ECE 695
Numerical Simulations
Lecture 21: Applications of S^4

Prof. Peter Bermel

March 3, 2017

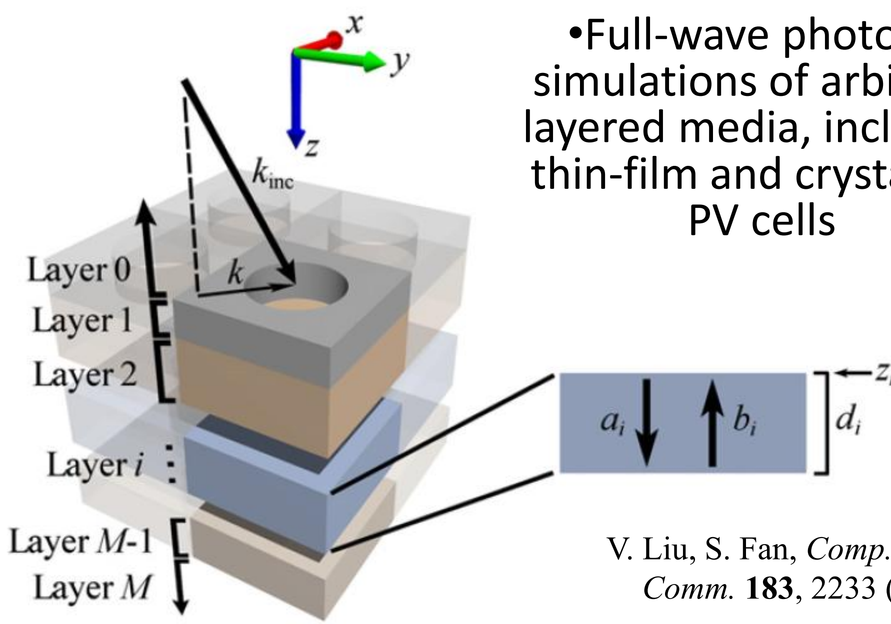
S-Matrix Method: Advantages

- No *ad hoc* assumptions regarding structures
- Applicable to wide variety of problems
- Suitable for eigenmodes or high-*Q* resonant modes at single frequency
- Can treat layers with large difference in length scales
- Computationally tractable enough on single core machines

S-Matrix Method: Disadvantages

- Accurate solutions obtained more slowly as the following increase:
  - Number of layers
  - Absolute magnitude of Fourier components (especially for metals)
  - Number of plane-wave components (~N^3)
- Relatively slow for broad-band problems (time-domain is a good alternative)

Photonic Simulations with S^4



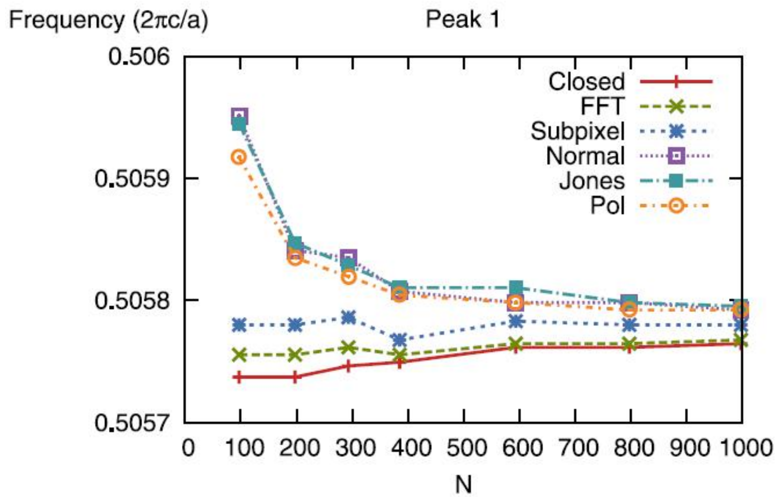
- Full-wave photonic simulations of arbitrary layered media, including thin-film and crystalline PV cells

