnetics with Perfectly-Matched Layers (PML)



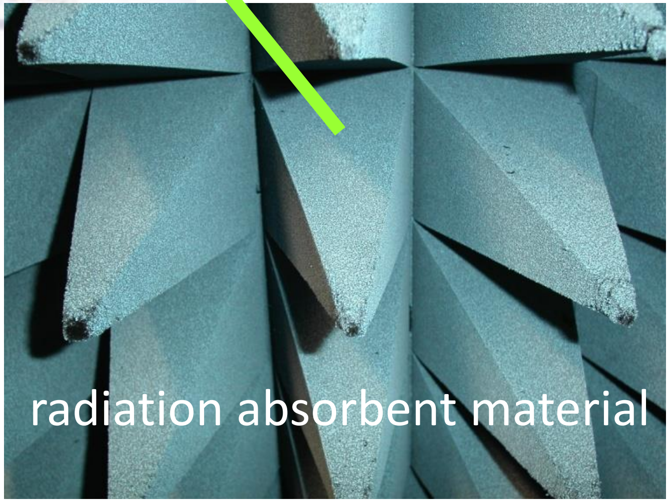
JP Berenger, *J. Comp. Phys.*, **114**, pp. 185-200 (1994)

PML widely used: cited 8000+ times

Simulating Open Boundaries with Anechoic Chambers

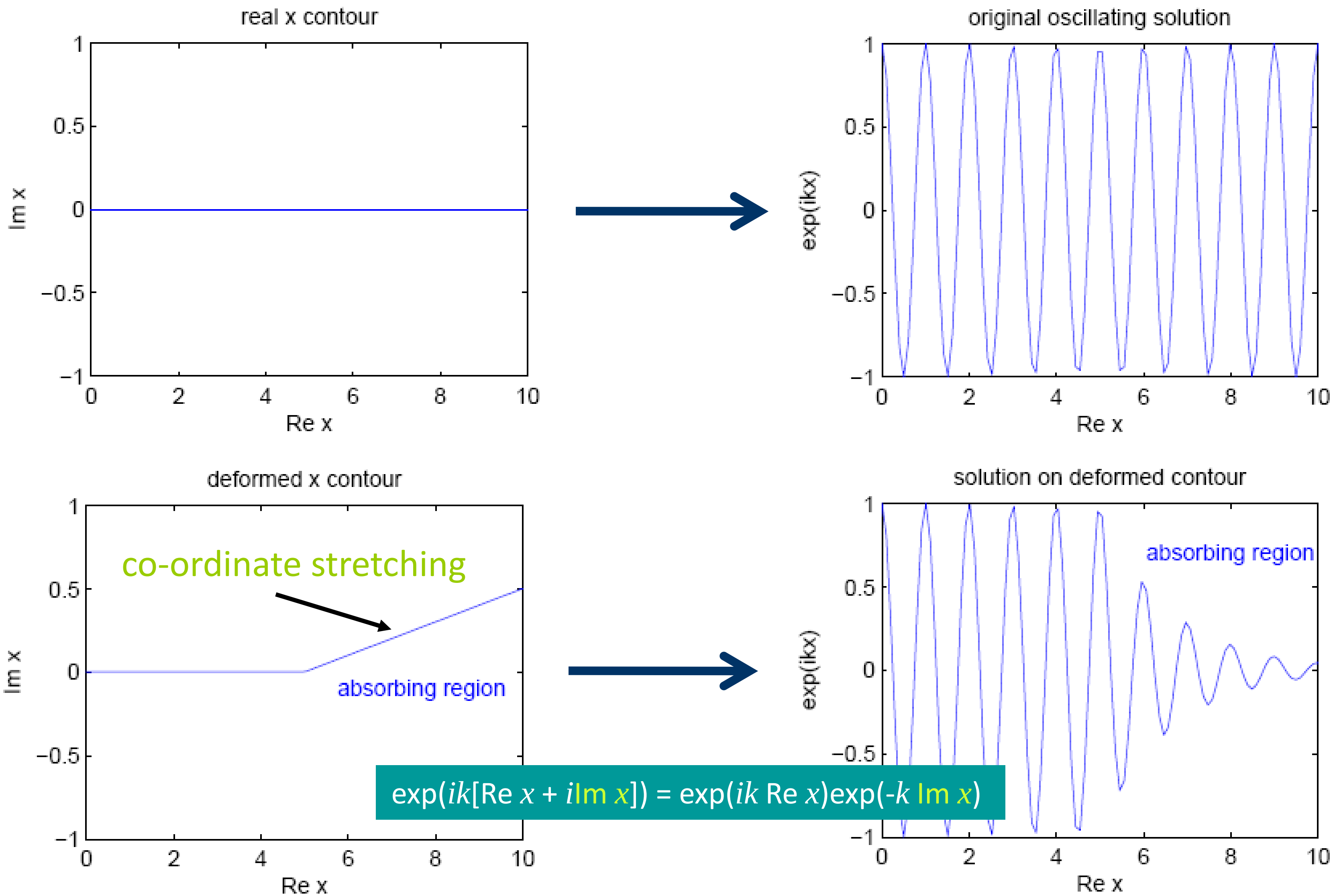


- minimize reflections from walls
- EM or sound waves
- used for testing antennas, radars, acoustic speakers, industrial machinery noise pollution



radiation absorbent material

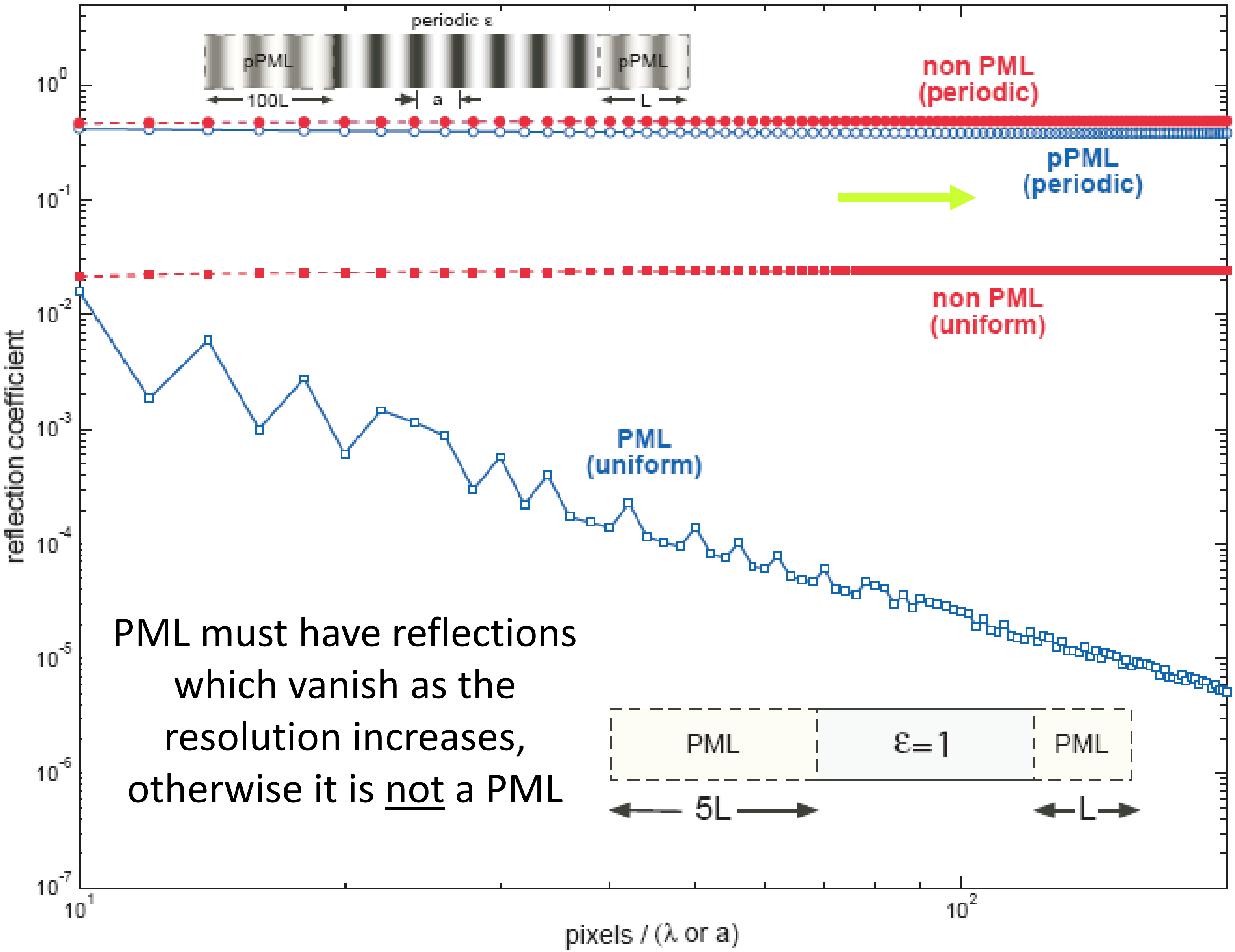
PML: *Stretching* Real into Complex Co-ordinates



$\exp(ik[\mathrm{Re}\ x + i\mathrm{Im}\ x]) = \exp(ik\ \mathrm{Re}\ x)\exp(-k\ \mathrm{Im}\ x)$

<u>zero</u> reflections between PML and adjacent non-PML region in the exact wave equation

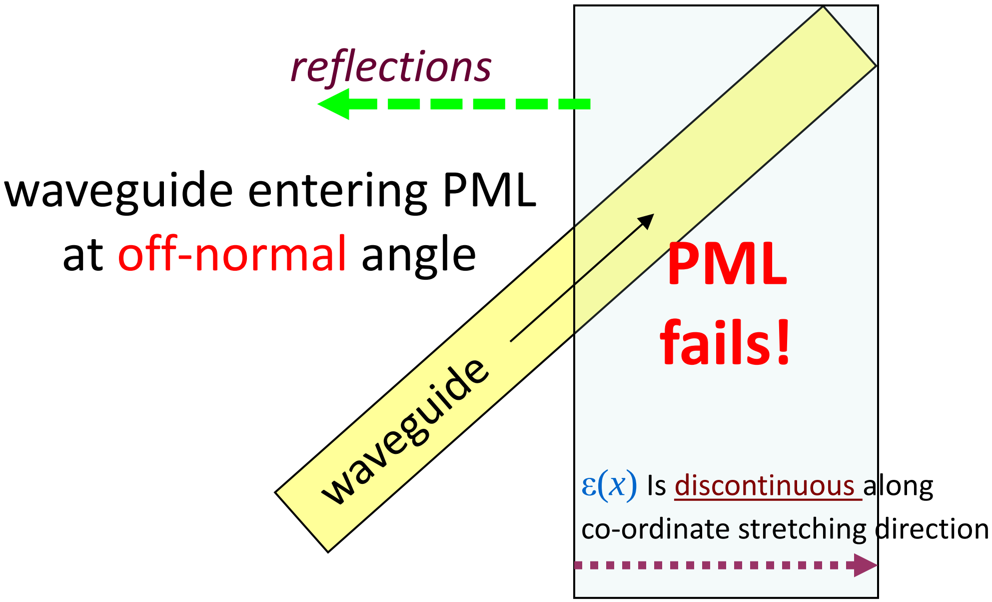
Problem: PMLs Fail for Inhomogeneous Media

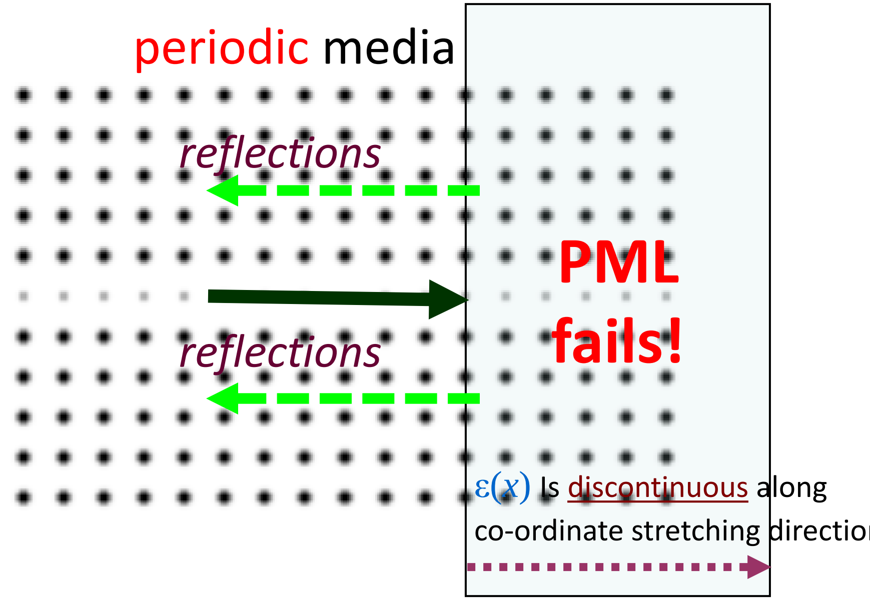


A. Oskooi et al., *Optics Express*, **16**, pp. 11376-92 (2008)

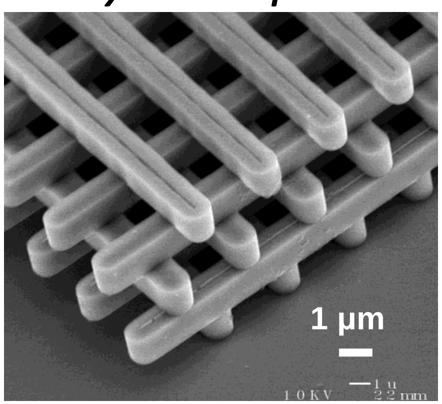
A. Oskooi & S.G. Johnson, *J. Comp. Phys.*, **230**, pp. 2369-77 (2011)

Problem: PMLs Fail for Inhomogeneous Media



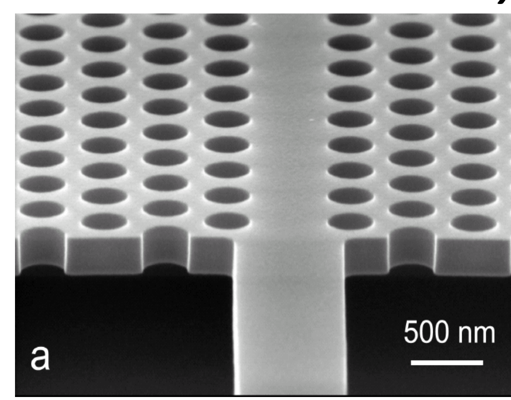


many nanophotonic devices are therefore challenging to simulate accurately



S. Lin et al. (Sandia)

G.A. Ozin et al. (U. Toronto)

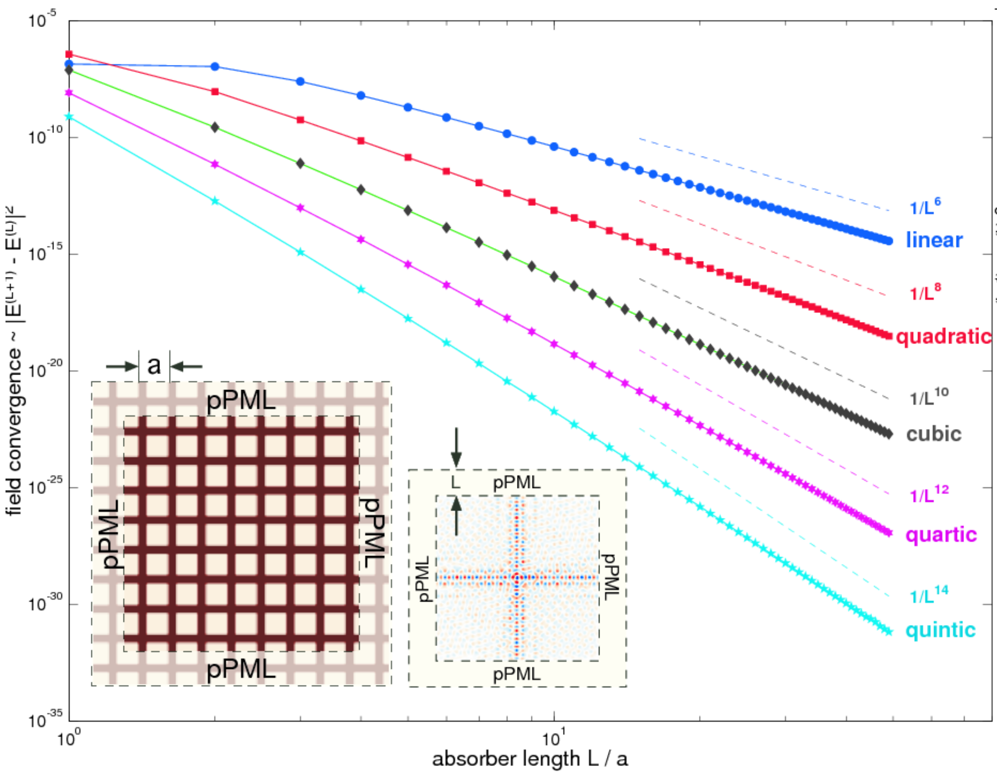


Y. Vlasov et al. (IBM)

A. Oskooi et al., *Optics Express*, **16**, pp. 11376-92 (2008)

A. Oskooi & S.G. Johnson, *J. Comp. Phys.*, **230**, pp. 2369-77 (2011)

When PMLs Fail, What Remains is an Adiabatic Absorber



by properly tuning the profile of the adiabatic absorber, numerical artifacts can be reduced when PMLs fail

absorbing boundary layers can be made much smaller thus reducing size of simulations while also improving accuracy

A. Oskooi et al., *Optics Express*, **16**, pp. 11376-92 (2008)

A. Oskooi & S.G. Johnson, *J. Comp. Phys.*, **230**, pp. 2369-77 (2011)

We incorporated the standard FDTD method as well as our enhancements (sub-pixel smoothing, adiabatic absorbers, and others) into an open-source software package…

MIT Electromagnetic Equation Propagation

`meep.readthedocs.io`

A. Oskooi et al., *Computer Physics Communications,* **181**, pp. 687-702 (2010)

downloaded **200,000+** times, cited **1500+** times, **7000+** posts to mailing list

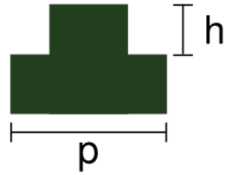
Overview of MEEP's features

- **Free and open-source software** under the GNU GPL
- Complete **scriptability** via Python, Scheme, or C++
- Simulation in **1d**, **2d**, **3d**, and **cylindrical** coordinates
- Distributed memory **parallelism** on any system supporting the MPI standard
- **Portable** to any Unix-like system (e.g., Linux or macOS)
- Arbitrary **anisotropic** electric permittivity ε and magnetic permeability μ, along with **dispersive** $\varepsilon(\omega)$ and $\mu(\omega)$ including loss/gain, **nonlinear** (Kerr & Pockels) dielectric and magnetic materials, and electric/magnetic **conductivities** σ
- **PML** absorbing boundaries and/or perfect conductor and/or **Bloch-periodic** boundary conditions
- Exploitation of **symmetries** to reduce the computation size – even/odd mirror symmetries, and 90°/180° rotations
- Field output in the **HDF5** standard scientific data format; supported by many visualization tools
- Arbitrary material and source distributions
- Field analyses including flux spectra, Maxwell stress tensor, frequency extraction, local density of states and energy integrals, near to far field transformations; completely programmable

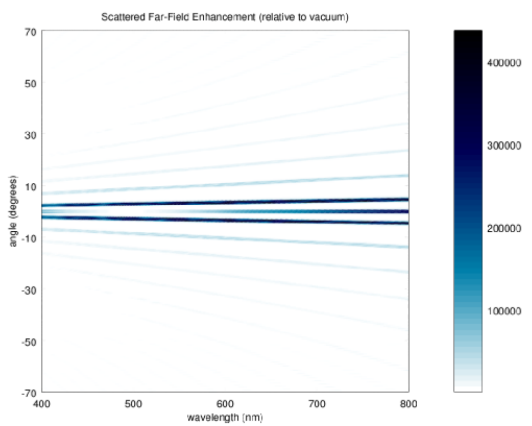
What kinds of problems can MEEP simulate?