V. Liu, S. Fan, *Comp. Phys. Comm.* **183**, 2233 (2012)

https://nanohub.org/tools/s4sim/

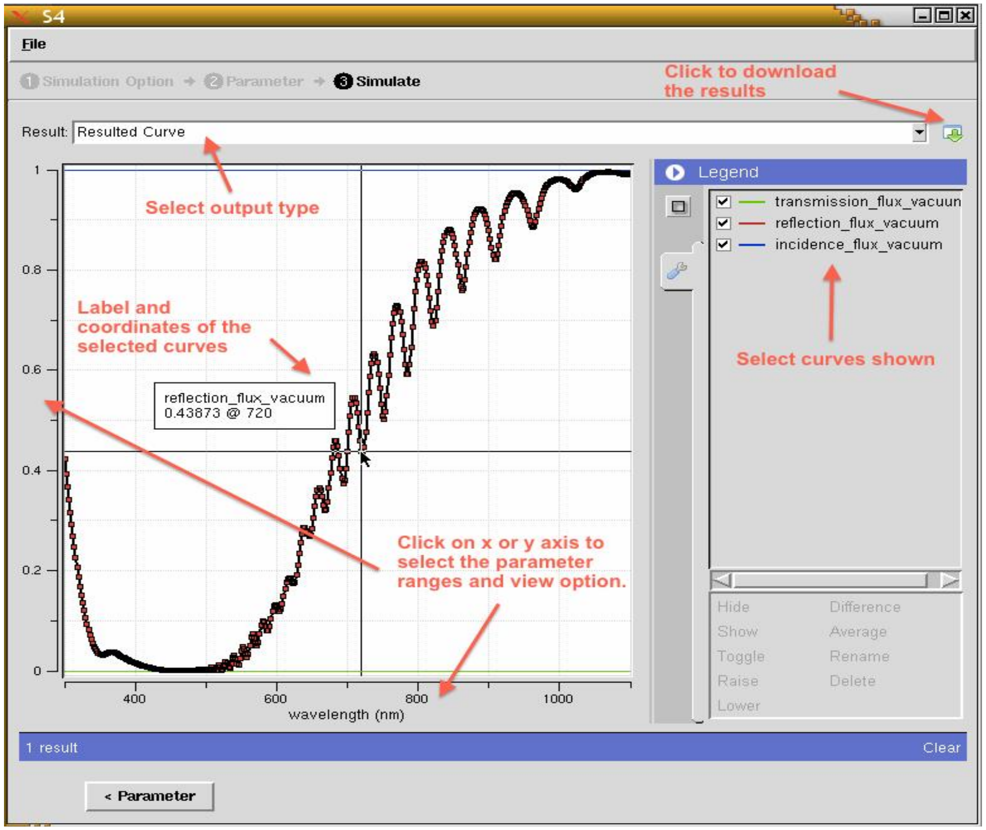
Photonic Simulations with S^4

Accuracy improves systematically
with computing power

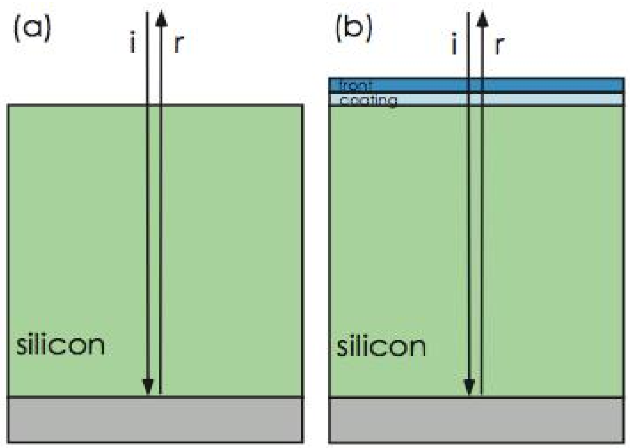


V. Liu, S. Fan, *Comp. Phys. Comm.* **183**, 2233 (2012)

S4sim: Output Window



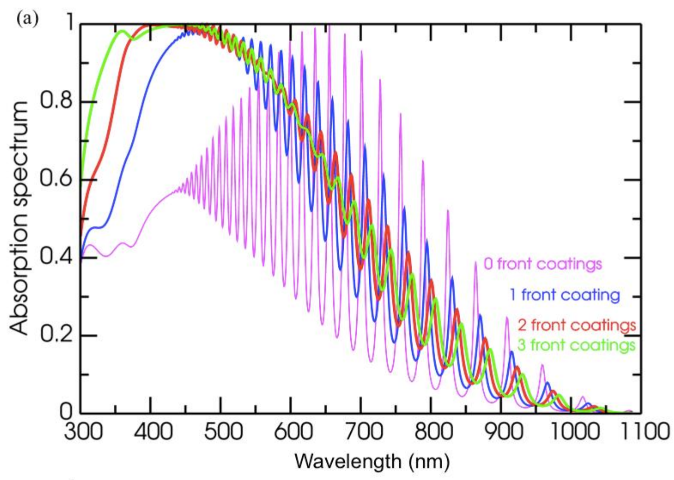
S4sim Example: PV Front Coating



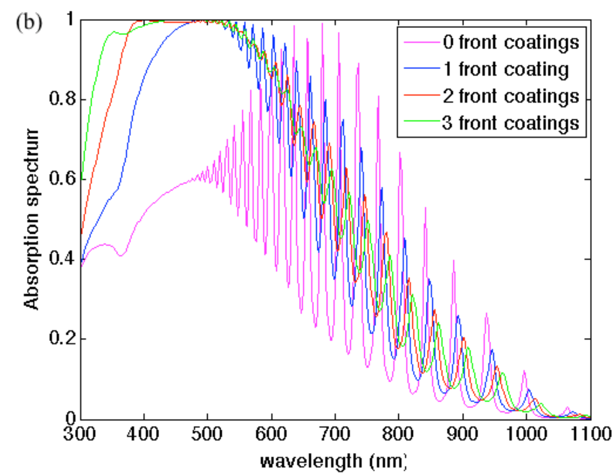
Number of front coating layers	1		2		3	
Relative permittivity	Real	Imag	Real	Imag	Real	Imag
Layer 1	4.32	0	2.37	0	1.80	0
Layer 2			9.12	0	5.71	0
Layer 3					14.36	0

Number of front coating layers	1	2	3
Thickness (nm)			
Layer 1	60	82.3	91.0
Layer 2		38.9	53.1
Layer 3			29.9

S4sim Example: PV Front Coating

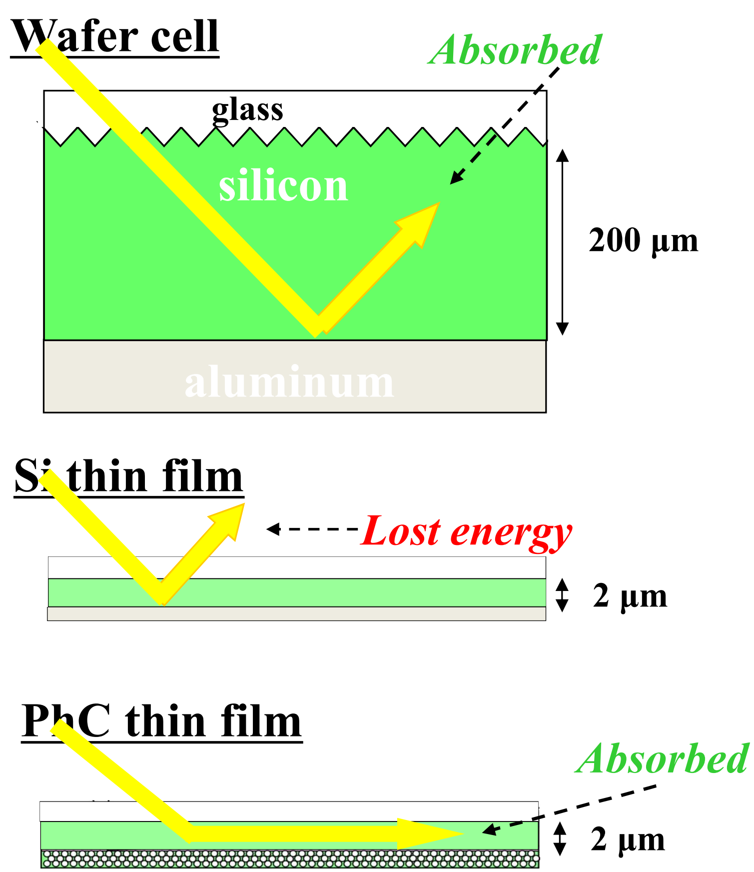


Results from M. Ghebrebrhan, P. Bermel, Y. Avniel, J. Joannopoulos, and S. Johnson, Optics Express 17, 7505-7518 (2009).