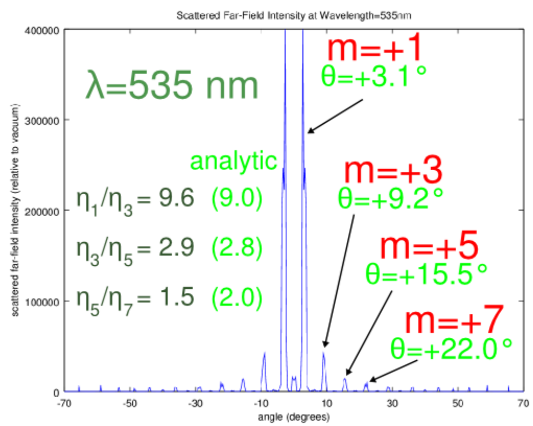
far-field scattering spectra

Binary Diffraction Grating

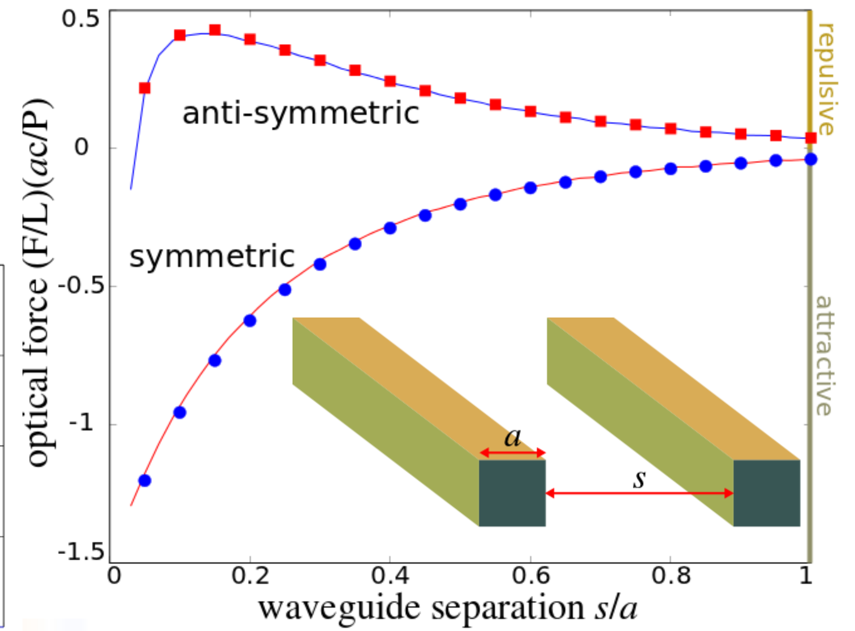


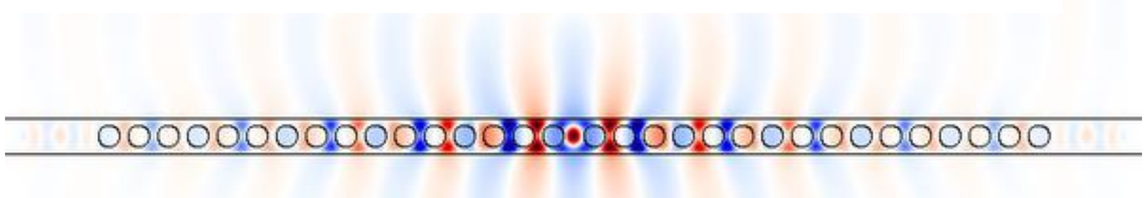
period=10µm, height=500nm, duty cycle=0.5, incident planewave angle=0°



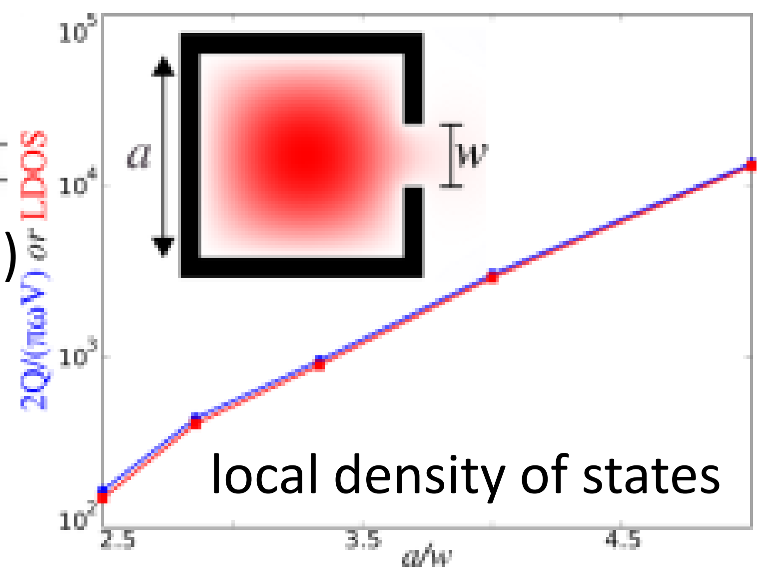


optical forces





resonant modes (Qs, freqs., field profiles, etc.)



local density of states

...& more

How to control MEEP simulations?

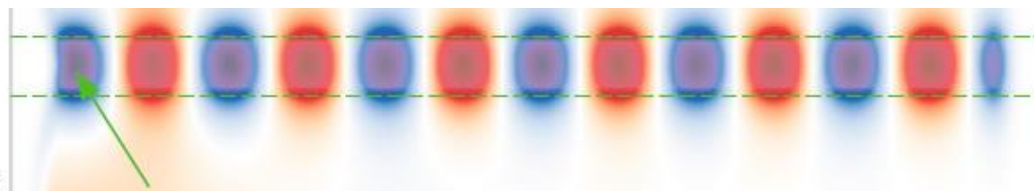
Python Interface

(Scheme & C++ also available)

computational cell & materials

```
import meep as mp

cell_size = mp.Vector3(16,8,0)
geometry = [mp.Block(mp.Vector3(mp.inf, 1, mp.inf), center=mp.Vector3(0, 0),
                     material=mp.Medium(epsilon=12))]
pml_layers = [mp.PML(thickness=1.0)]
```



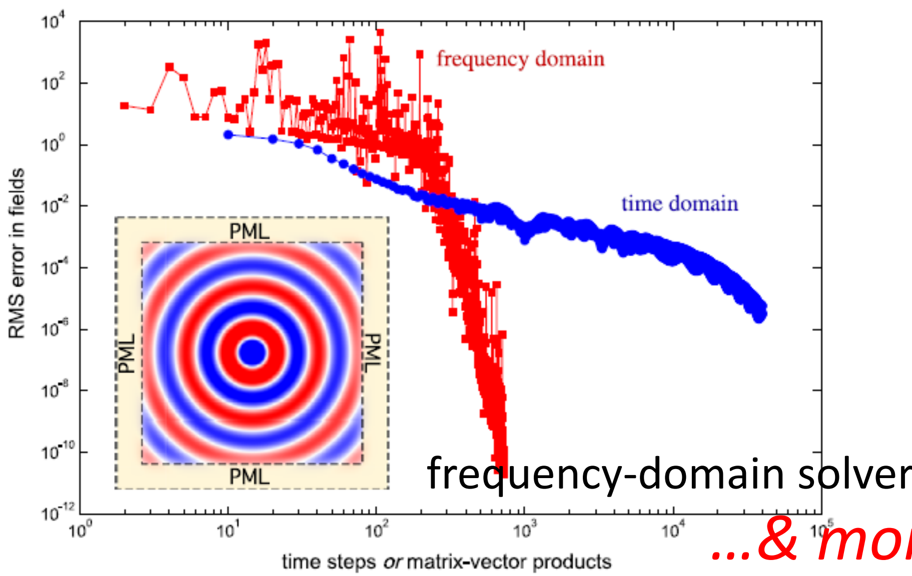
current source

```
sources = [mp.Source(mp.ContinuousSource(frequency=0.15),
                     component=mp.Ez, center=mp.Vector3(-7,0))]
resolution = 10
```

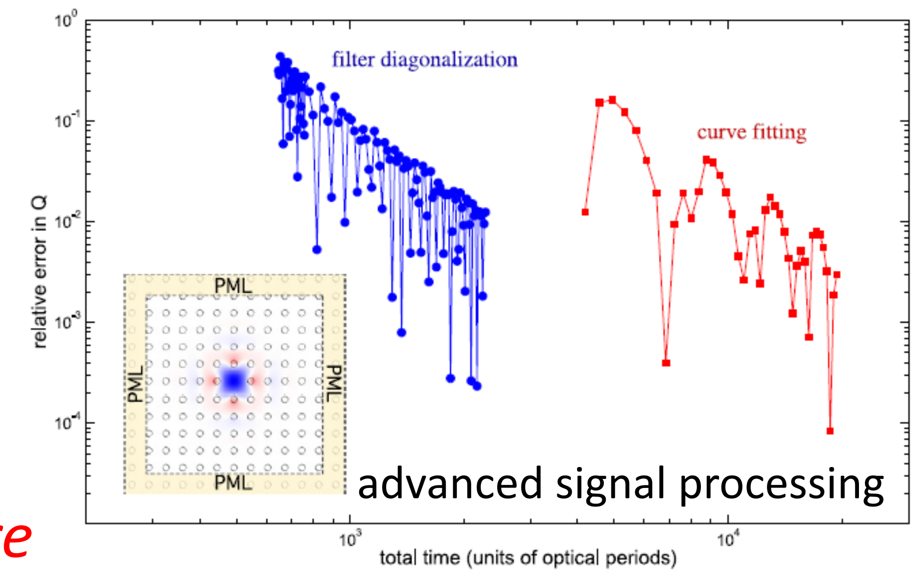
run & output

```
sim.run(mp.at_beginning(mp.output_epsilon),
        mp.at_end(mp.output_efield_z), until=200)
```

other unique features



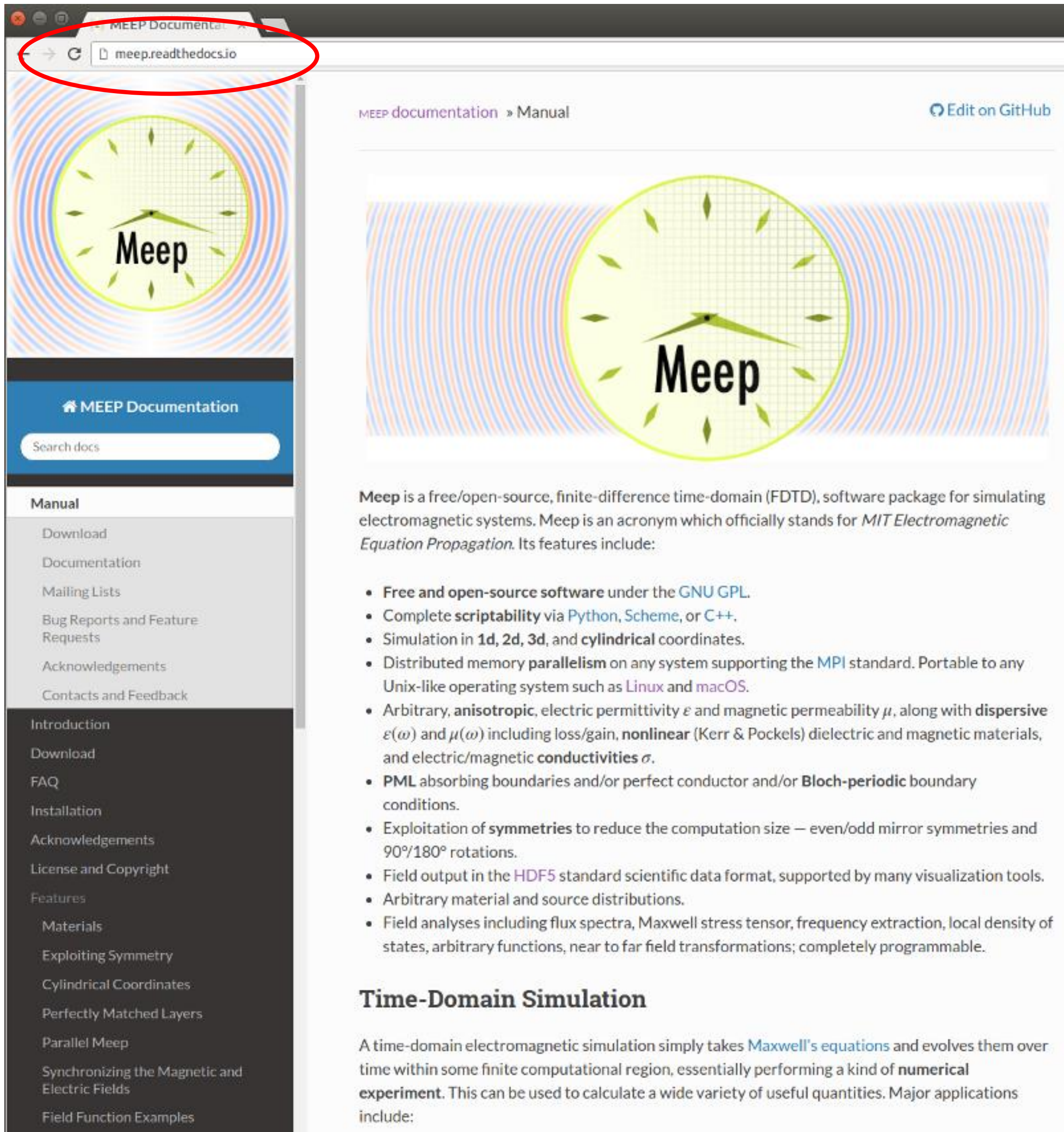
…& more

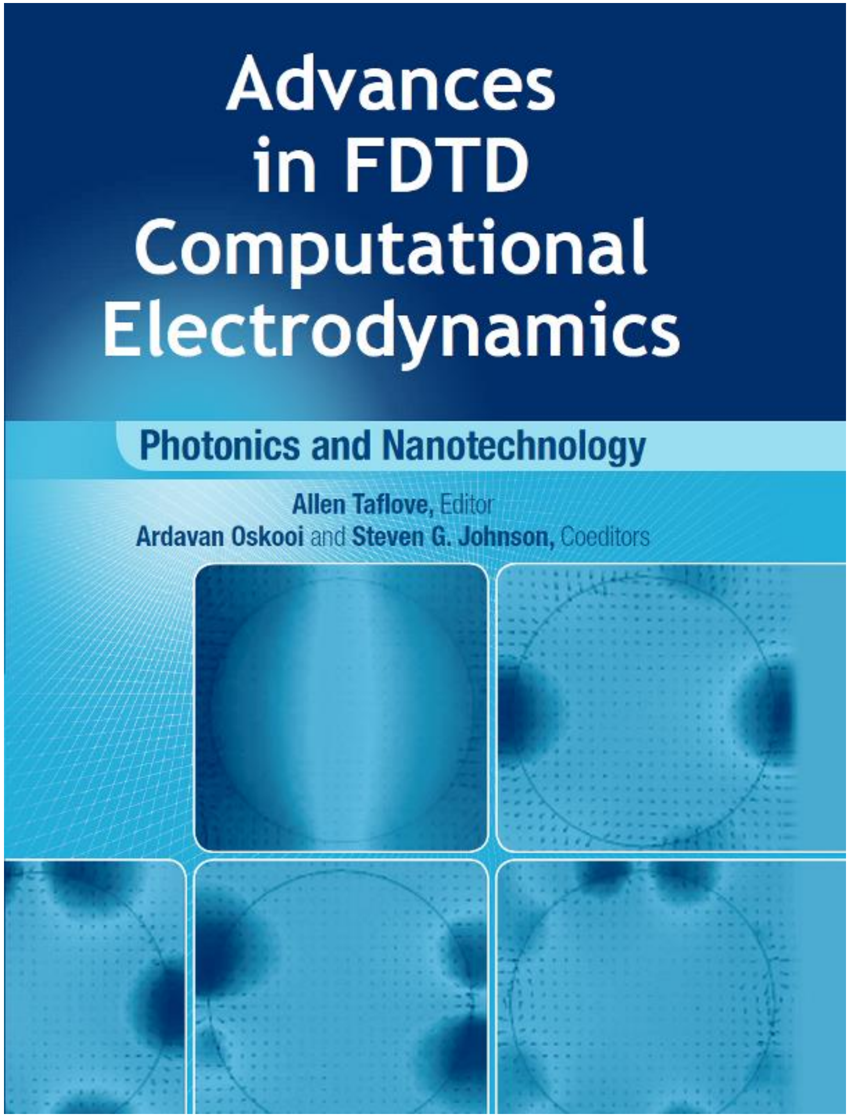


MEEP Homepage

install guide, user tutorials, FAQs, & more

source code on GitHub





670 pages. Hardcover and Kindle formats.
Published by Artech House in 2013.
Available on Amazon.com

book reviews latest advances in sub-pixel smoothing of dielectric interfaces, PMLs and adiabatic absorbers for inhomogeneous media, MEEP, and more.

Editors

Allen Taflove (Northwestern U.)
Ardavan Oskooi (Simpetus)
Steven G. Johnson (MIT)

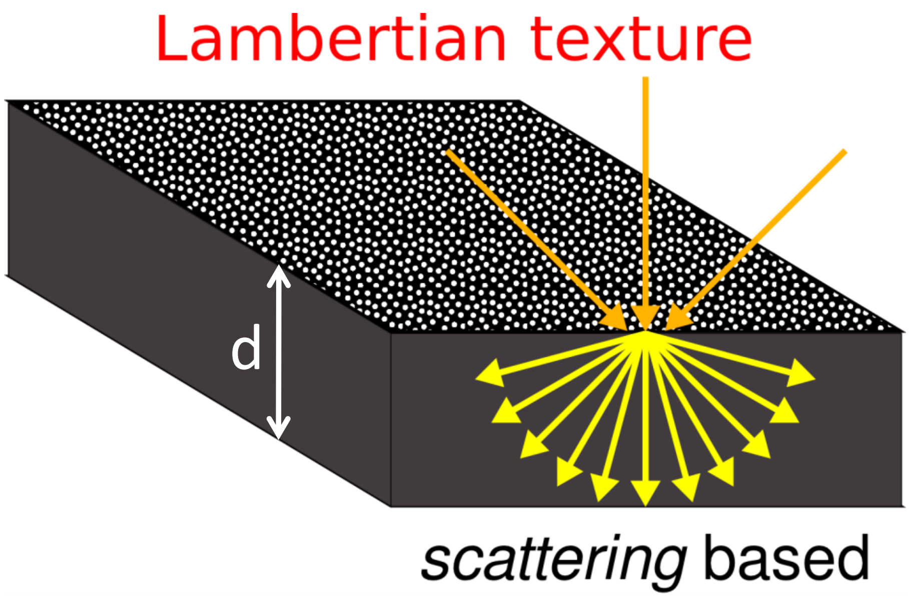
includes contributions
from over 20 researchers

Leveraging Advances in Computational Electrodynamics to Enable New Kinds of Nanophotonic Devices

Thin-Film Solar Cells

What is the maximum absorption of solar radiation over the broadest range of frequencies and angles using the thinnest material possible?