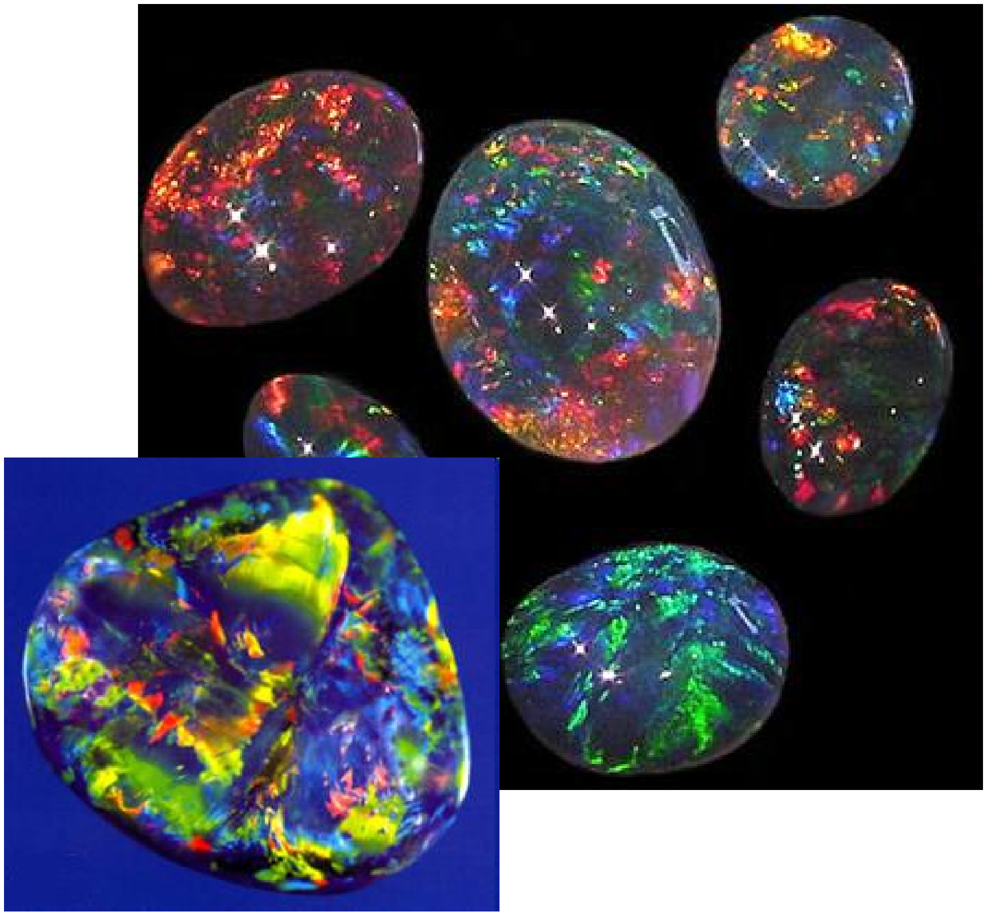
Results generated by S4sim

Application: Improving Solar Cells



Nature was the First…

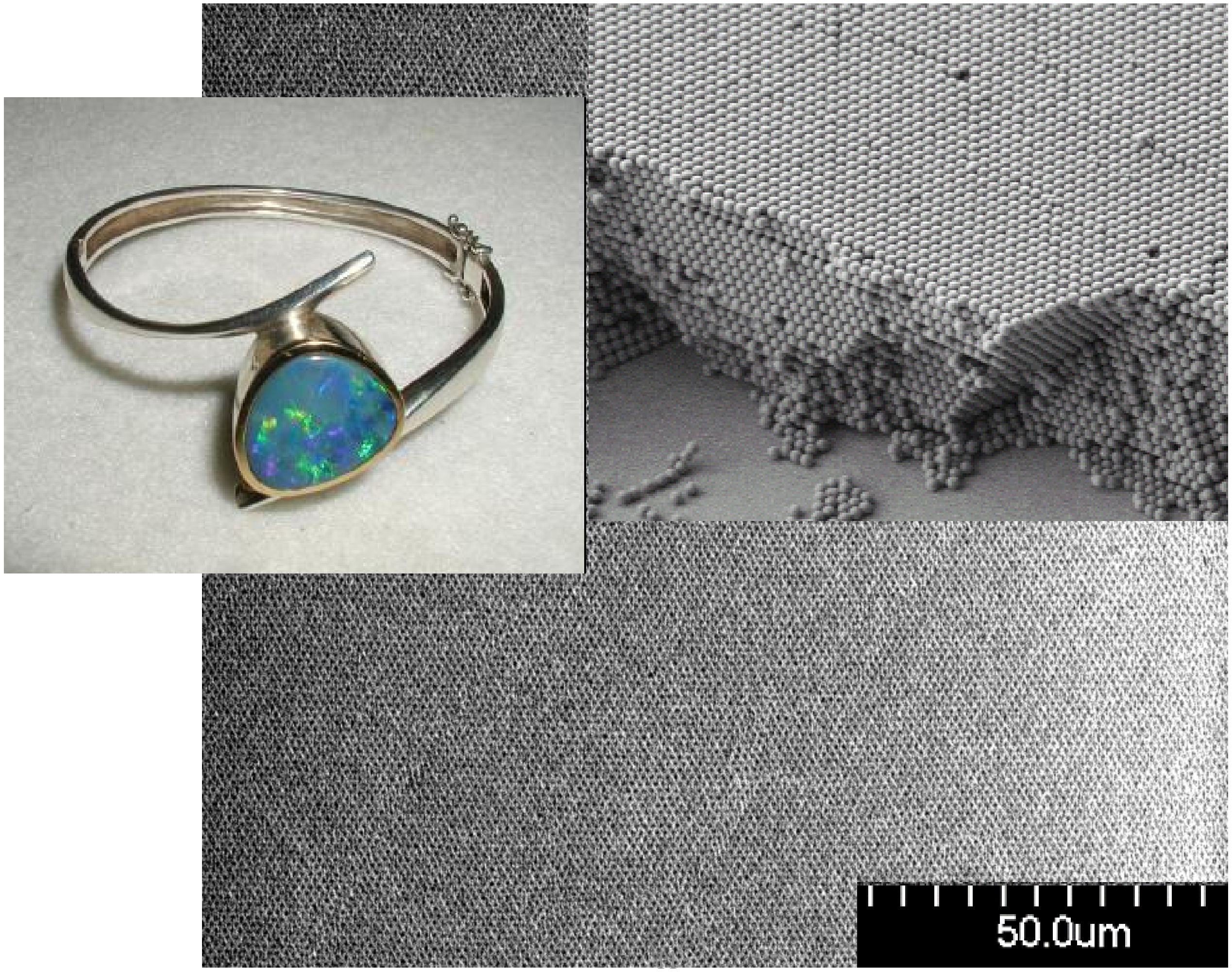
Natural opal



Artificial direct and inverse opals

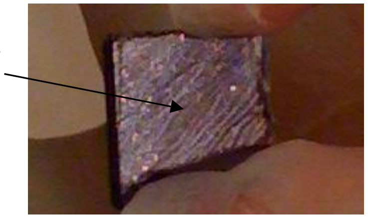
http://www.australianblackopals.com/images
http://www.opals-of-light-and-fire.com/web_images/black-opal-1.jpg

Self-Assembled 3D Photonic Crystal Structures: Opals

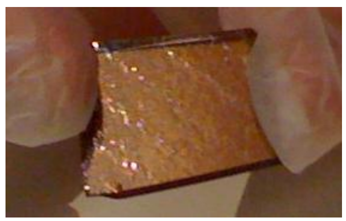


Benefits of Opal PhCs in Solar Cells

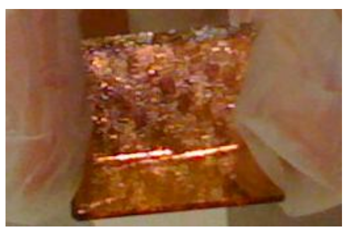
Noticeably darker than controls!