Two Different Approaches to Light Trapping



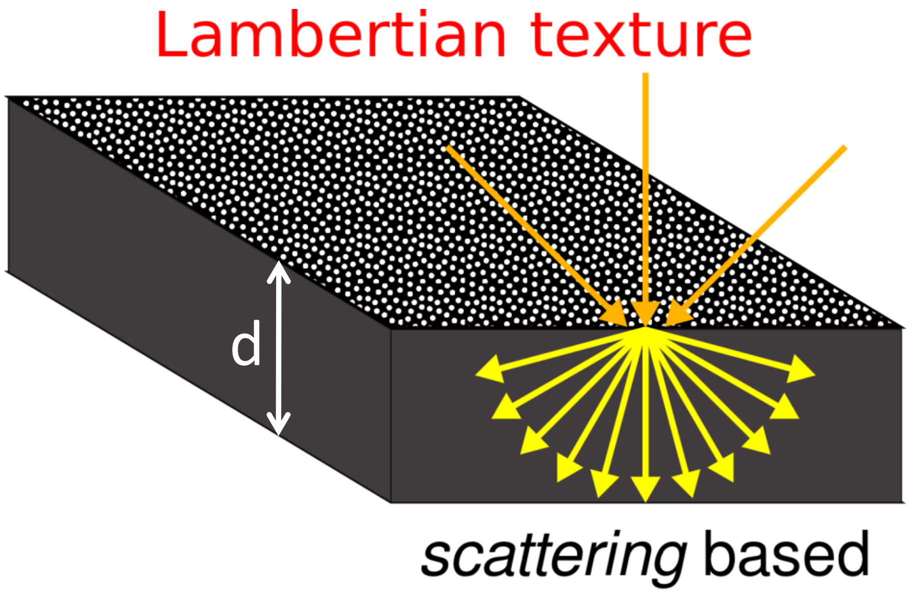
- scattering light rays into index-guided modes
- optical path length effectively doubled (d→2d)
- works over widest set of conditions
- an ideal design: cannot be made in practice
- widely used by solar industry in crystalline silicon designs (d ~ 100s of μms)

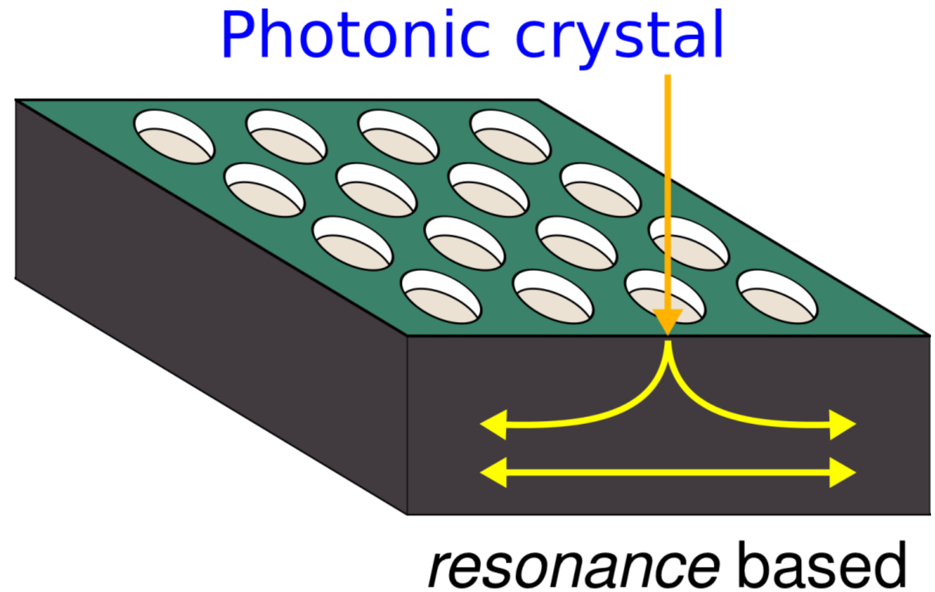
E. Yablonovitch & G.D. Cody, *IEEE Trans. Elec. Dev.*, **29**, pp. 300-5 (1982)

E. Yablonovitch , *J. Opt. Soc. Am.*, **72**, pp. 899-907 (1982)

P. Campbell & M.A. Green, *J. App. Phys.*, **62**, pp. 243-9 (1987)

Two Different Approaches to Light Trapping





- scattering light rays into index-guided modes
- optical path length effectively doubled (d→2d)
- works over widest set of conditions
- an ideal design: cannot be made in practice
- widely used by solar industry in crystalline silicon designs (d ~ 100s of μms)

- coupling light waves into coherent modes
- nearly 100% absorption but only for a narrow bandwidth, single angle & polariz.
- delicate interference effects require precise fabrication for good performance
- **applicable to thin films (d < 1 μm)**

E. Yablonovitch & G.D. Cody, *IEEE Trans. Elec. Dev.*, **29**, pp. 300-5 (1982)

E. Yablonovitch , *J. Opt. Soc. Am.*, **72**, pp. 899-907 (1982)

P. Campbell & M.A. Green, *J. App. Phys.*, **62**, pp. 243-9 (1987)

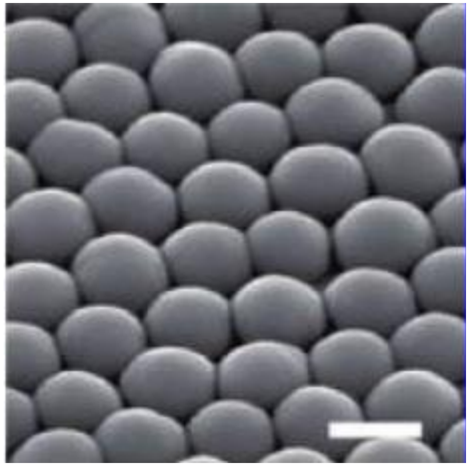
A. Chutinan et al., *Opt. Express*, **17**, pp. 8871-8 (2009)

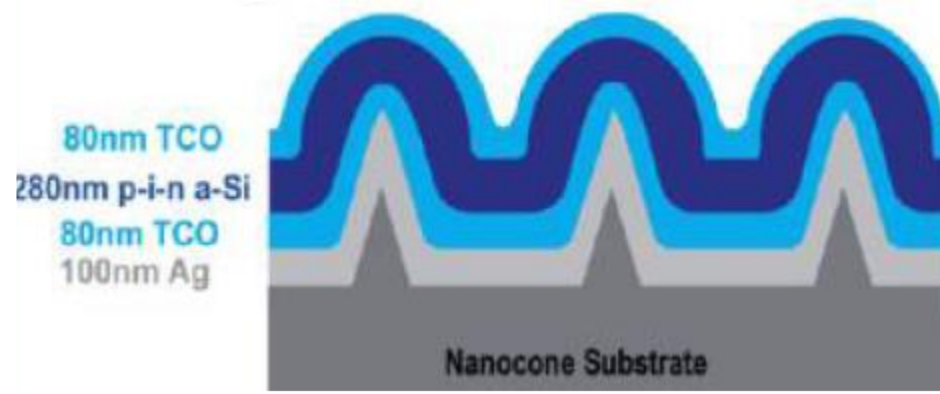
S.B. Mallick et al., *Opt. Express*, **18**, pp. 5691-706 (2010)

Z. Yu et al., *PNAS*, **107**, pp. 17491-17496 (2010)

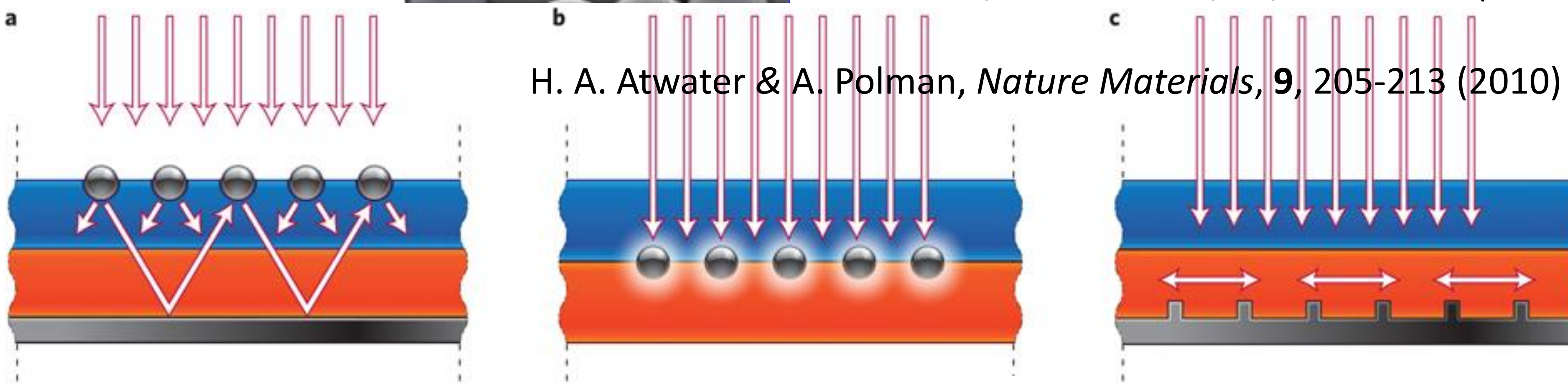
& many more (nanowires, plasmonics, ...)

Resonance-Based Approaches to Light Trapping

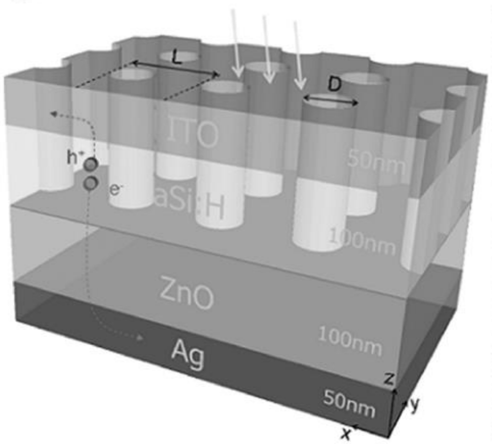


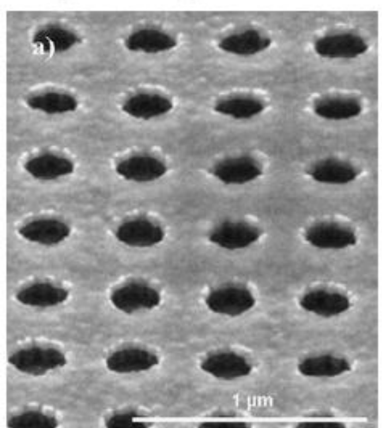


Y. Cui et al., *Nano Letters*, **10**, 1979-1984 (2009)



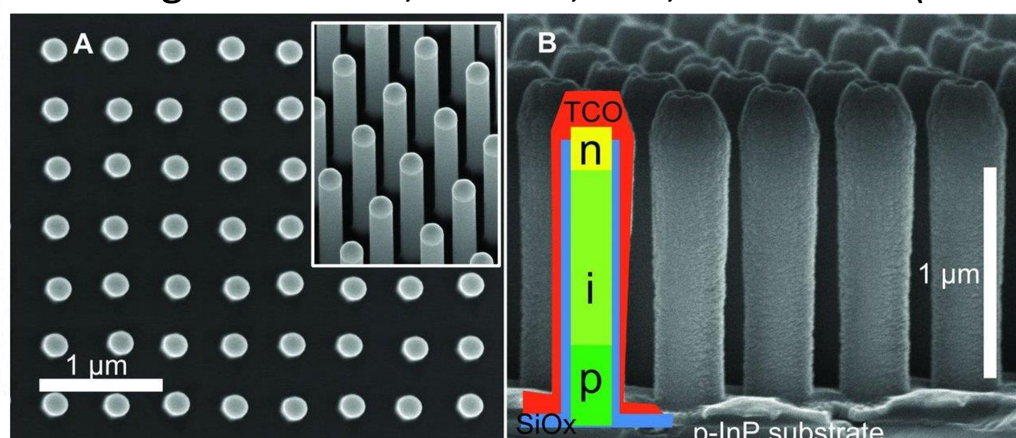
H. A. Atwater & A. Polman, *Nature Materials*, **9**, 205-213 (2010)



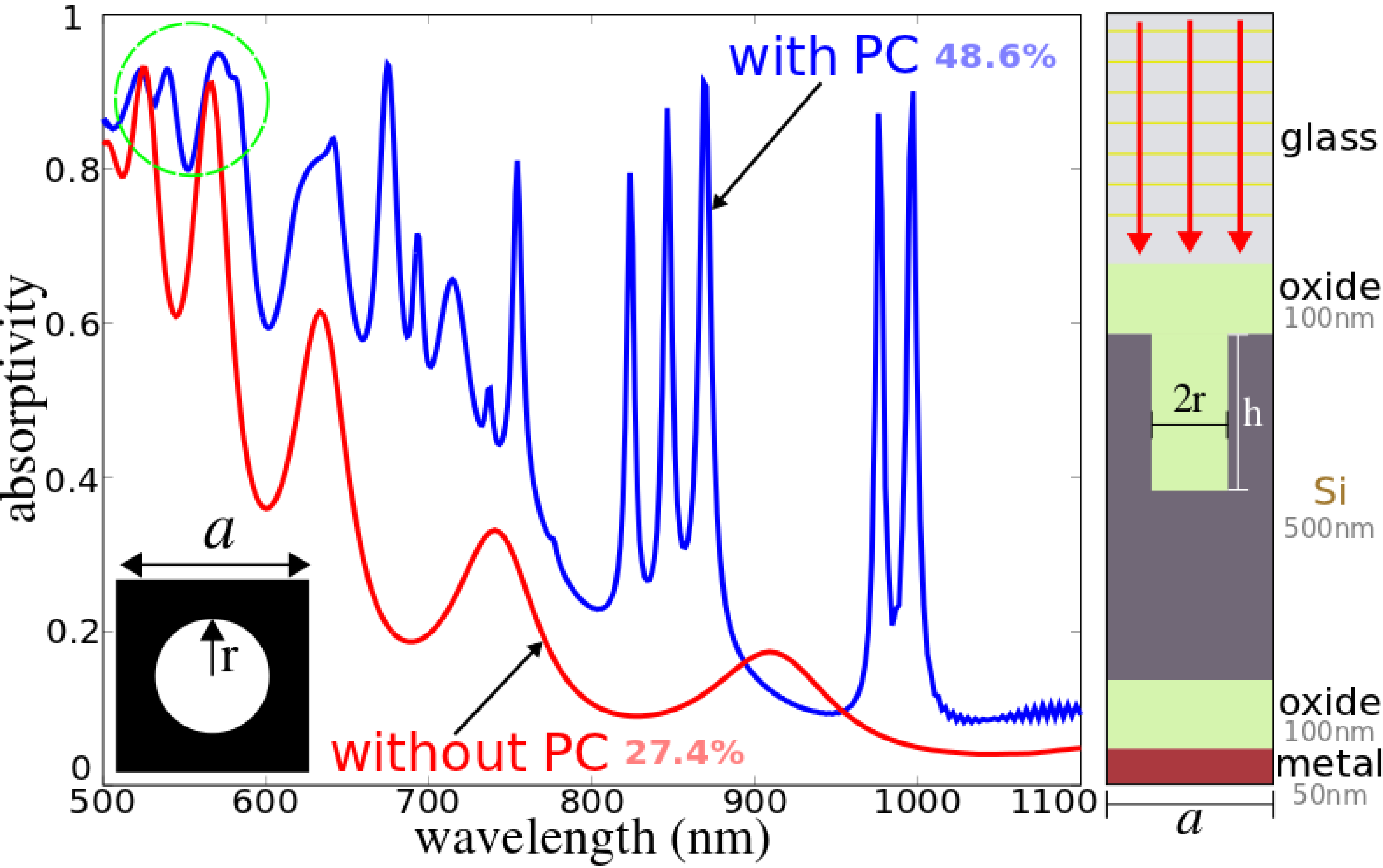


C. Seassal et al., *Sol. Energy Mater. & Sol. Cells*, **95**, S32-S38 (2011)

M.T. Borgstrom et al., *Science*, **339**, 1057-1060 (2013)



Light Trapping in Nanostructured Thin Films



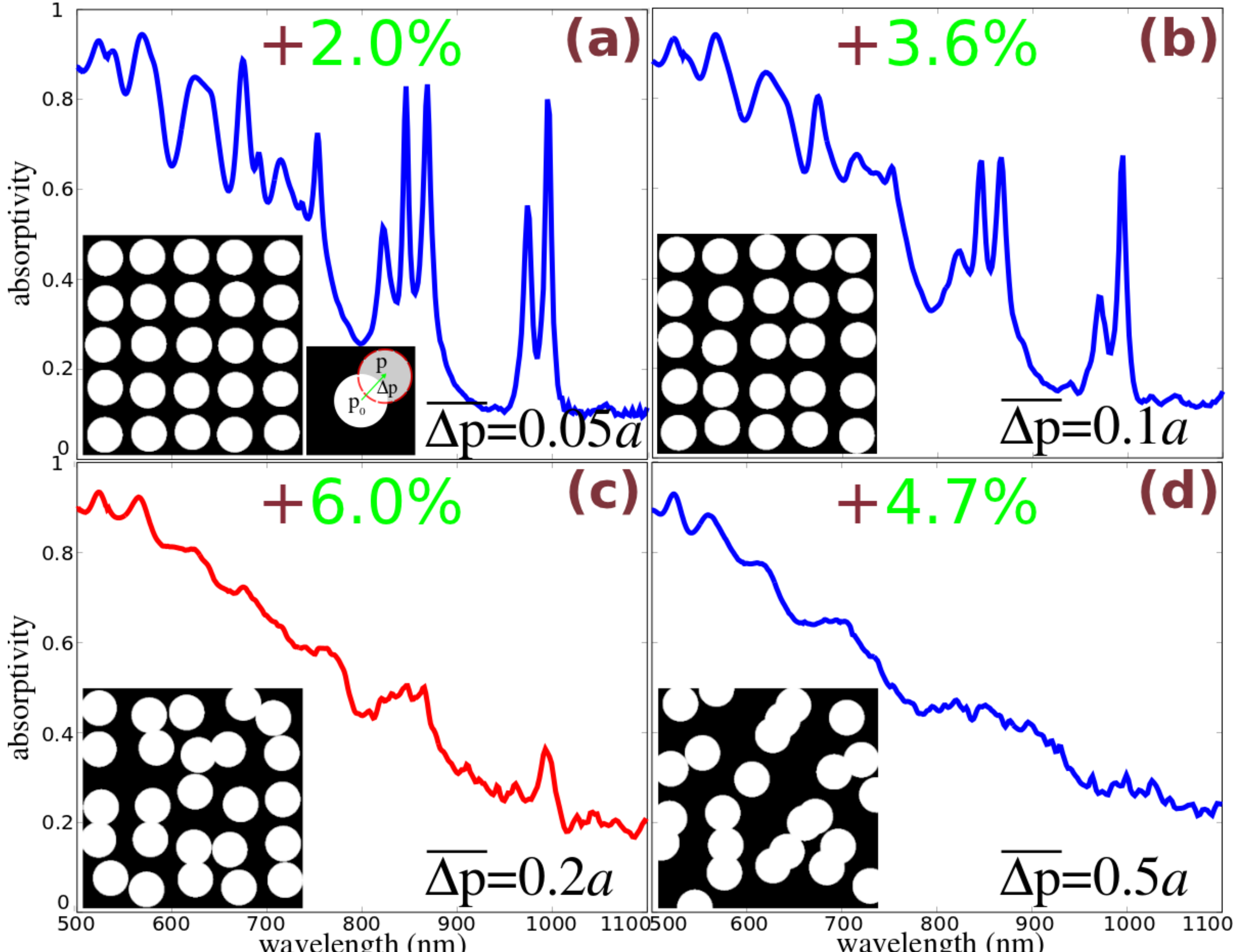
A. Oskooi et al., *Applied Physics Letters,* **100**, 181110 (2012)

How can narrow peaks be broadened

and

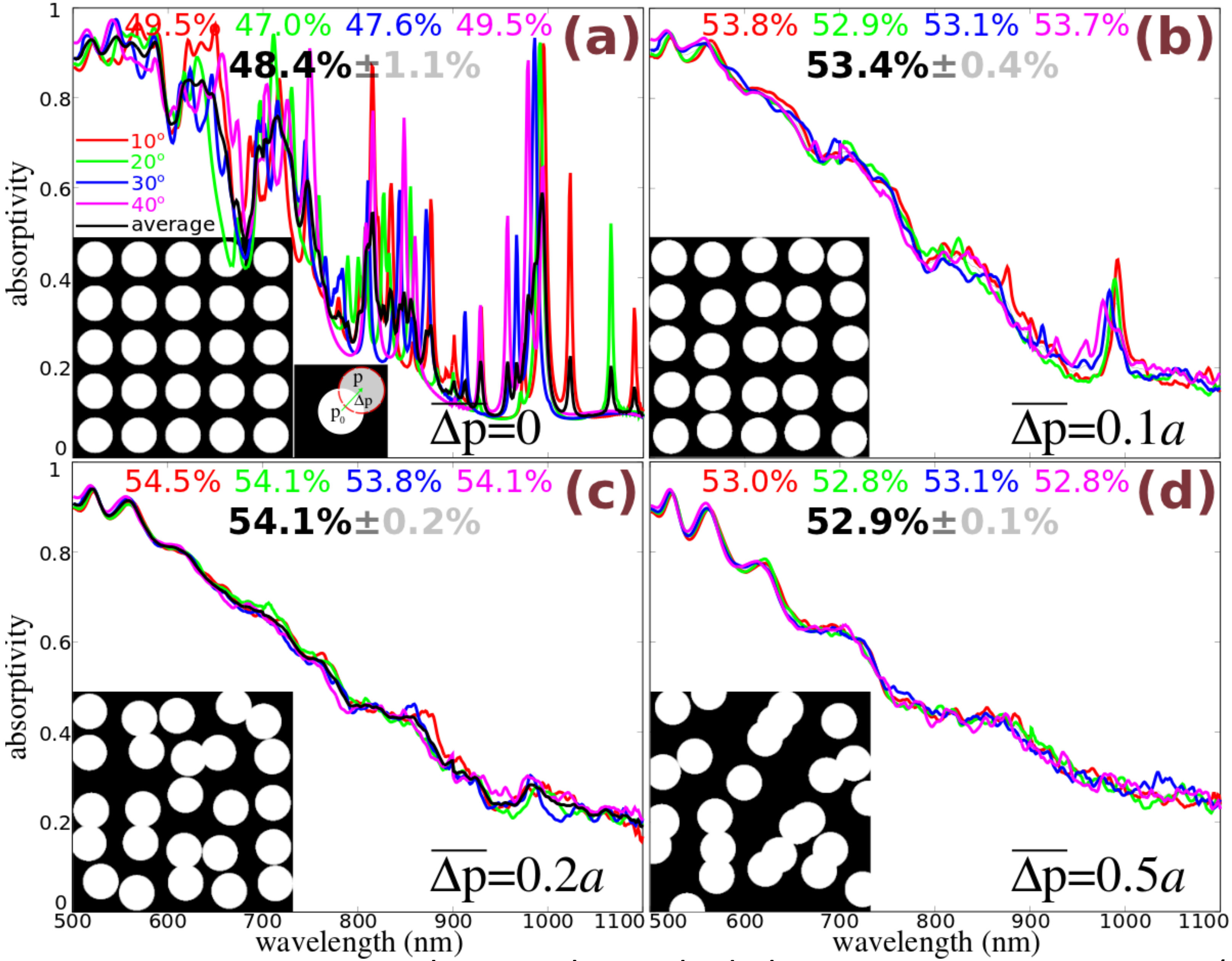
device made more robust?

1. positional disorder broadens peaks



A. Oskooi et al., *Applied Physics Letters,* **100**, 181110 (2012)

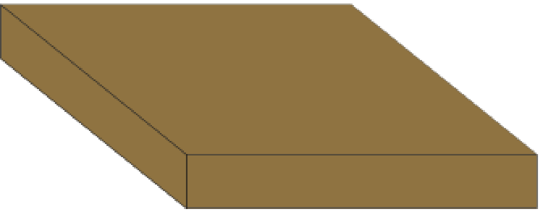
2. positional disorder reduces angle/pol sensitivity



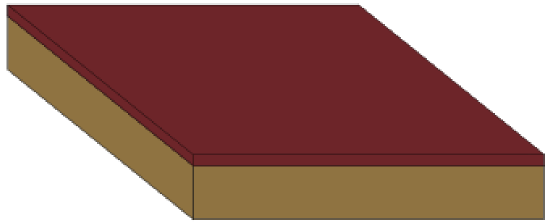
A. Oskooi et al., *Applied Physics Letters*, **100**, 181110 (2012)

Experimental Demonstration of Quasi-Resonant Absorption

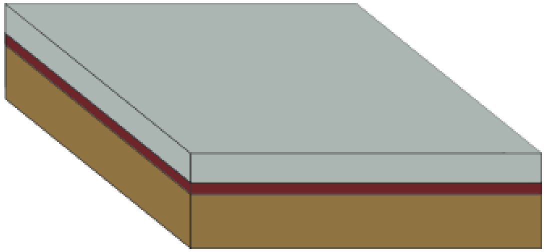
device fabrication using semiconductor processing
via thin-film deposition & lithography



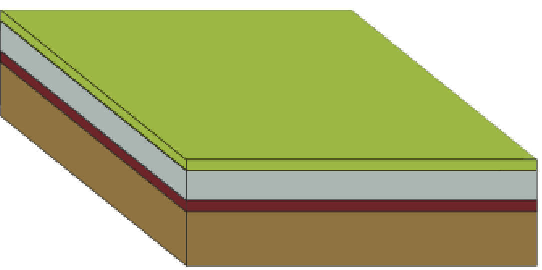
0. substrate



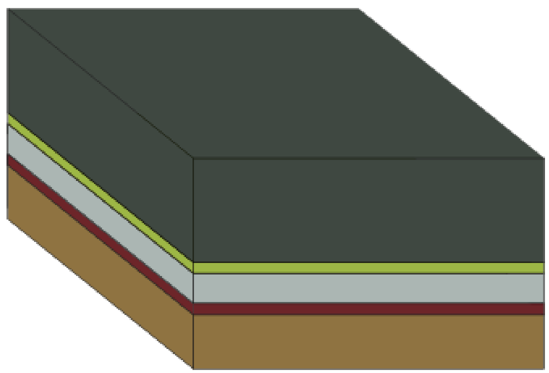
1. +30nm Ti
via EB PVD



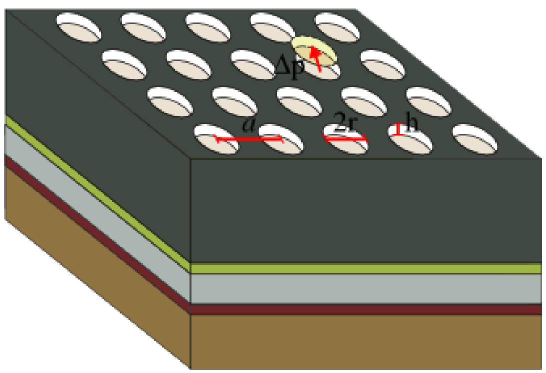
2. +250nm Ag
via EB PVD



3. +50nm GZO
via sputtering



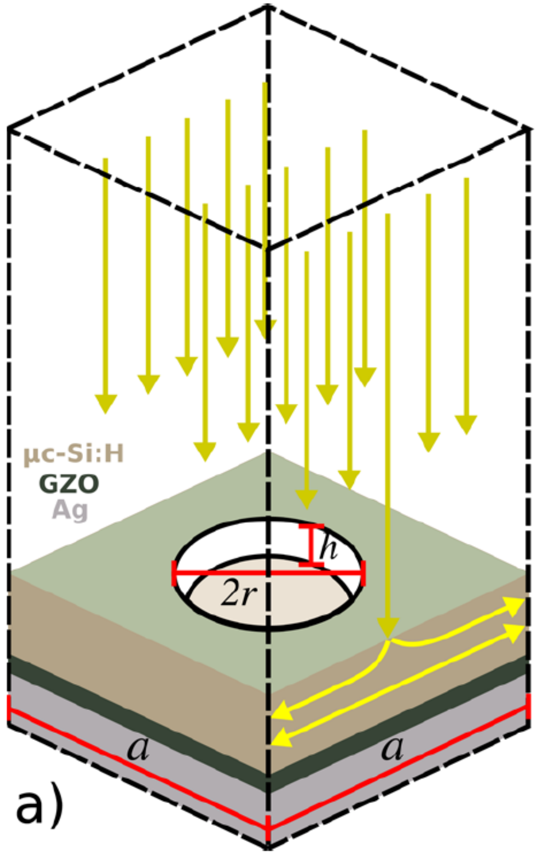
4. +520nm mc-Si
via PECVD



5. EBL *followed by*
dry etch & resist strip

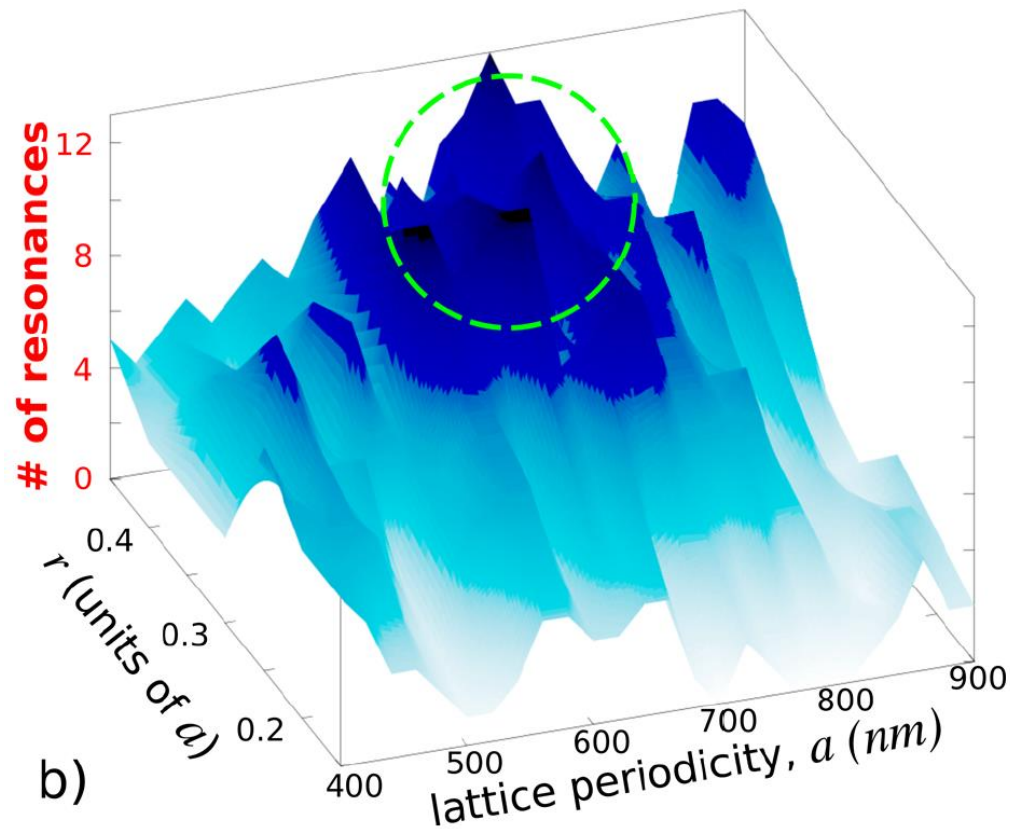
A. Oskooi et al., *ACS Photonics*, **1**, pp. 304-9 (2014)

Photonic Crystal Designed Ab-initio to Produce Large Number of Resonant Absorption Peaks



a)

optimize **2** parameters of square-lattice PC slab: *a* and *r* (*h* =180 nm, fixed)



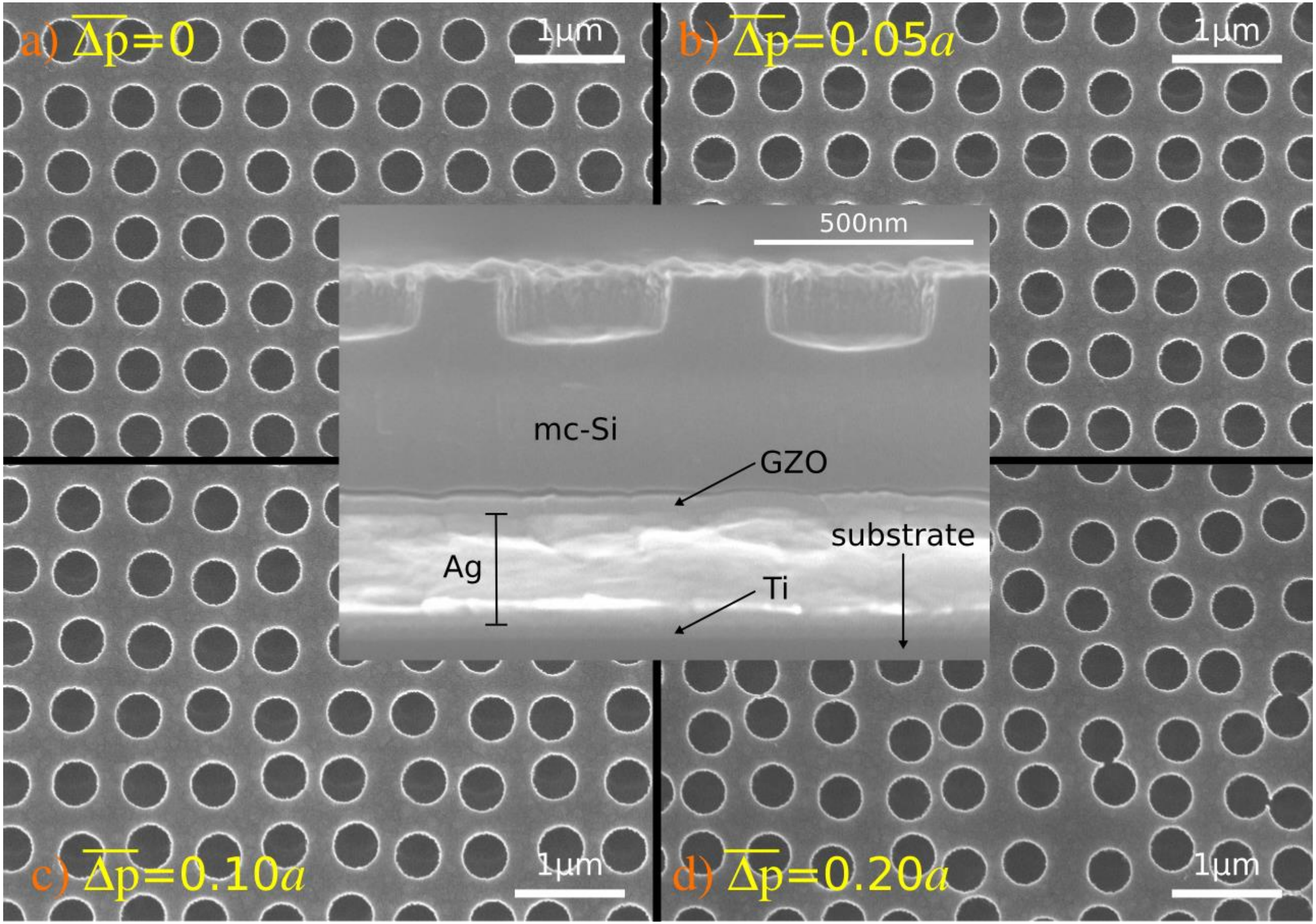
b)

optimum: *a*=650 nm, *r*=208 nm

A. Oskooi et al., *ACS Photonics,* **1**, pp. 304-9 (2014)

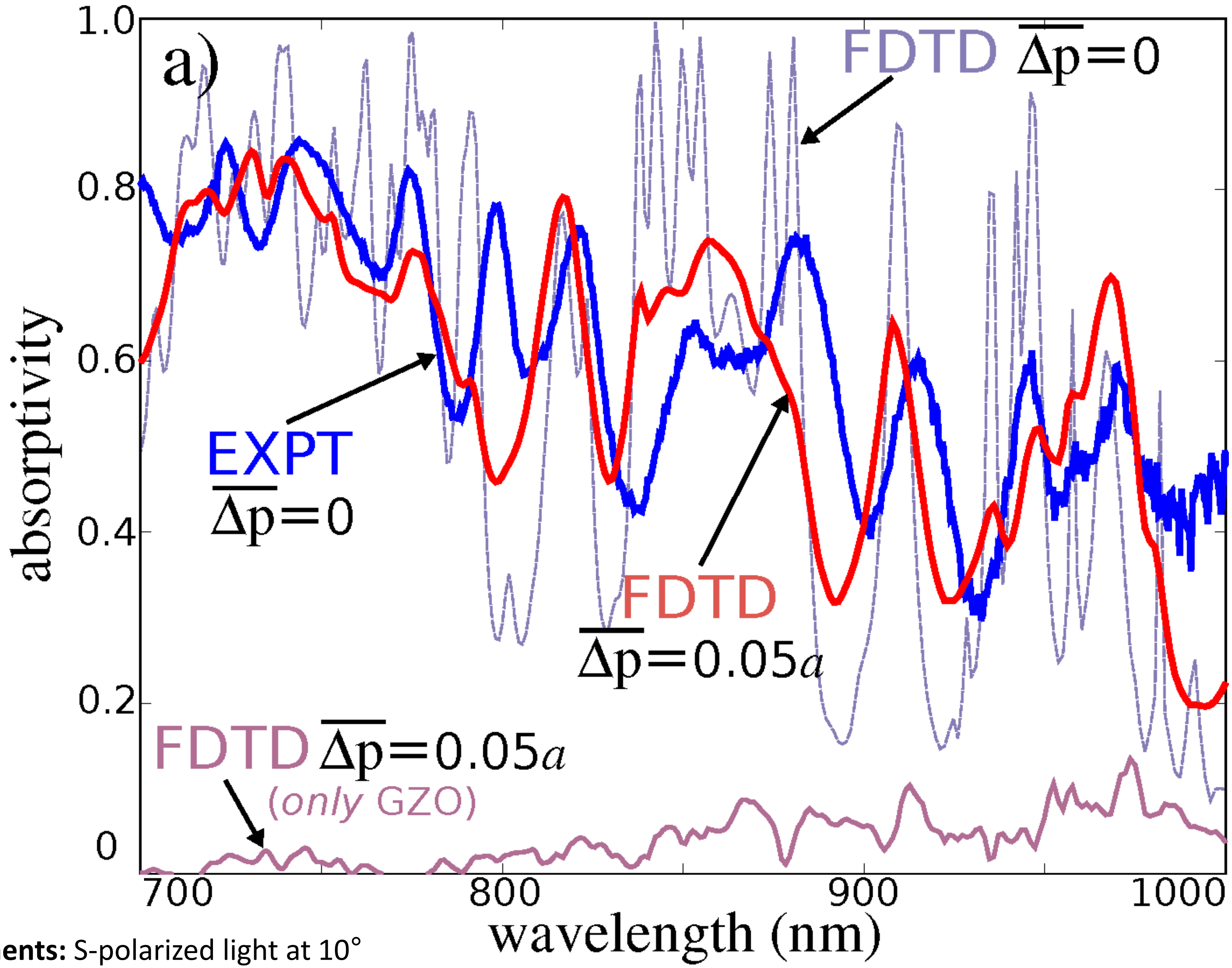
Experimental Demonstration of Quasi-Resonant Absorption

partially-disordered PC lattices in micro-crystalline Si



A. Oskooi et al., *ACS Photonics,* **1**, pp. 304-9 (2014)

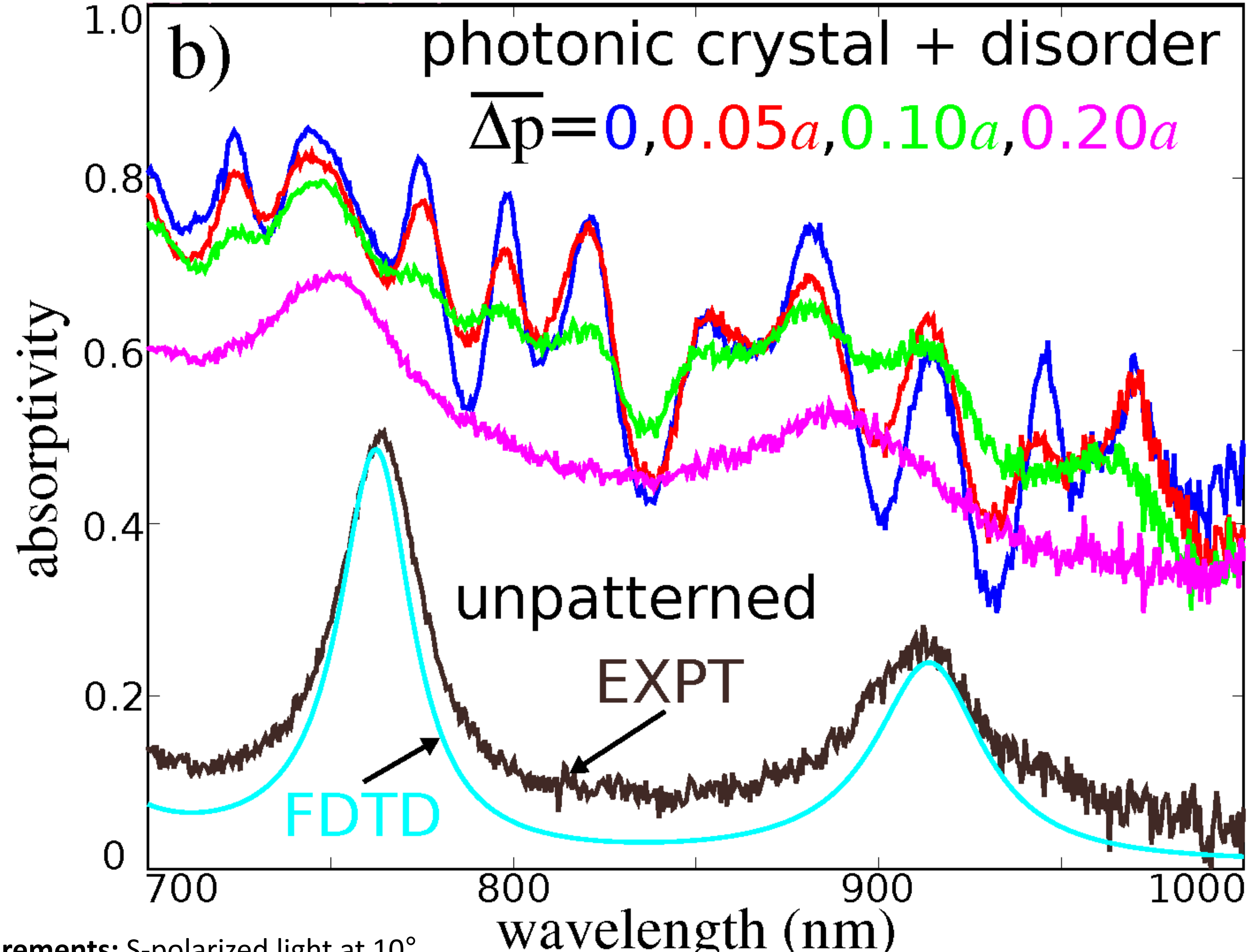
Comparison of Experimental and Simulation Results