Expt'l cell with texturing and PhC



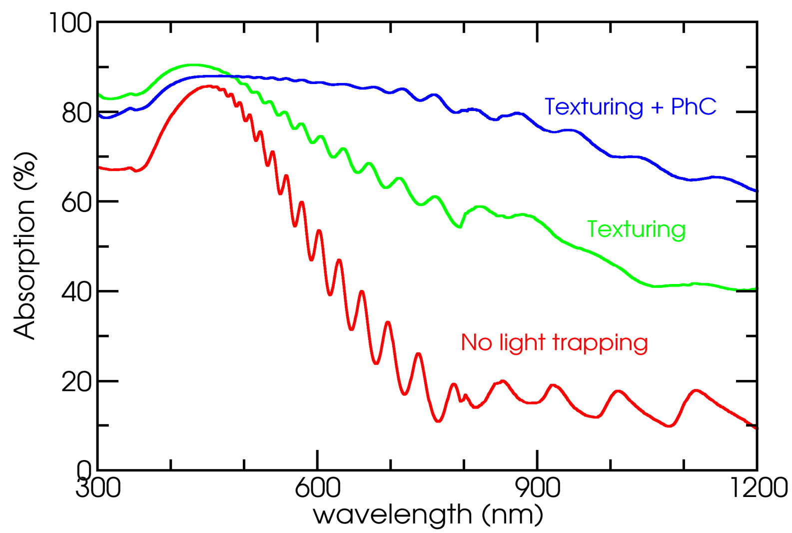
Control cell with texturing



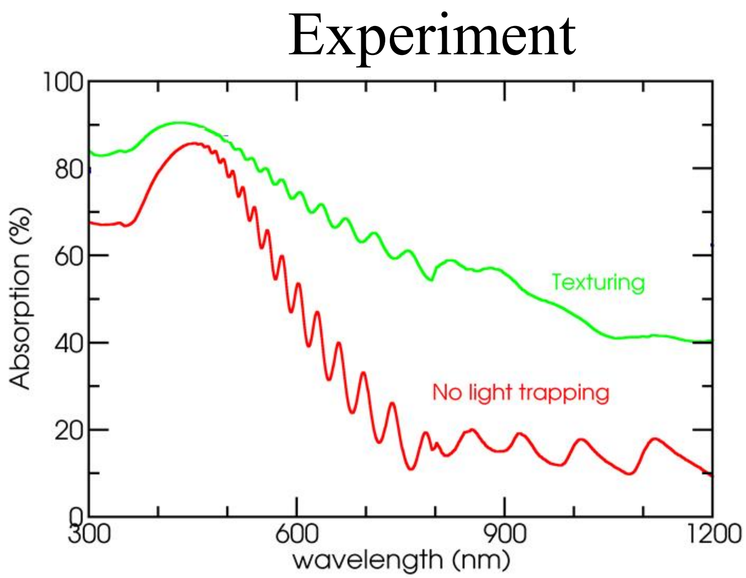
Control cell without light trapping

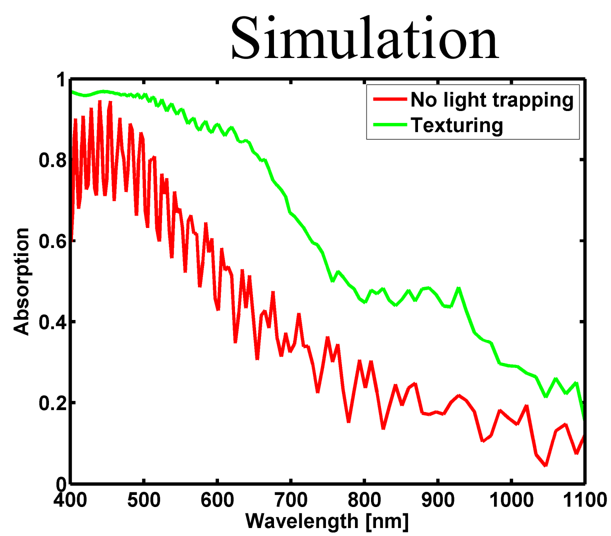
PhC enhanced cell →

30% higher J_{sc} than texturing



Experimental absorption vs simulated absorption





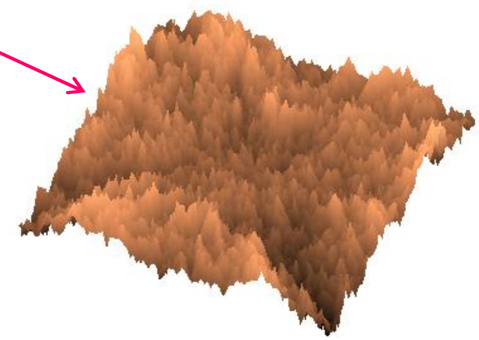