measurements: S-polarized light at 10° angle of incidence in integrating sphere

A. Oskooi et al., *ACS Photonics,* **1**, pp. 304-9 (2014)

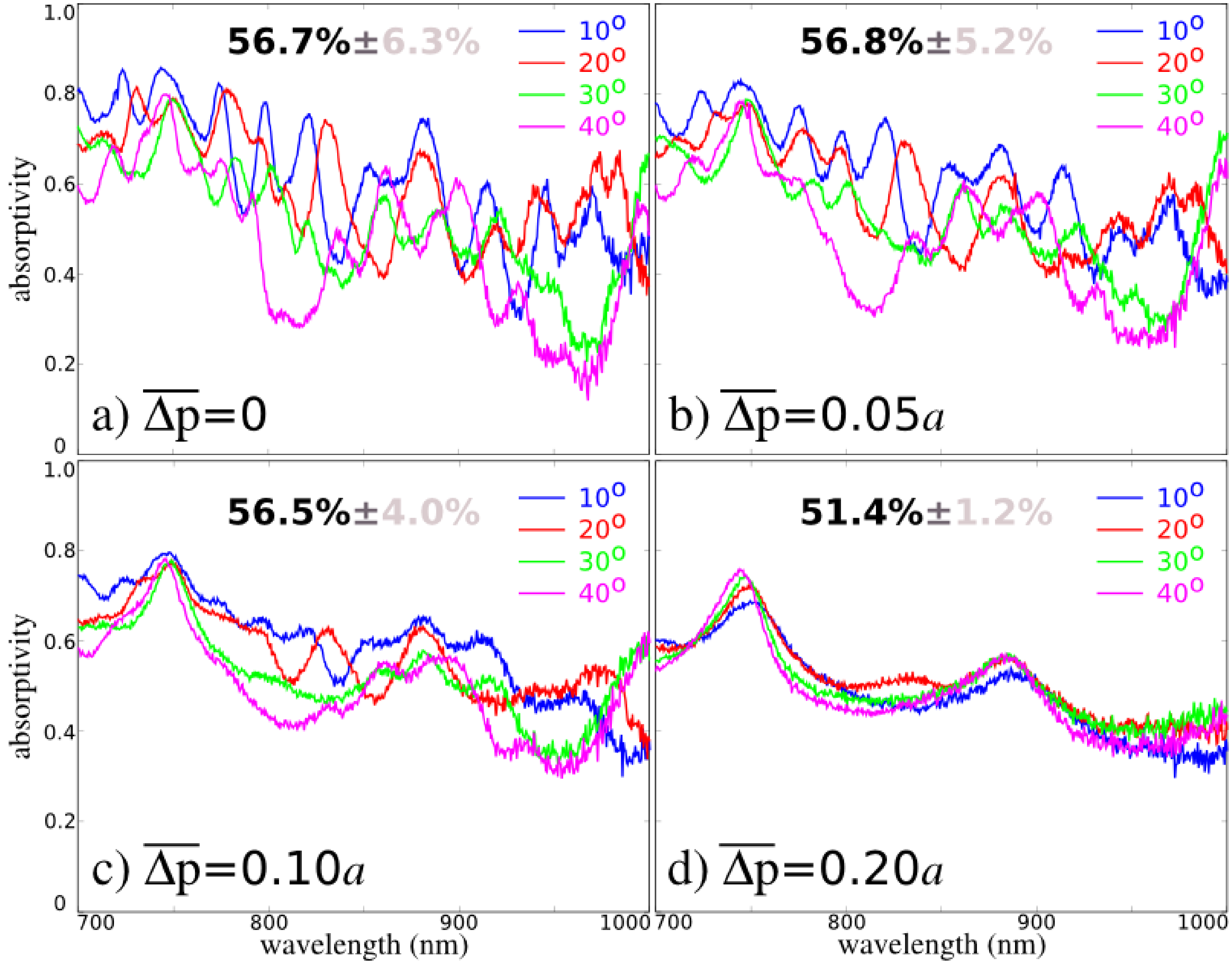
Comparison of Experimental and Simulation Results



measurements: S-polarized light at 10° angle of incidence in integrating sphere

A. Oskooi et al., *ACS Photonics,* **1**, pp. 304-9 (2014)

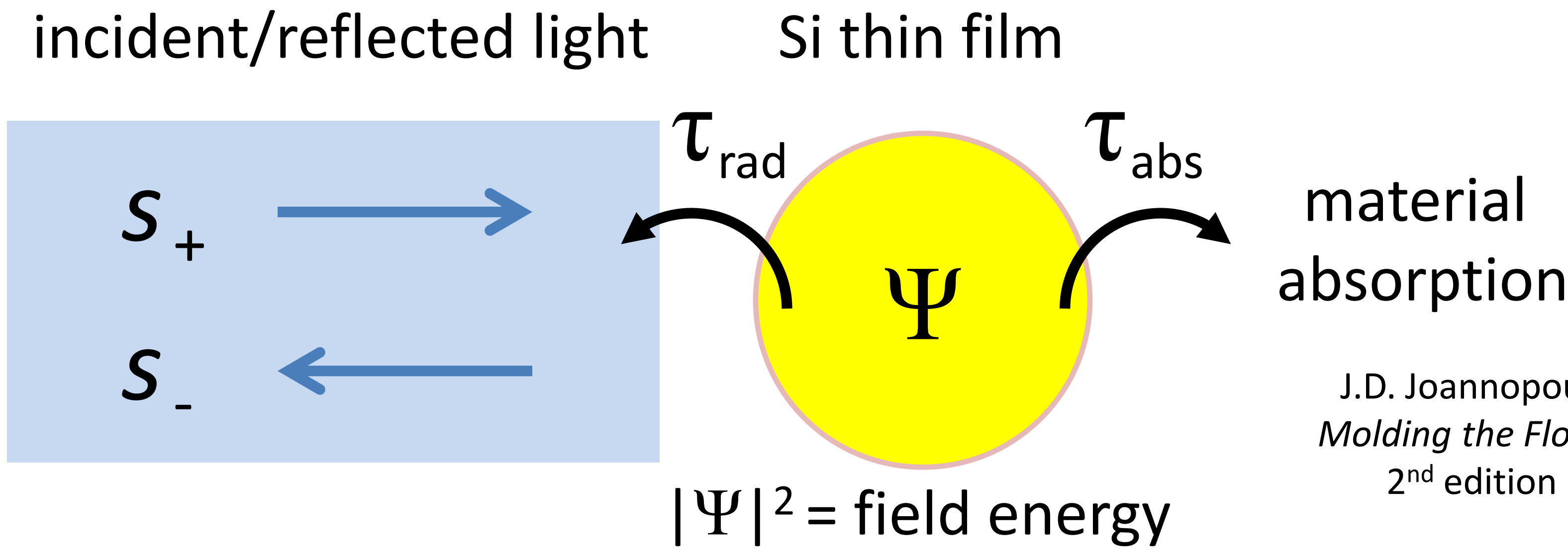
Improved Robustness from Increased Disorder



A. Oskooi et al., *ACS Photonics,* **1**, pp. 304-9 (2014)

Effect of Disorder on Broadband Light Trapping

consider *weak* coupling to single **resonant** mode of the PC

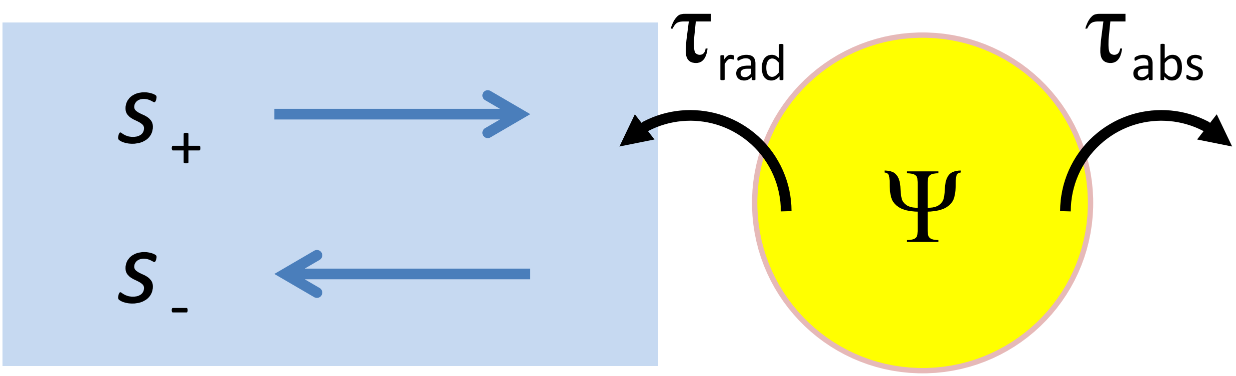


J.D. Joannopoulos et al, *Molding the Flow of Light*, 2nd edition (2008)

Effect of Disorder on Broadband Light Trapping

consider *weak* coupling to single **resonant** mode of the PC

incident/reflected light Si thin film



material absorption

$|\Psi|^2$ = field energy

J.D. Joannopoulos et al, *Molding the Flow of Light*, 2nd edition (2008)

Lorentzian Absorption

$$A(\omega) = \frac{\frac{4}{\tau_{rad}\tau_{abs}}}{(\omega-\omega_0)^2 + \left(\frac{1}{\tau_{rad}} + \frac{1}{\tau_{abs}}\right)^2}$$

$$A(\omega_0) = \frac{4\tau_{rad}\tau_{abs}}{(\tau_{rad}+\tau_{abs})^2}$$

$$\int_{-\infty}^{\infty} A(\omega)d\omega = \frac{4\pi}{\boxed{\tau_{rad}}+\tau_{abs}}$$

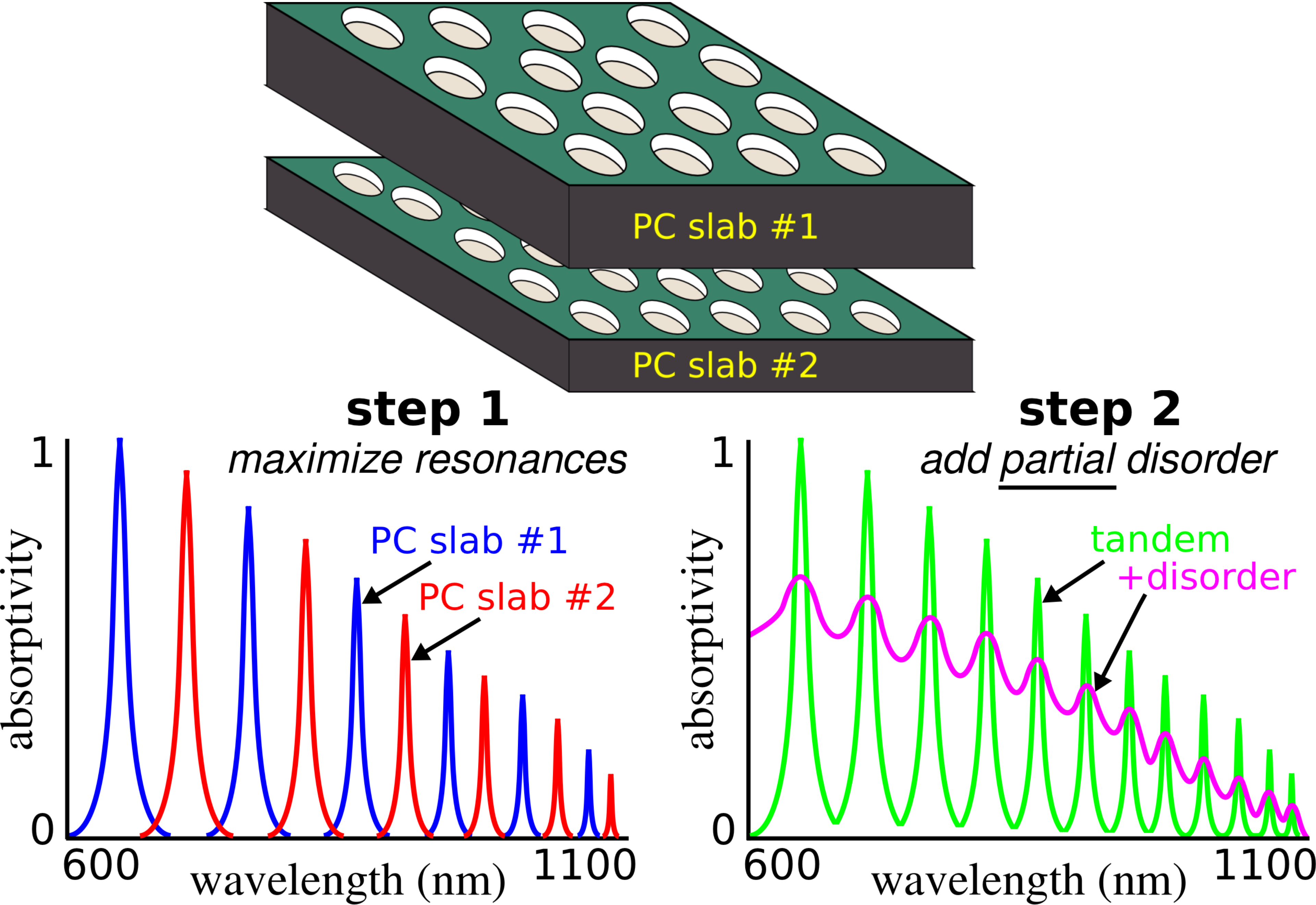
…peak broadening via decreasing τ_{rad} **always** increases wideband light trapping!

Q: How to *most effectively* make use of partial disorder for light-trapping enhancement in a thin film?

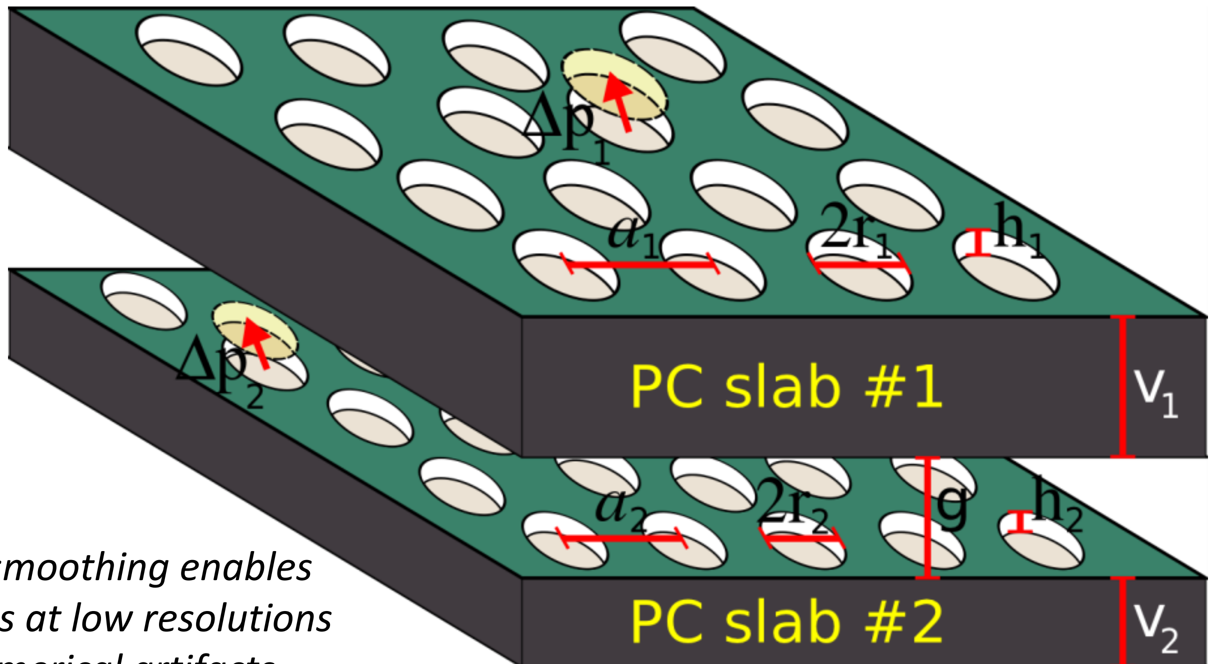
Q: How to *most effectively* make use of partial disorder for light-trapping enhancement in a thin film?

A: First, *maximize number of resonances* so there is little bandwidth separation between peaks and then *add disorder*

Tandem Partially-Disordered Photonic-Crystal Slabs



Geometry Optimization in MEEP



MEEP's sub-pixel smoothing enables accurate simulations at low resolutions & eliminates numerical artifacts

7 design parameters of tandem PC slabs

lattice periodicity a_1 (= a_2), hole radii r_1 & r_2, hole heights h_1 & h_2

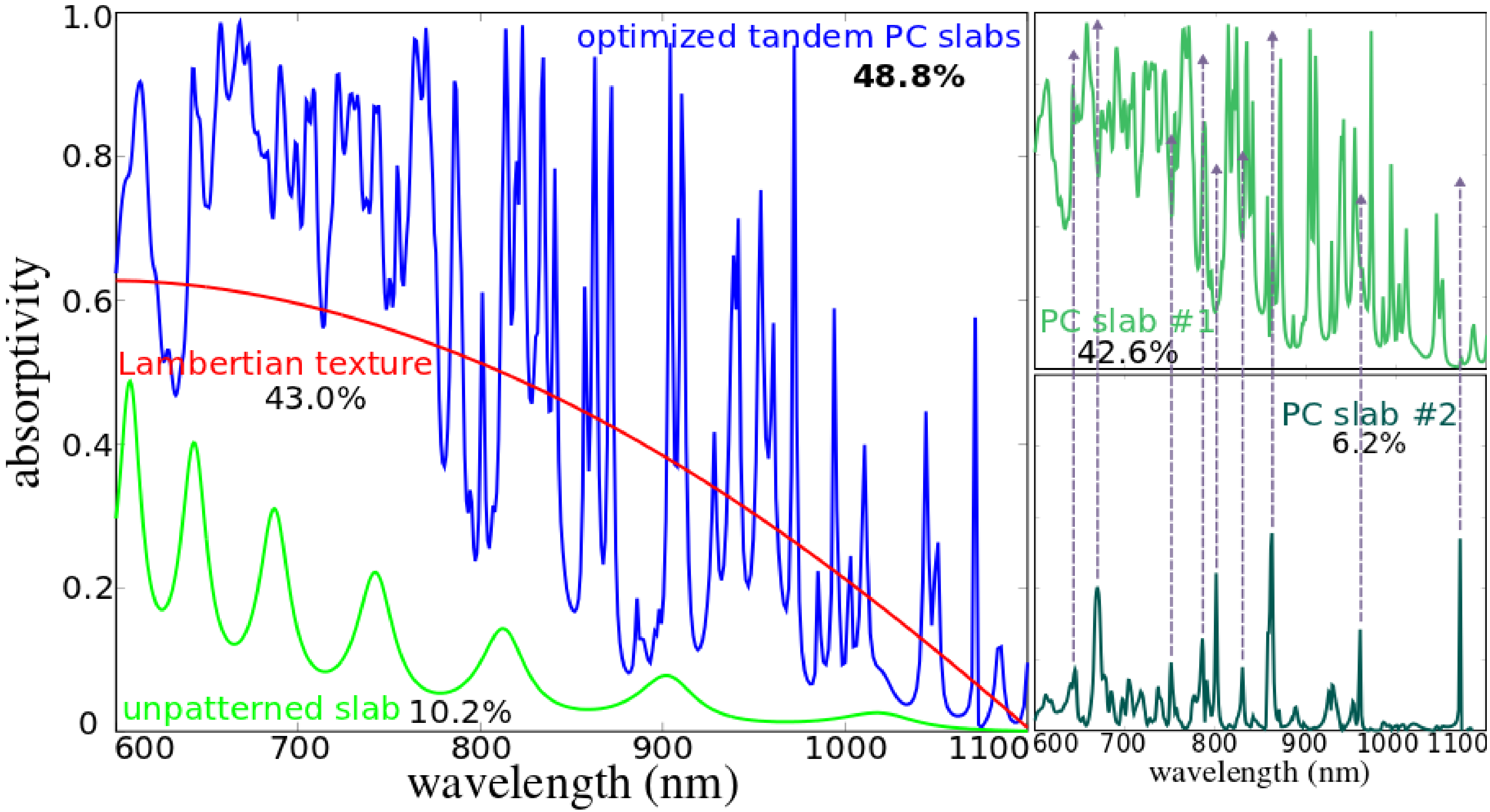
slab thickness v_1 (v_2=1μm-v_1) , separation gap *g*

- compute broadband absorption spectra at normal incidence & from this *count* number of large-amplitude peaks
- repeat many times with random initial values to explore different local minima

A. Oskooi et al., *Applied Physics Letters*, **105**, 091121 (2014)

Geometry-Optimized Tandem Design with Maximized Peak Density

Resonances Add Complimentarily Over Wideband Spectra

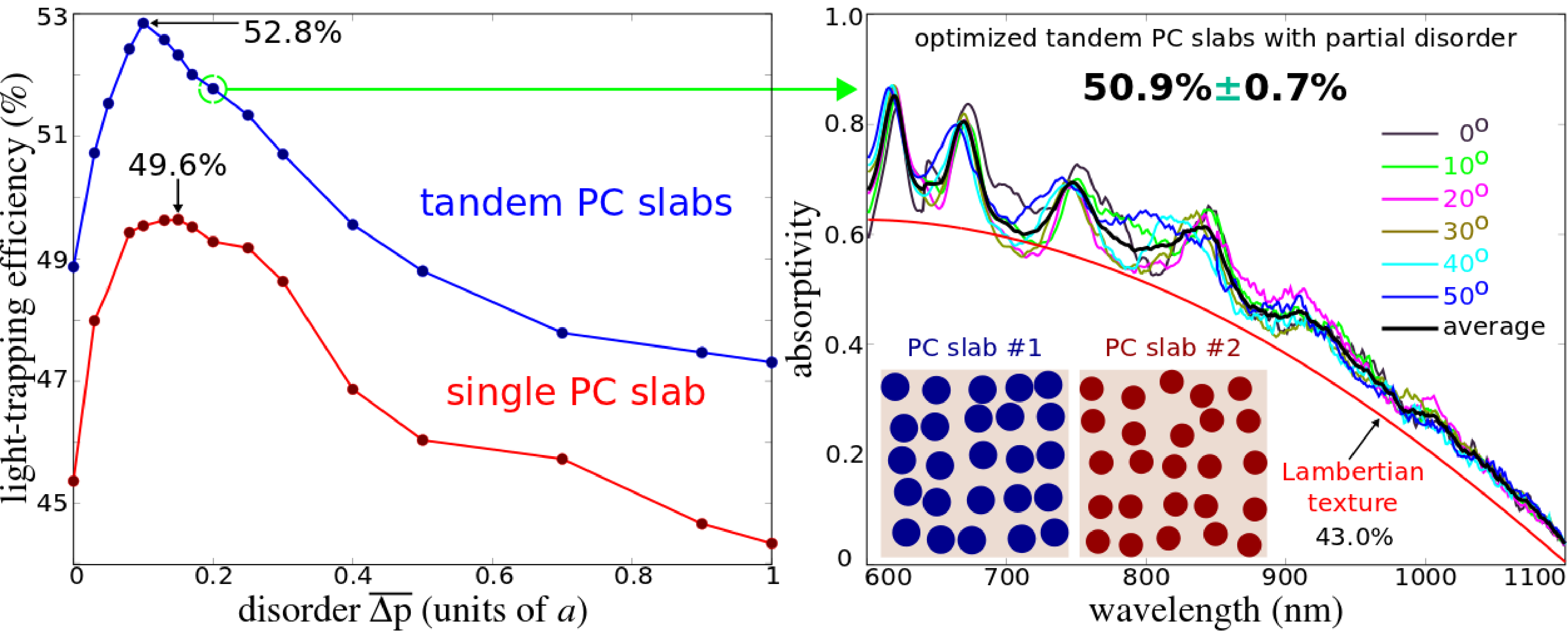


now apply partial disorder to increase light trapping and robustness...