- The left figure indicates the experimental absorption rate for a 1500 nm thick c-Si solar cell. It is adapted from recently published research [4]. The right figure indicates the absorption rate obtained by the simulation.
- 3-D QCRF-FDTD simulation is performed using the same geometry in order to prove its accuracy

[4] 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).

Random surface texturing algorithm

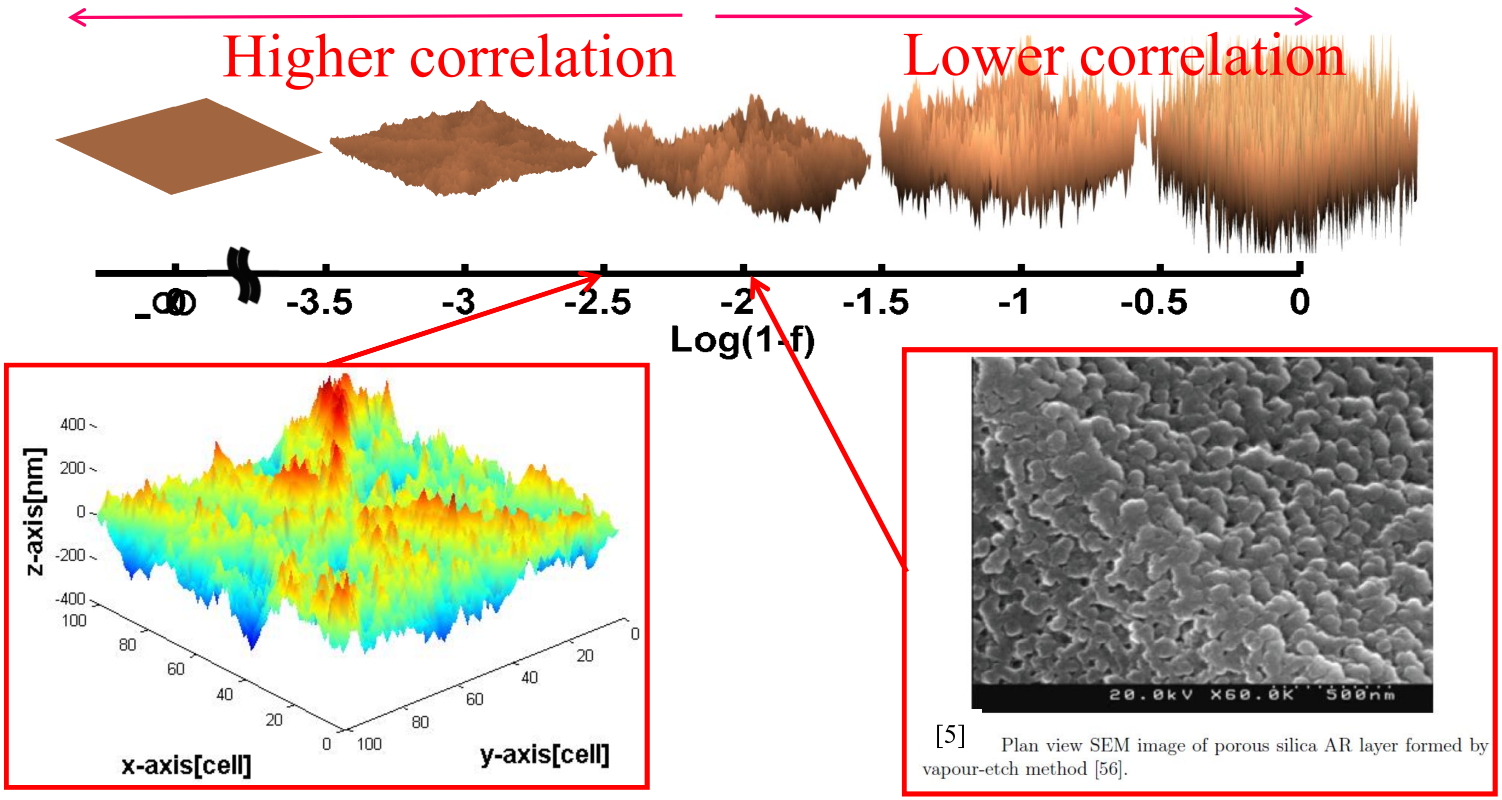
$$Z_{n+1} = f * Z_n - \sqrt{1 - f^2} * r_n$$