A. Oskooi et al., *Applied Physics Letters*, **105**, 091121 (2014)

Geometry-Optimized Tandem Design with Partial Disorder

Oblique Angular Response and Comparison with Lambertian Texture



single MEEP simulation required 168 cores & ~8 hours on Kyoto University Cray Supercomputer

tandem PC thin films' absorption exceeds Lambertian texture at nearly every wavelength and angle with a total broadband light-trapping efficiency almost 10% larger

A. Oskooi et al., *Applied Physics Letters*, **105**, 091121 (2014)

Leveraging Advances in Computational Electrodynamics to Enable New Kinds of Nanophotonic Devices

Displays and Solid-State Lighting

Organic Light-Emitting Diodes (OLEDs) for Energy-Efficient Displays and Solid-State Lighting

Samsung

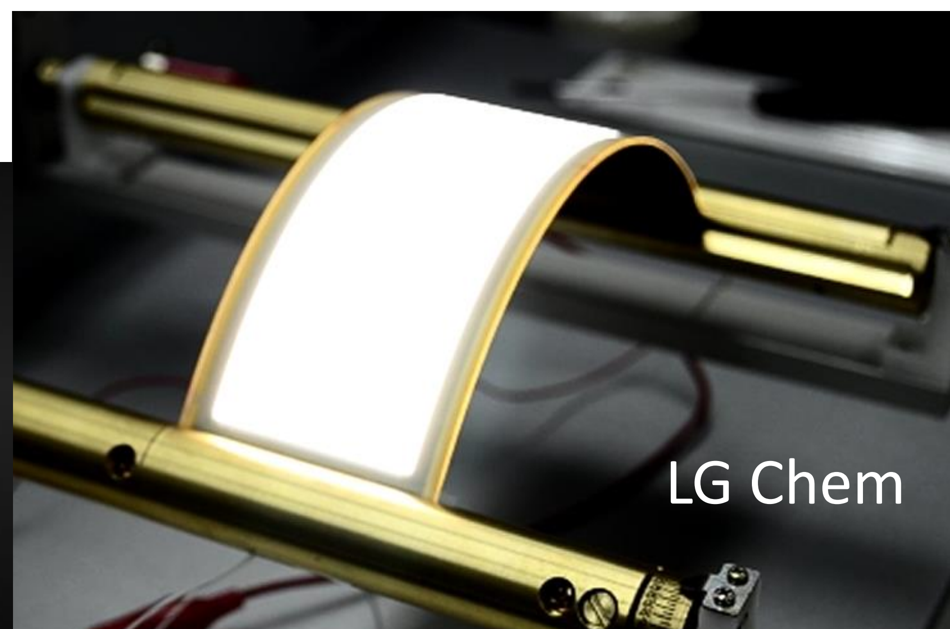
- thin, lightweight, can be fabricated on a variety of substrates (even flexible ones)
- Displays: better color, higher contrast ratio, broader viewing angle
- Lighting: large-area, low-brightness source

Apple

Applications

smartphone displays, tablet displays, TVs, lighting, …

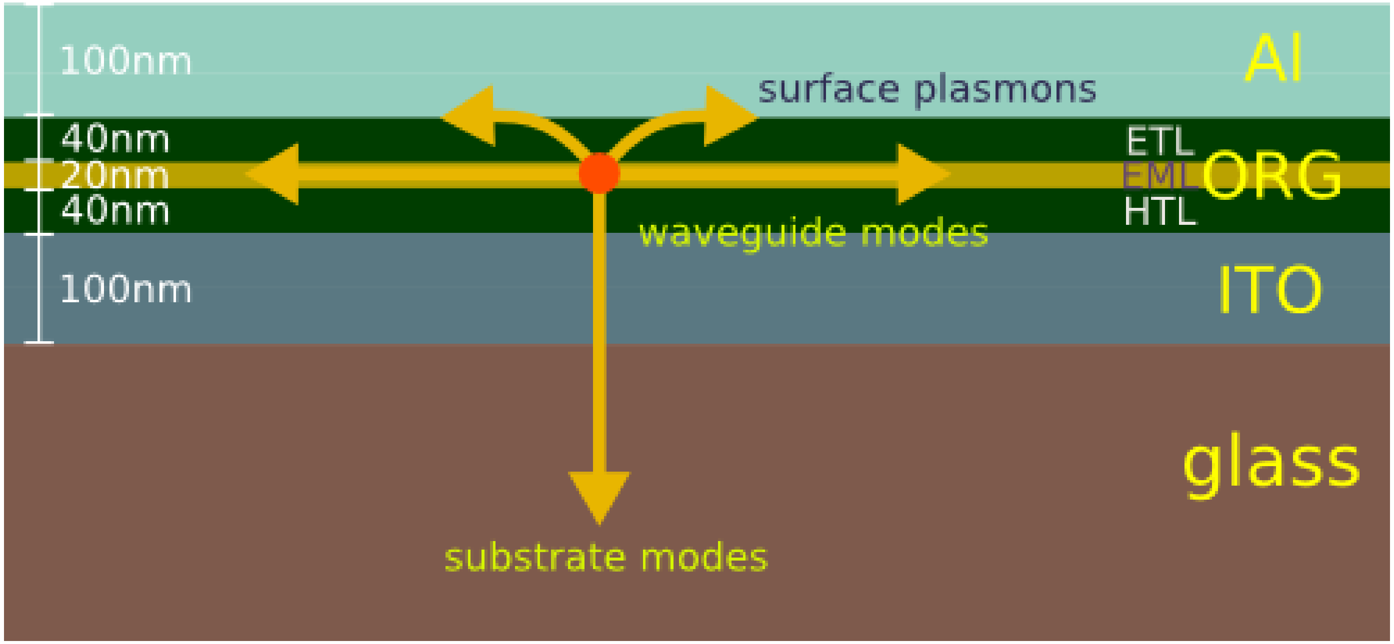
Philips



LG Chem

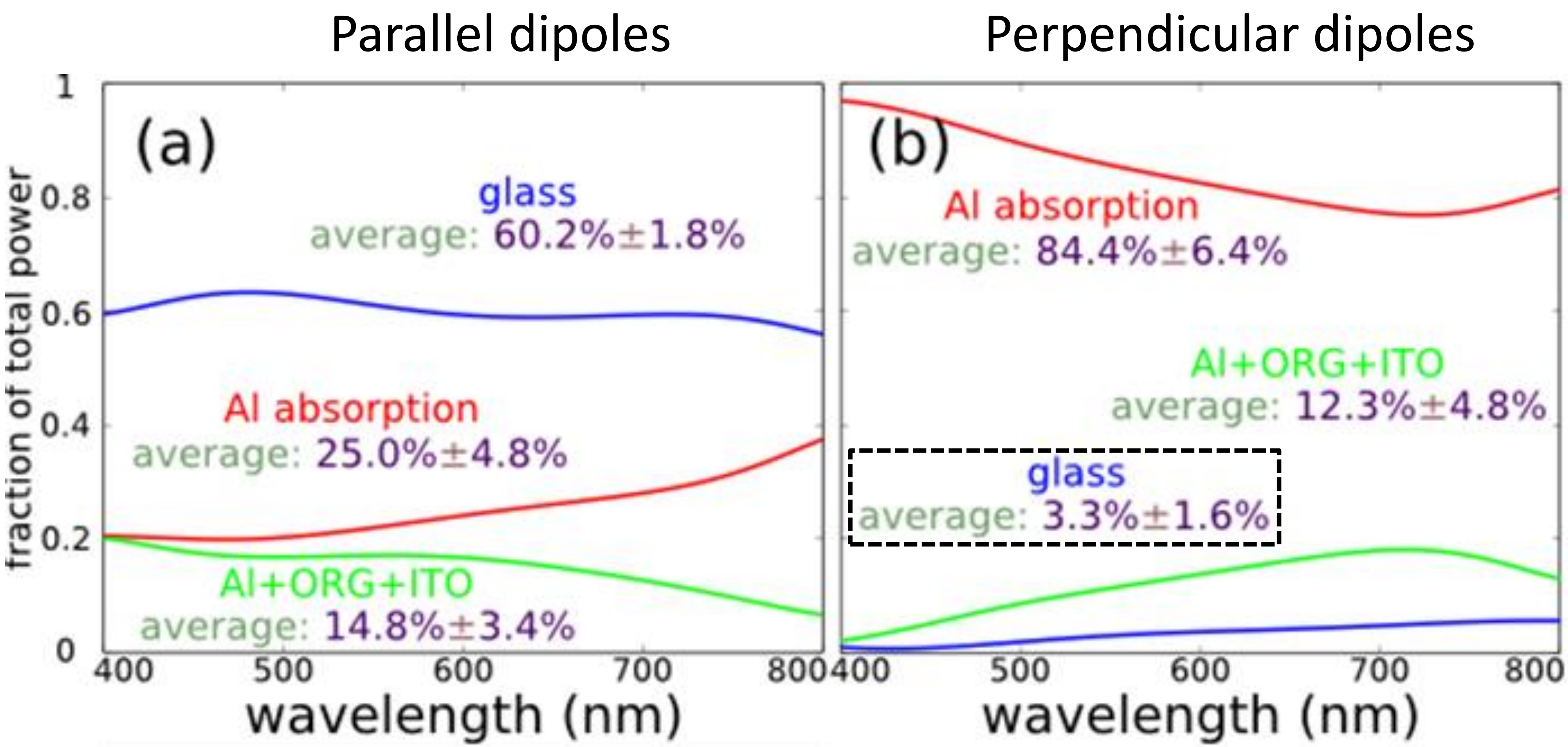
OLED Device Structure and Operation

Electrons injected from Al cathode, holes from ITO anode. Charges reach emissive layer (EML) and form excitons (bound states of electrons & holes) which spontaneously recombine to emit photons. Extracted light emerges through the glass substrate.



Primary limitation to external quantum efficiency is light extraction which is dominated by losses due to surface plasmons at the metal/organic interface

Low Light-Extraction in a Planar OLED

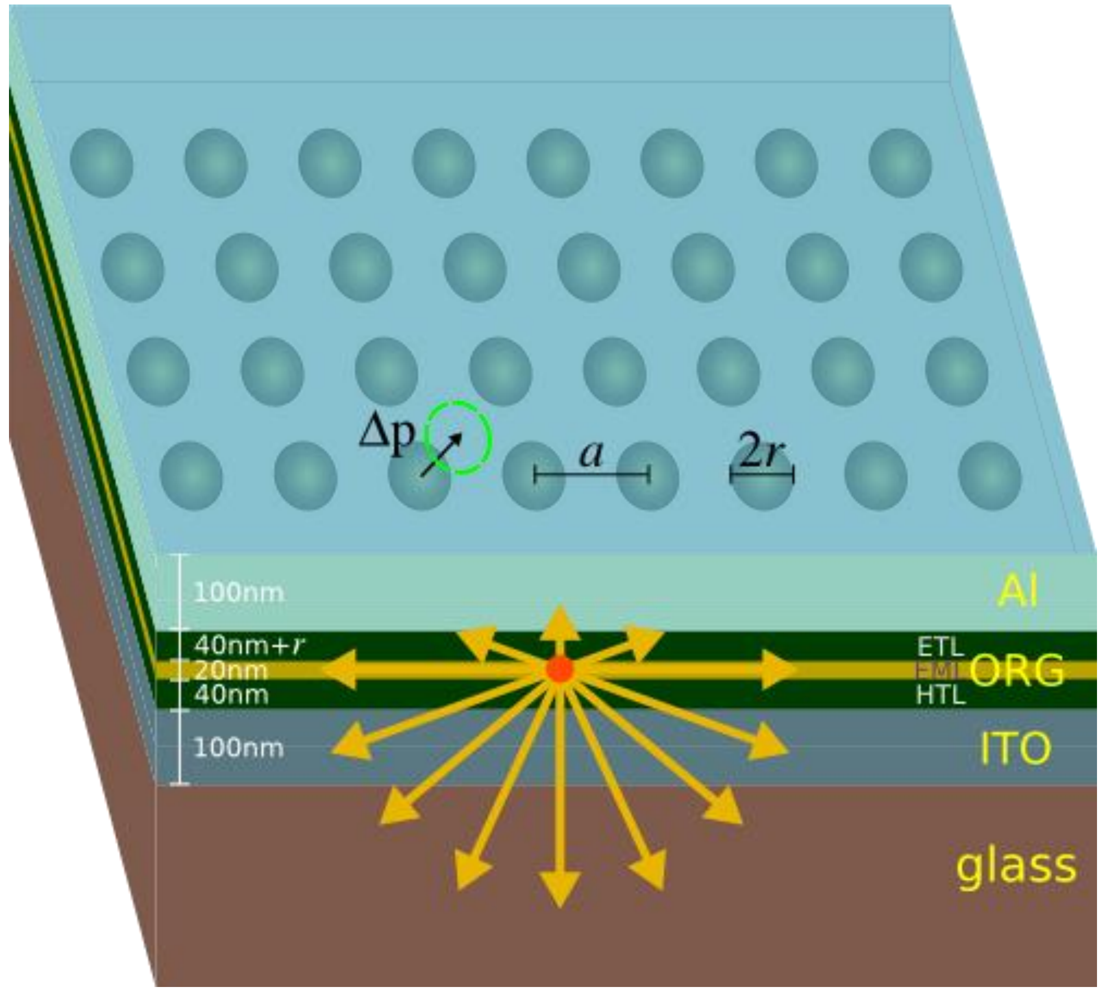


Losses in the metal cathode due to surface plasmons are dominant, particularly for the *perpendicular* dipoles which degrades light extraction

A. Oskooi, *Applied Physics Letters*, **106**, 041111 (2015)

Texturing the Cathode of OLEDs using a Lattice of Nanoscale Scatterers

objective:
find a cathode texture that enhances both light-extraction efficiency *and* exciton radiative-recombination rate



Key Texture Parameters

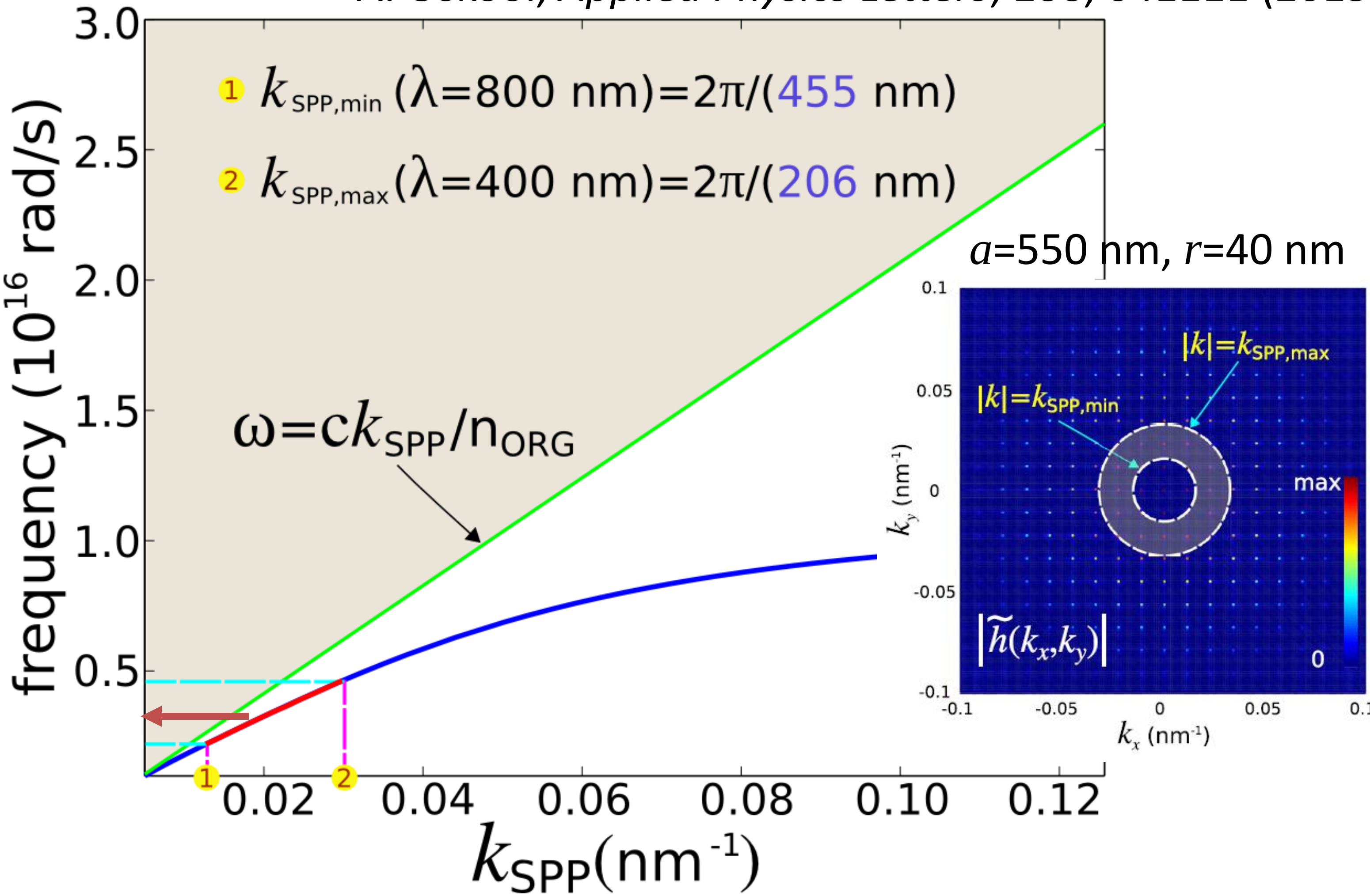
- lattice periodicity
- scatterer morphology
- degree of disorder

organic layers can be textured using hard or soft stamps

A. Oskooi, *Applied Physics Letters*, **106**, 041111 (2015)

Scattering Surface-Plasmon Polariton Modes Out from the Cathode Surface

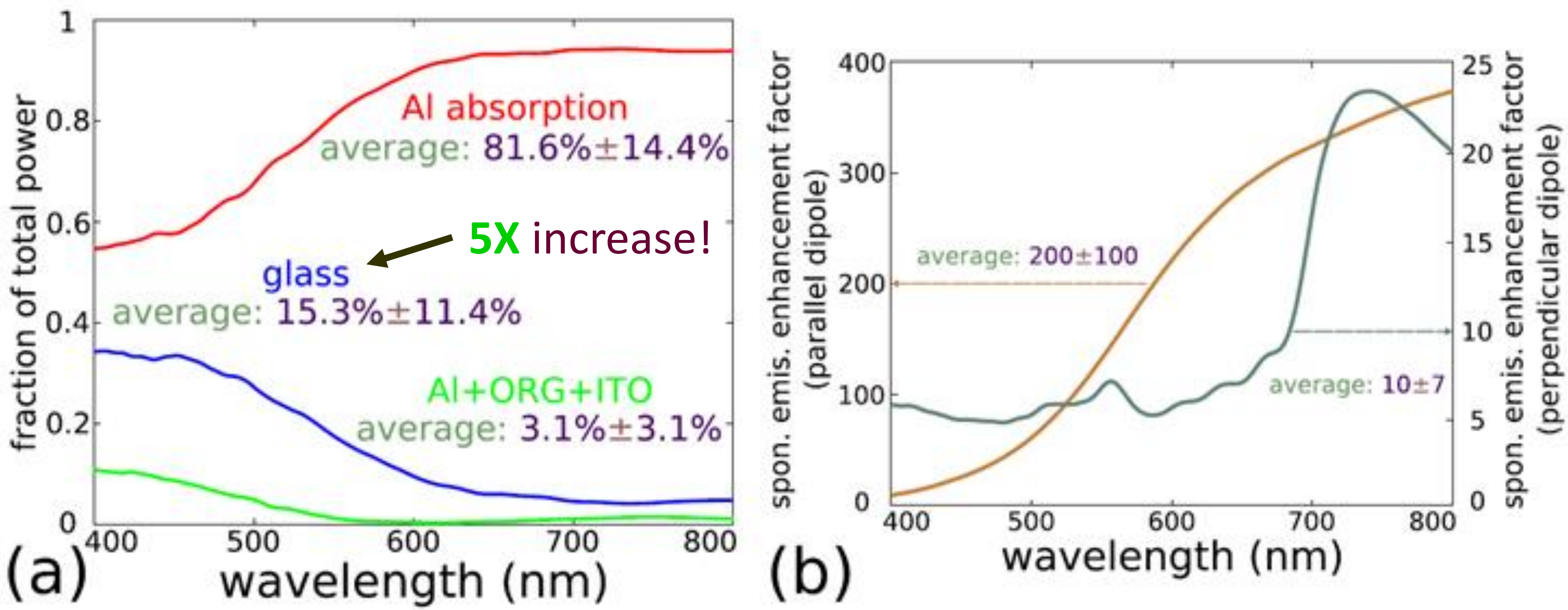
A. Oskooi, *Applied Physics Letters*, **106**, 041111 (2015)



An effective texture at the cathode surface should scatter *all* SPP modes into a normal direction: Fourier transform of texture should span *all* k_{SPP}

Cathode-Textured OLED Boosts Light Extraction

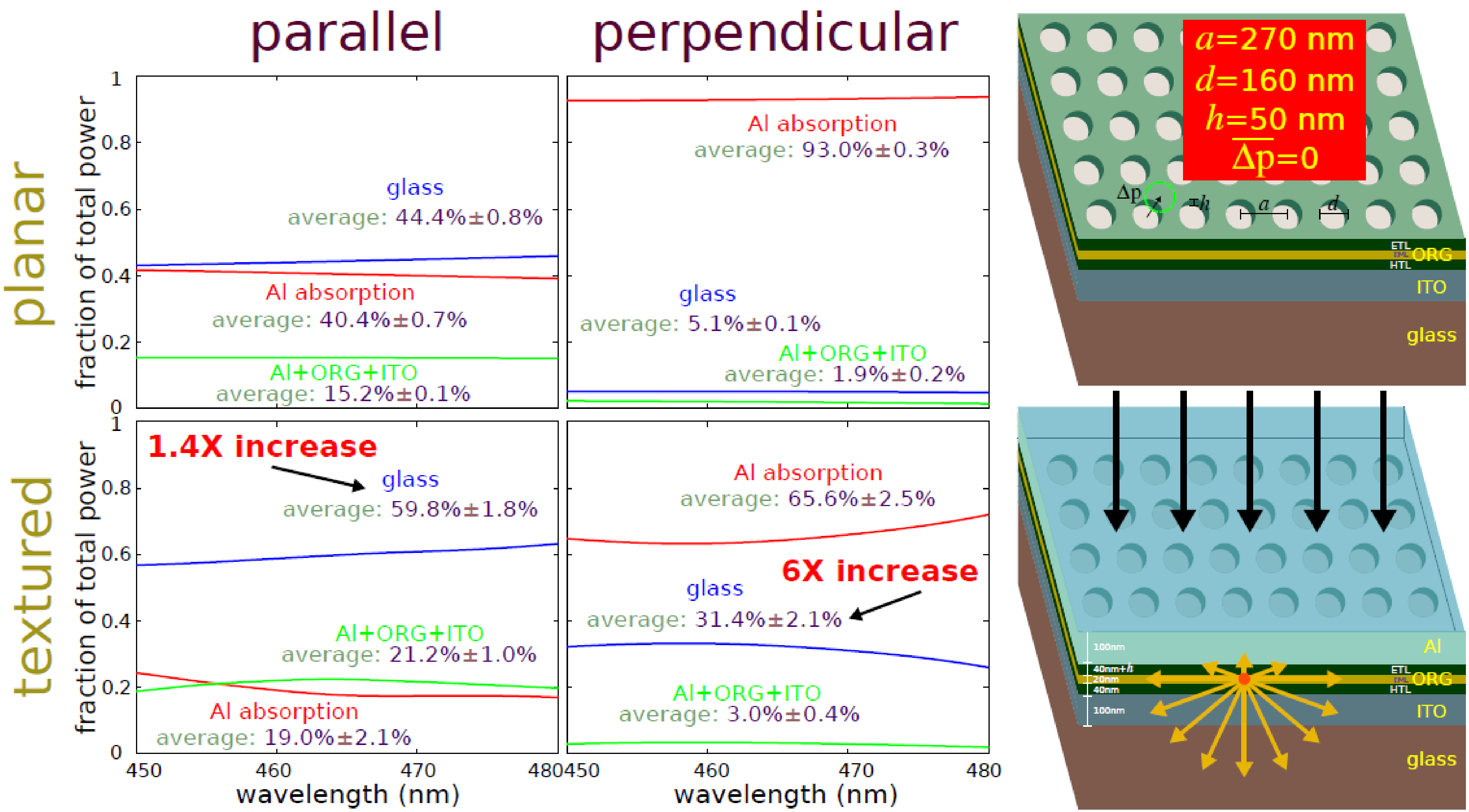
2D lattice of hemispheres protruding into organic film:
a=550 nm, r=40 nm, no disorder



…faster excitons may lead to increase in device lifetime

A. Oskooi, *Applied Physics Letters*, **106**, 041111 (2015)

Large, Uniform Light Extraction for Blue OLED



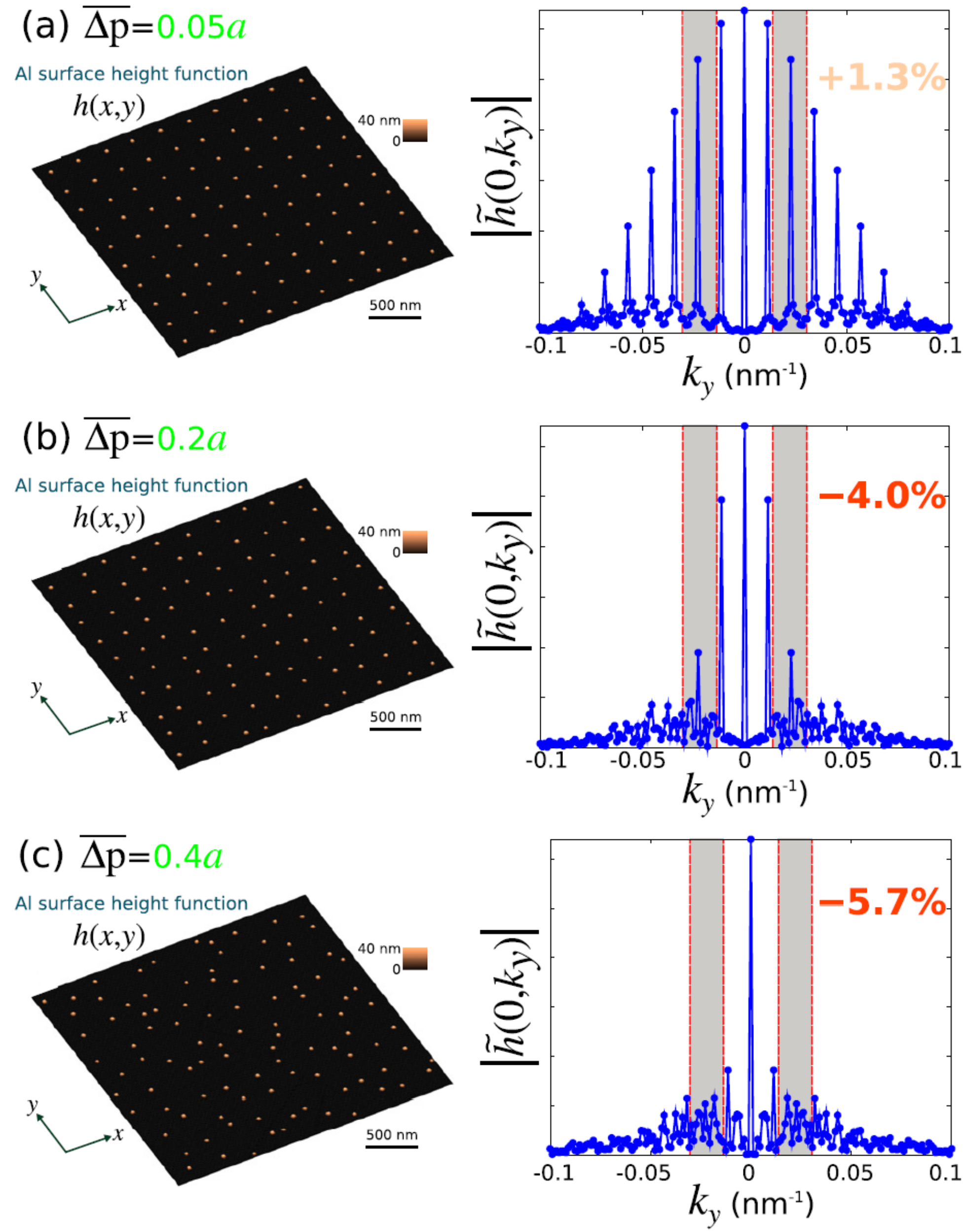
enhanced radiative recombination rate could boost overall device **lifetime**

Effect of Disorder on Light Extraction

Partial disorder maximizes light-extraction efficiency by *broadening* texture's spectral peaks leading to *enhanced scattering* of surface plasmons...

...but too much disorder eliminates spectral peaks and degrades performance.

single MEEP simulation required 180 cores & ~10 hours on Stampede cluster at Texas Advanced Computing Center



A. Oskooi, *Applied Physics Letters*, **106**, 041111 (2015)

Leveraging Advances in
Computational Electrodynamics to
Enable New Kinds of Nanophotonic Devices

New Opportunities for
Large-Scale Device Design using
High-Performance Computing
In the Public Cloud

The Commercial Opportunity

Limitations of Current Simulation Software

1. Restrictive and Expensive Licenses

- fixed term, per seat/core; "*more you use, more you pay*"

2. Steep Learning Curve to Leverage Full Capabilities of Tool

- flashy GUI makes it easy to believe results are meaningful

3. Difficult to Customize and Integrate with Third-Party Software

- cannot "look under the hood" to hack code, proprietary formats

4. Require Significant Hardware Investment to Deploy Large Simulations

- build up and maintain on-site infrastructure; not scalable

Our focus is to challenge this existing paradigm by providing simulation software that is accessible, easy to use, and in sync with today's pervasive, scalable, and low-cost HPC

Simpetus Company Profile

- Launched in August 2015; commercializing 10+ years of MIT graduate research in computational electromagnetics
- Based in San Francisco, CA
- Seed Funding: NSF SBIR Phase I ($225K) and Phase II ($750K)
- **What We Provide: Simulations as a Service**
  - Under Development: Automated Simulation Platform powered by Machine Learning, Cloud HPC, & State-of-the-Art EM Solvers
  - Consulting Services for Photonics Design & Modeling
- Clients include R&D groups in industry & academia
- Founding Team:
  - CEO: Ardavan Oskooi (Sc.D., MIT)
  - CTO: M.T. Homer Reid (Ph.D., MIT)
  - Chief Scientist: Steven G. Johnson, Prof. of Applied Math & Physics, MIT
- **Open-Source Physics Engines**
  - MEEP (finite-difference time-domain)
  - MPB (planewave-expansion mode solver)
  - SCUFF (boundary-element integral equation solver)

Simulations as a Service

How We Enhance Our Clients' R&D

- provide **custom**, **turn-key** simulation modules for *any* application; input are device parameters, rest is automated
- modules integrated with **nonlinear optimization** libraries to enable large-scale design involving 100s of parameters
- design and prototype **robust** devices that are insensitive to intrinsic variations in fabrication or operating conditions
- provide **technical support** for suite of simulation tools with typical response times of less than 24 hours
- offer hands-on **workshops**, **training sessions**, and **code review** on site or remotely
- assist with **deploying simulations** using on-site cluster and/or public cloud with focus on maximizing job throughput
- **enterprise platform with machine learning under development**

Cloud Computing for Research & Development

- rent virtual machines for pennies per hour via AWS EC2 spot instances
- on-demand access, pay only for resources used, size cluster for any application, re-size on the fly
- eliminates need for costly on-site hardware acquisition and maintenance

Open Source Provides Flexibility to
Leverage Full Capabilities of Cloud-Based HPC

Summary

1. **Enhancements to Core Capabilities of FDTD**
   - *Sub-pixel Smoothing of Dielectric Interfaces*
   - *Absorbing Boundary Layers for Inhomogeneous Media*

2. **MEEP: A Flexible Free-Software Package for Electromagnetic Simulations by the FDTD method**

3. **New Kinds of Nanophotonic Devices**
   - *Light Trapping in Silicon Thin Films for Enhanced Solar Cells*
   - *Light Extraction from Organic Light-Emitting Diodes for Energy-Efficient Displays and Solid-State Lighting*

4. **New Opportunities for Large-Scale Device Design using High-Performance Computing (HPC) in the Public Cloud**

The Future of Computational Electromagnetics promises many more interesting things to come!

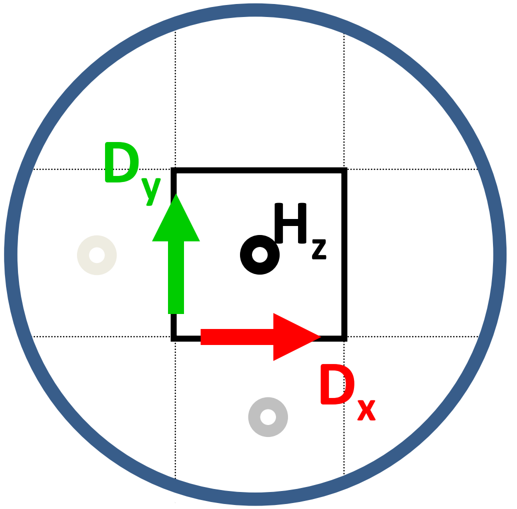
extra slides

FDTD: Leapfrog Algorithm

1) at time t: Update **D** fields everywhere using spatial derivatives of **H**, then find $\mathbf{E}=\varepsilon^{-1}\mathbf{D}$

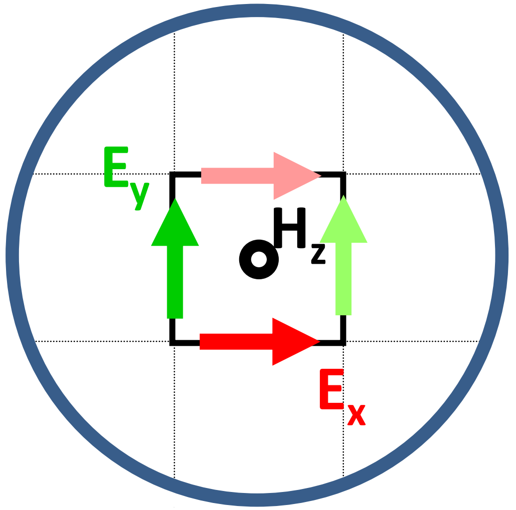
$$D_x \mathrel{+}= \frac{\Delta t}{\Delta y}\left(H_z^{j+0.5} - H_z^{j-0.5}\right)$$

$$D_y \mathrel{-}= \frac{\Delta t}{\Delta x}\left(H_z^{i+0.5} - H_z^{i-0.5}\right)$$



2) at time t+0.5: Update **H** fields everywhere using spatial derivatives of **E**

$$H_z \mathrel{+}= \frac{\Delta t}{\mu}\left(\frac{E_x^{j+1} - E_x^{j}}{\Delta y} + \frac{E_y^{i} - E_y^{i+1}}{\Delta x}\right)$$



Challenges

- Accuracy requires high resolution (small Δx, Δy, Δz)
- Small Δx, Δy, Δz forces small Δt (Courant stability)
- Many time-steps required for high-frequency resolution (Fourier Uncertainty)
- Modeling objects with complex shapes and geometries

PMLs in Maxwell's Equations

An ordinary PML in Cartesian co-ordinates is derived by a complex co-ordinate stretching of MEs, where each co-ordinate is stretched by a factor:

$$s_{x,y,z} = 1 + \frac{i\sigma_{x,y,z}}{\omega}$$

$\sigma > 0$ is the PML "**conductivity**"

*the **absorption profile σ** is the key to reducing reflections from discretization*

Using transformation optics, co-ordinate stretching can be absorbed into MEs as a change in both ε and μ:

$$\varepsilon' = \frac{\mathcal{J}\varepsilon(\omega)\mathcal{J}}{\det \mathcal{J}} \qquad \mu' = \frac{\mathcal{J}\mu(\omega)\mathcal{J}}{\det \mathcal{J}}$$

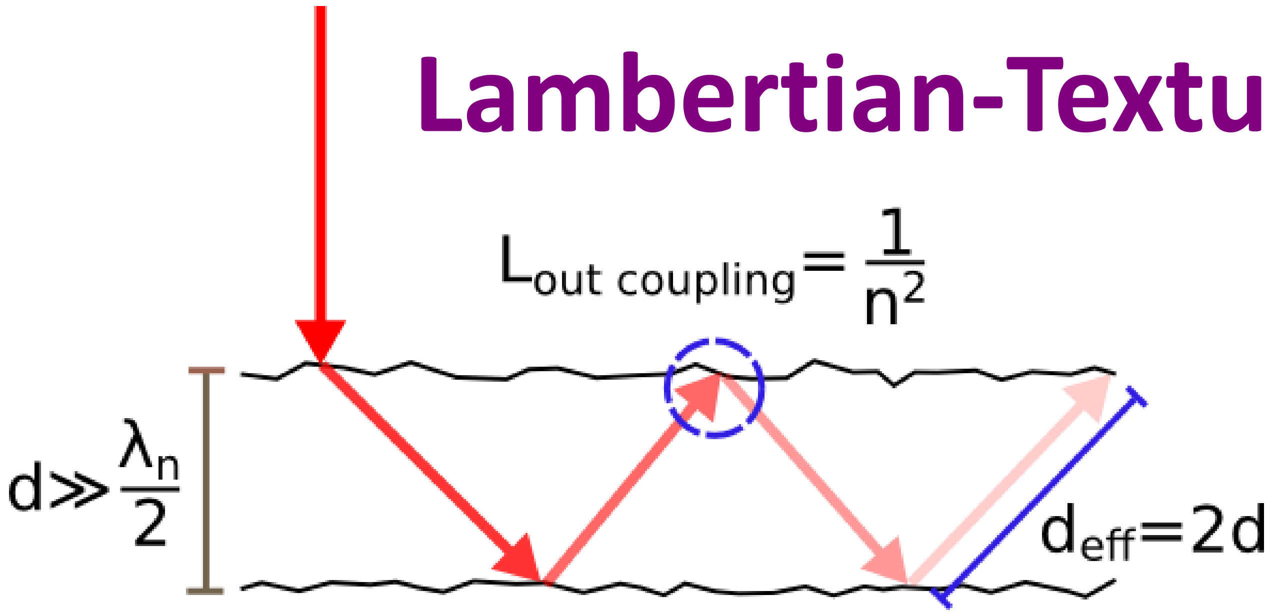
Jacobian matrix of co-ordinate stretching

$$\mathcal{J} = \mathrm{diag}\left(s_x^{-1}, s_y^{-1}, s_z^{-1}\right)$$

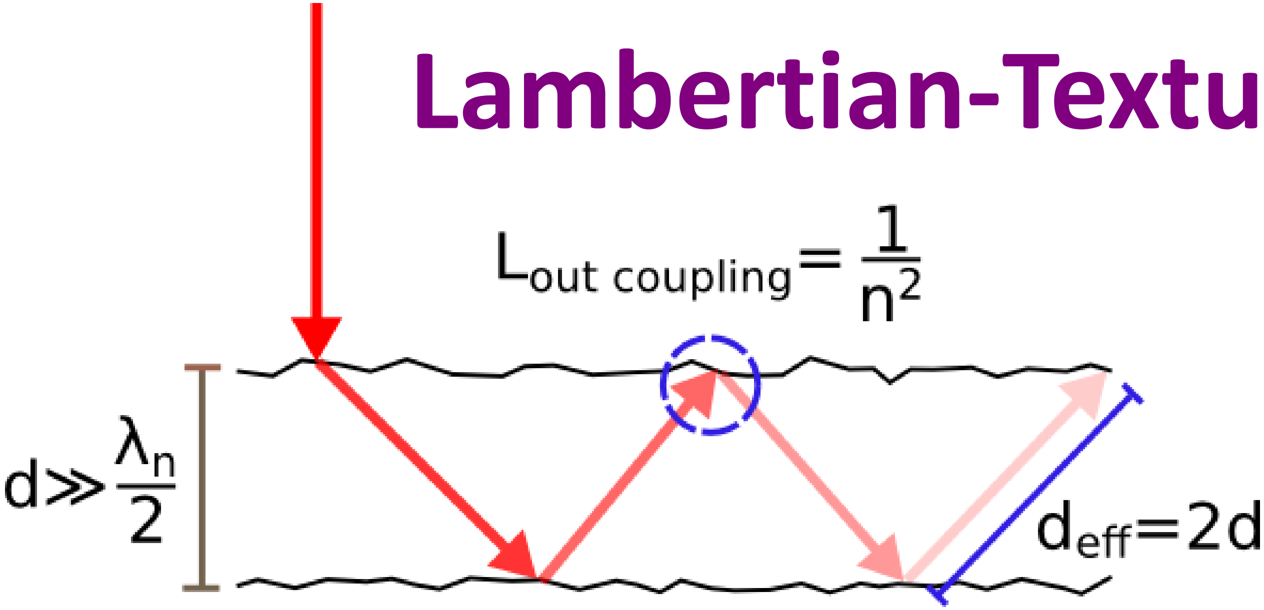
A.J. Ward & J.B. Pendry, *J. Mod. Optics*, **43**, pp. 773-93 (1996)

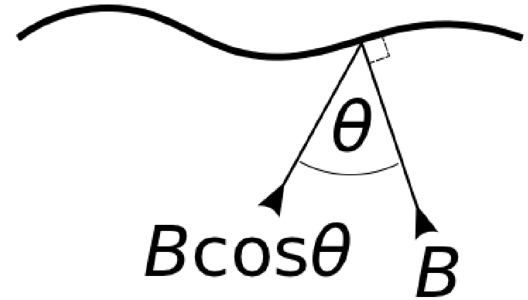
PML is very successful for absorbing waves in homogeneous media but…

Lambertian-Textured Film



Lambertian-Textured Film



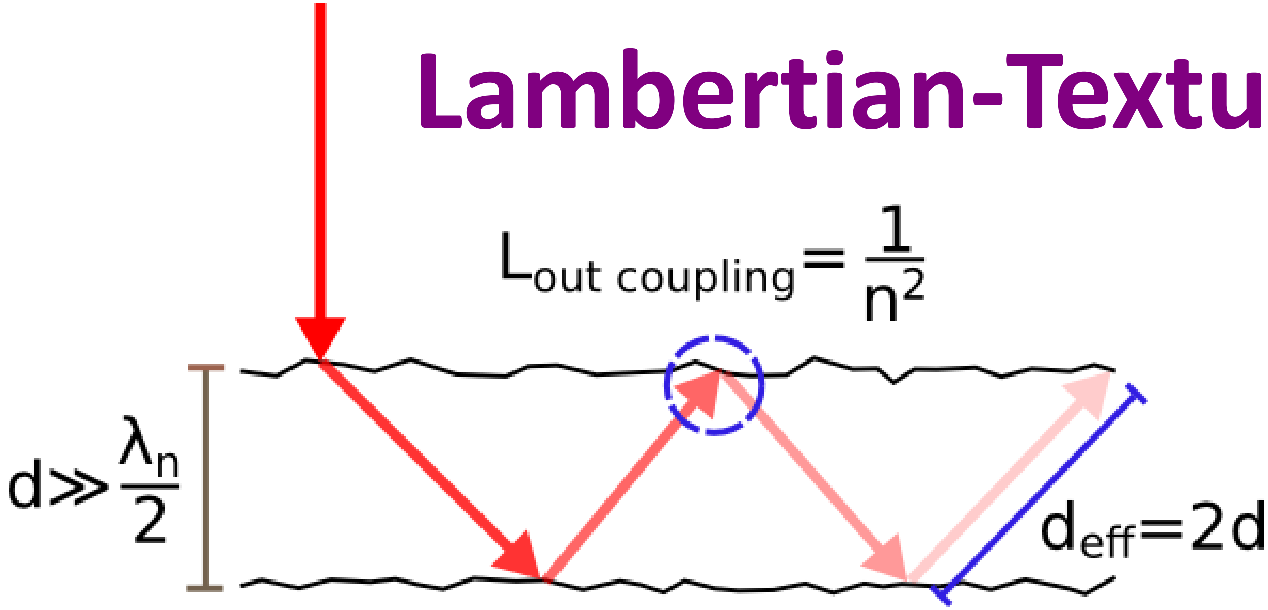


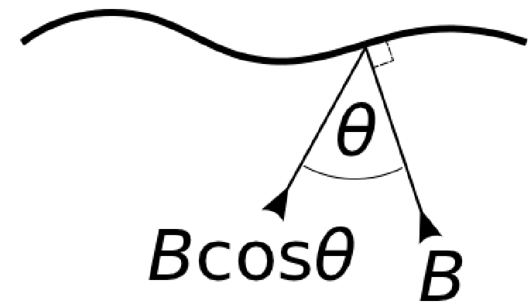
B: internal light intensity

$$d_{eff} = \frac{\int_0^{\pi/2} \frac{d}{\cos\theta} \cos\theta \sin\theta d\theta}{\int_0^{\pi/2} \cos\theta \sin\theta d\theta} = 2d \qquad L_{out-coupling} = \frac{\int_0^{\theta_c} B\cos\theta \sin\theta d\theta}{\int_0^{\pi/2} B\cos\theta \sin\theta d\theta} = \frac{1}{n^2}$$

P. Campbell & M.A. Green, *J. App. Phys.*, **62**, pp. 243-9 (1987)

Lambertian-Textured Film





B: internal light intensity

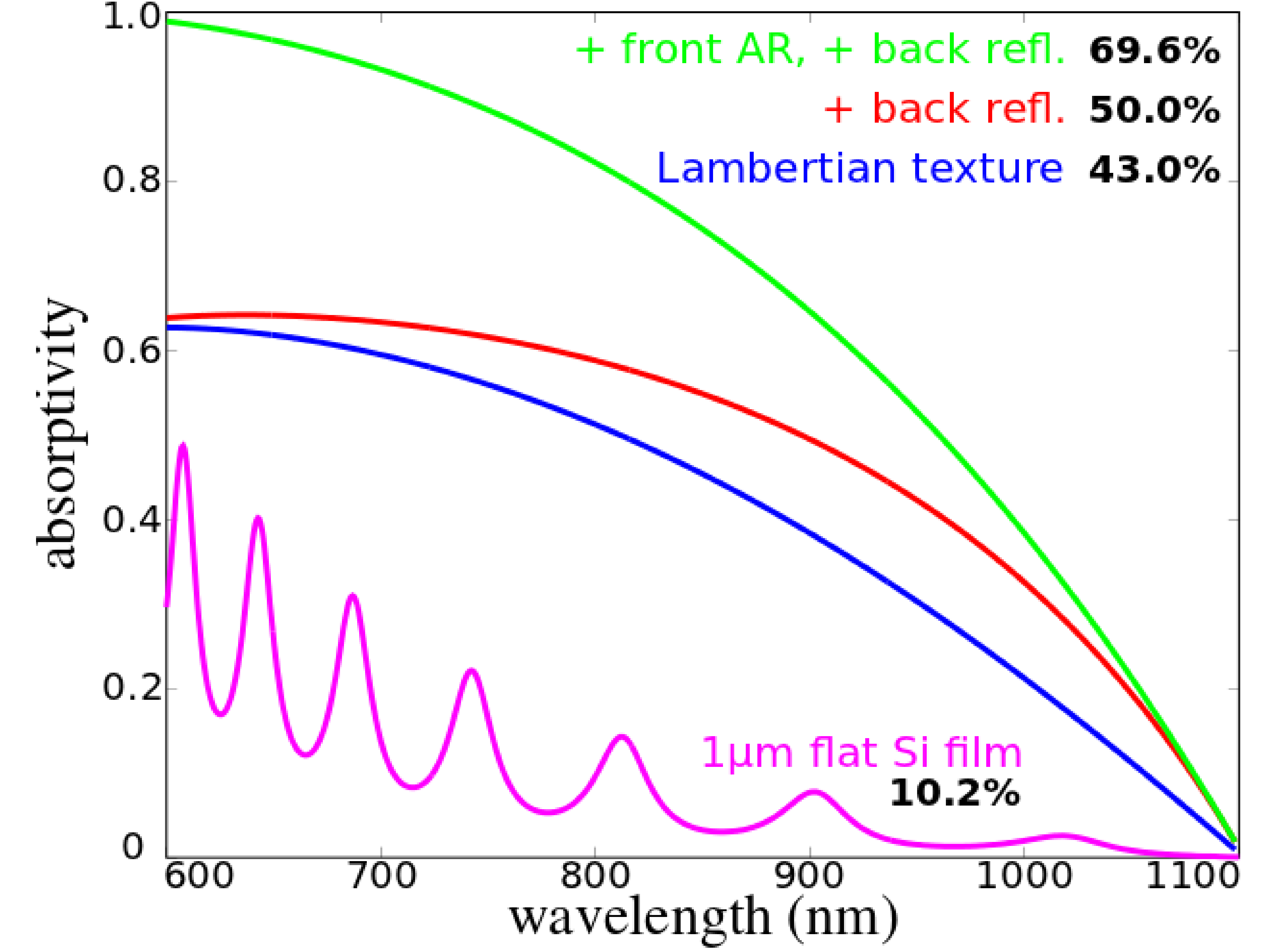
$$d_{eff} = \frac{\int_0^{\pi/2} \frac{d}{\cos\theta} \cos\theta \sin\theta d\theta}{\int_0^{\pi/2} \cos\theta \sin\theta d\theta} = 2d \qquad L_{out-coupling} = \frac{\int_0^{\theta_c} B\cos\theta \sin\theta d\theta}{\int_0^{\pi/2} B\cos\theta \sin\theta d\theta} = \frac{1}{n^2}$$

$$A_{lamb} = T\left(1 - e^{-2\alpha d}\right)\sum_{m=0}^{\infty}\left[e^{-2\alpha d}\left(1 - \frac{1}{n^2}T\right)\right]^m = \frac{T\left(1 - e^{-2\alpha d}\right)}{1 - e^{-2\alpha d}\left(1 - \frac{1}{n^2}T\right)}$$

Fresnel transmission

single-pass absorption

H. W. Deckman, C.B. Roxlo and E. Yablonovitch, *Optics Letters*, **8**, pp. 491-3 (1983)

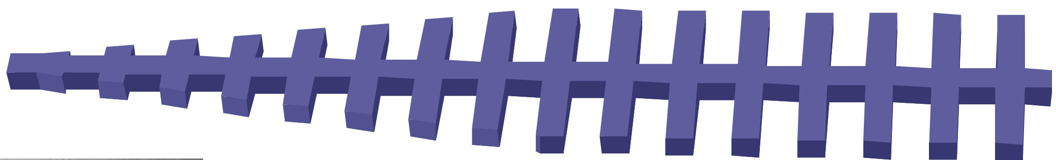


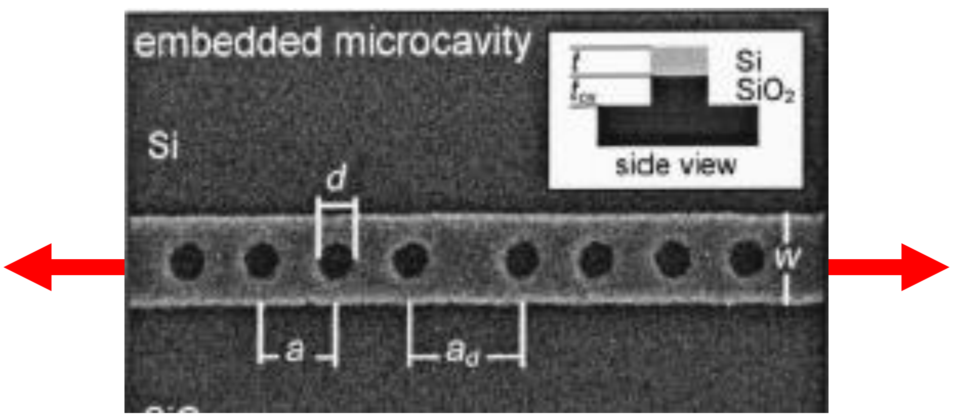
+ front AR, + back refl. 69.6%
+ back refl. 50.0%
Lambertian texture 43.0%
1μm flat Si film
10.2%
absorptivity
wavelength (nm)
1.0
0.8
0.6
0.4
0.2
0
600
700
800
900
1000
1100

A Distinguishing Feature of MEEP: Illusion of Continuity

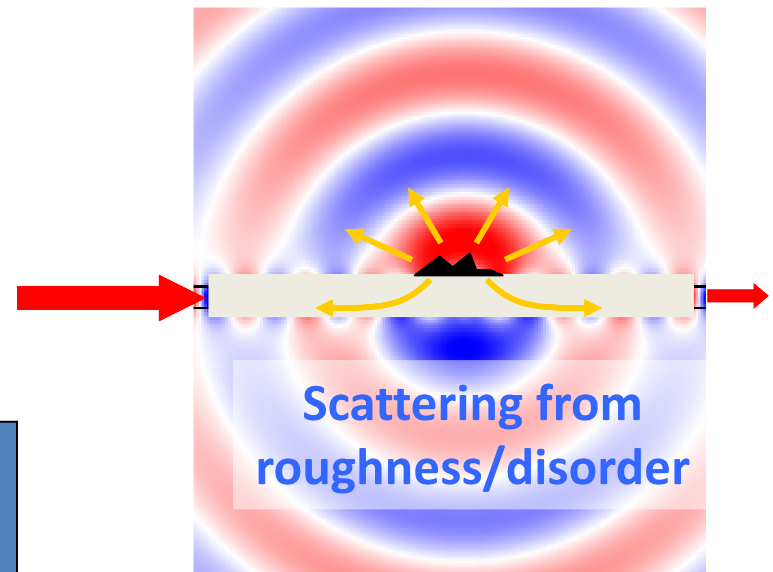
- continuously-varying inputs leads to continuously-varying outputs
- geometric properties (e.g., flux planes, dielectric objects, volume sources)
- important for topology optimization

Slow taper transitions

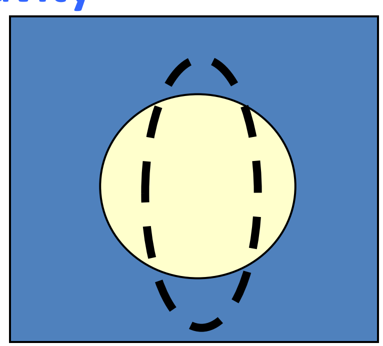




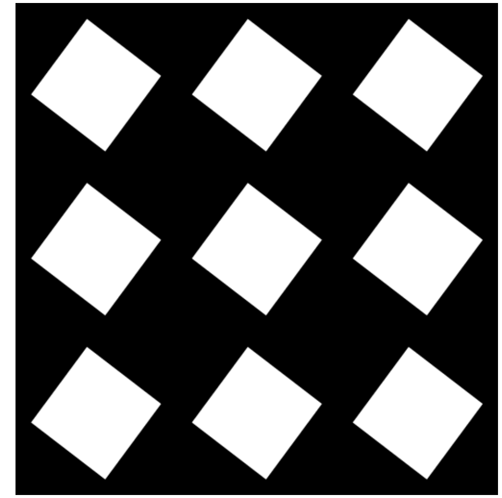
“stretched” microcavity



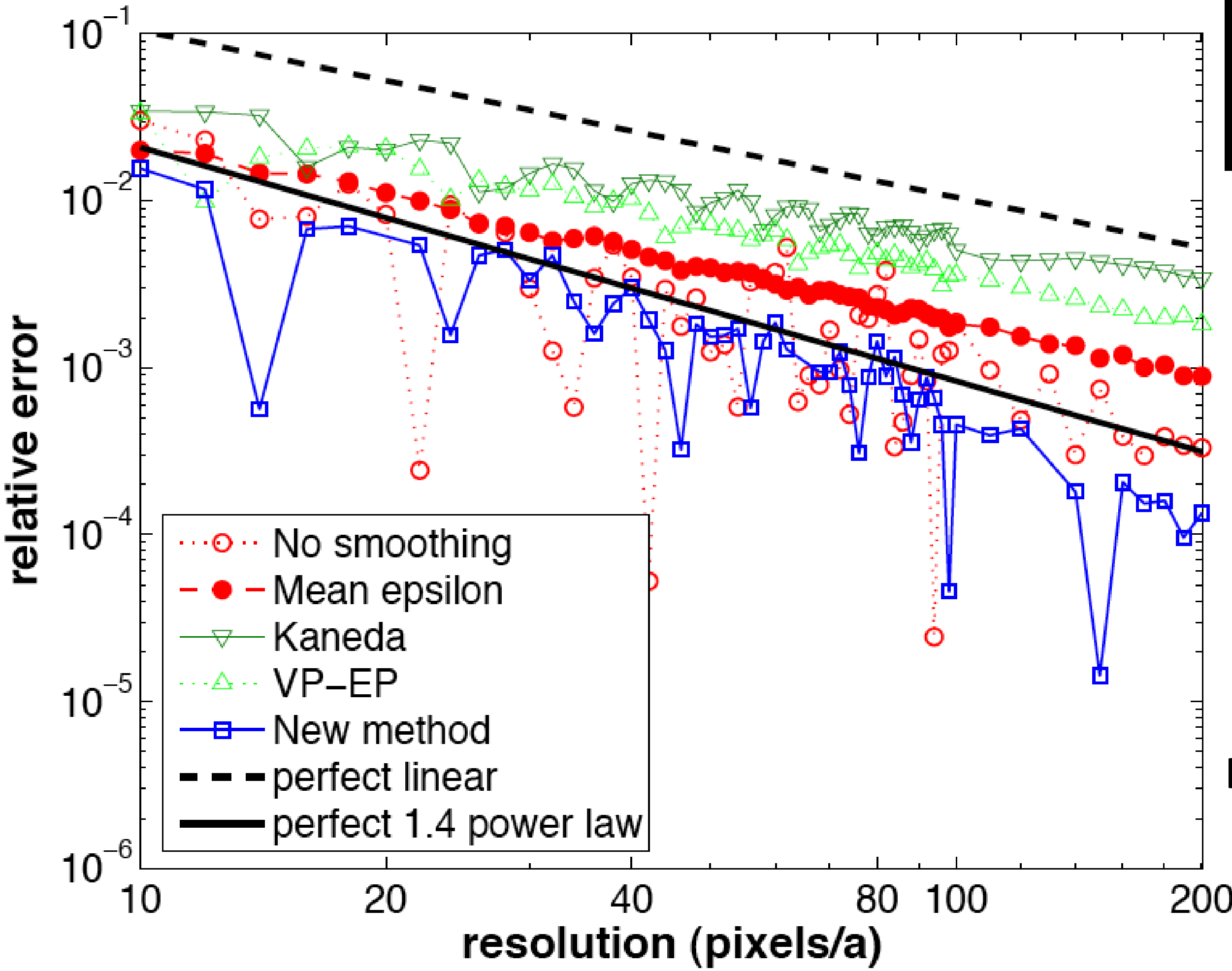
Effect of
deformations



A Qualitatively Different Case: Corners



still lowest error, but **not** quadratic



zero-perturbation criterion *not* satisfied due to **E** divergence at corner analytically, error ~ $\Delta x^{1.4}$

Anderson et al., IEEE T. Ant. Prop. 26, 1978