- Where $Z_1 = r_1$, r_n is an independent sampling from a random distribution of Gaussian variables with zero mean and unit variance.
- We expended this algorithm to 2-D and applied periodic boundary condition for each edge.
- Add double-sided correlation equation



- Two variables:
  - Maximum texturing height
  - Correlation factor

From the flat structure to the totally random structure via random surface texturing algorithm



[5] Plan view SEM image of porous silica AR layer formed by vapour-etch method [56].

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

Refraction: Epsilon Near Zero

Image of a swimming pool filled with water (n=1.33) (computer-generated)

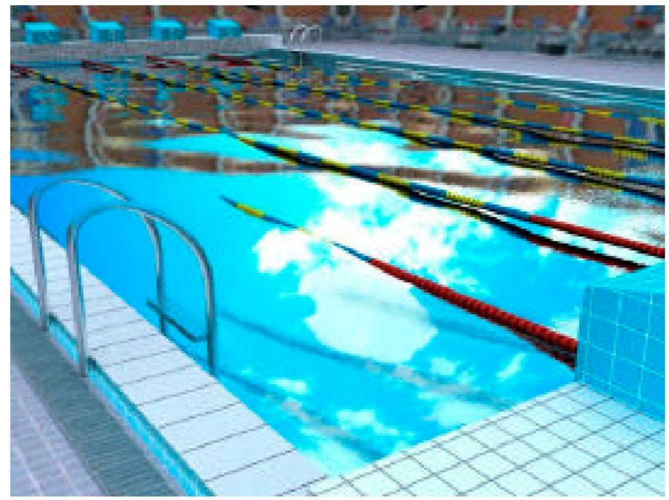
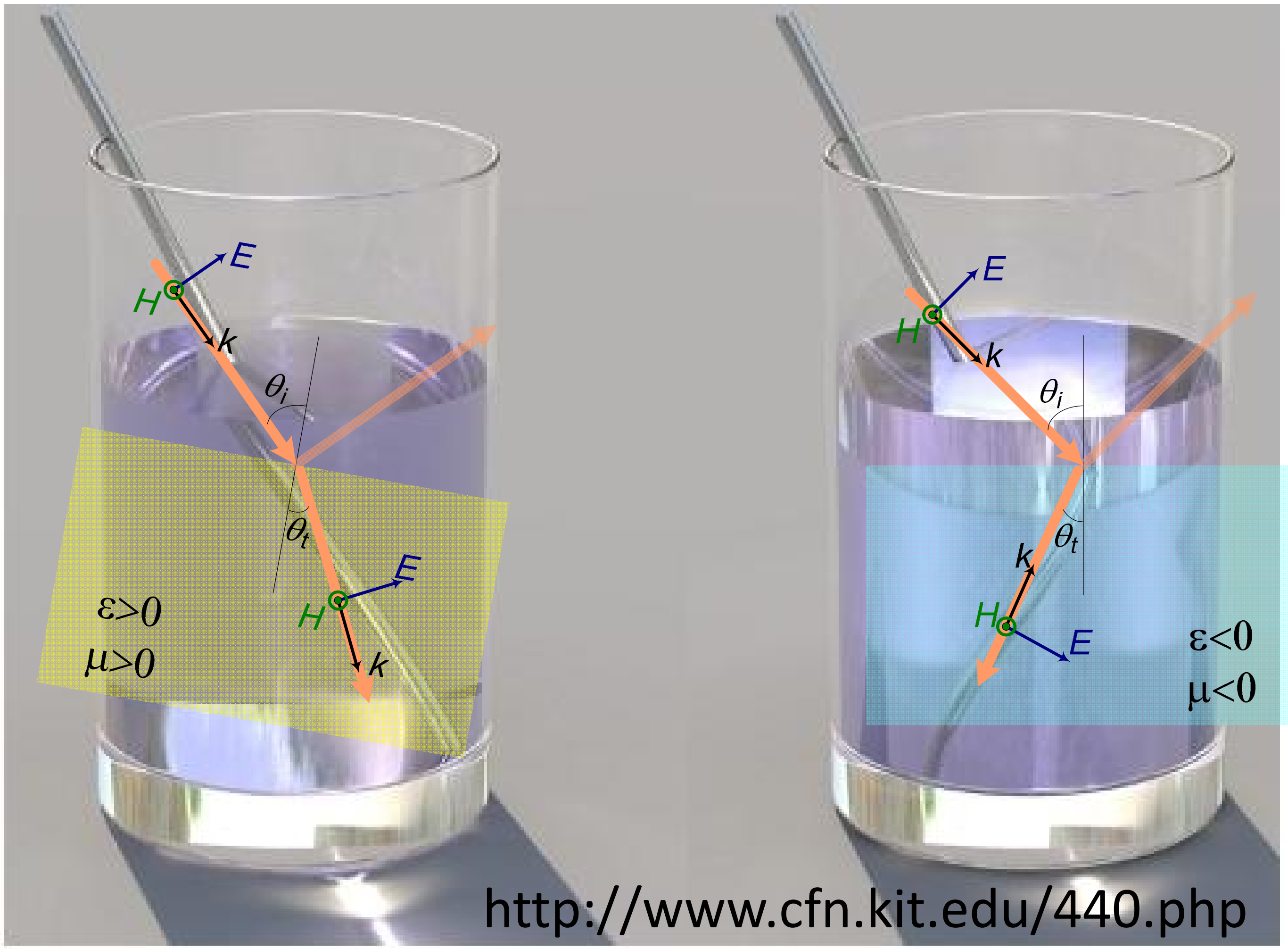


Image of a swimming pool filled with a substance having n=0.9.

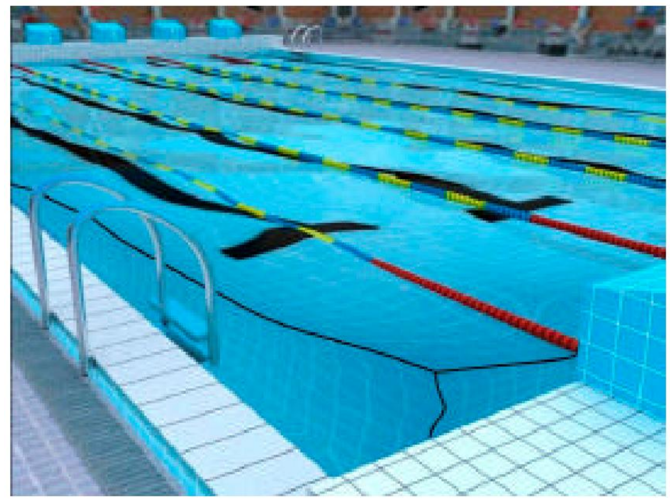
Aaron Danner, **"Photorealistic ray tracing aids understanding of metamaterials,"** 12 March 2009, SPIE Newsroom. DOI: 10.1117/2.1200903.1525

Negative Refractive Index



Refraction: Negative Index

Image of a swimming pool filled with water (n=1.33) (computer-generated)



Pool filled with negative-index 'water' (n=- 1.33). A black line: location of the pool bottom edge and corner. The bottom of the pool seems to 'float' above ground level.

Aaron Danner, **"Photorealistic ray tracing aids understanding of metamaterials,"** 12 March 2009, SPIE Newsroom. DOI: 10.1117/2.1200903.1525

Refraction: Negative Index

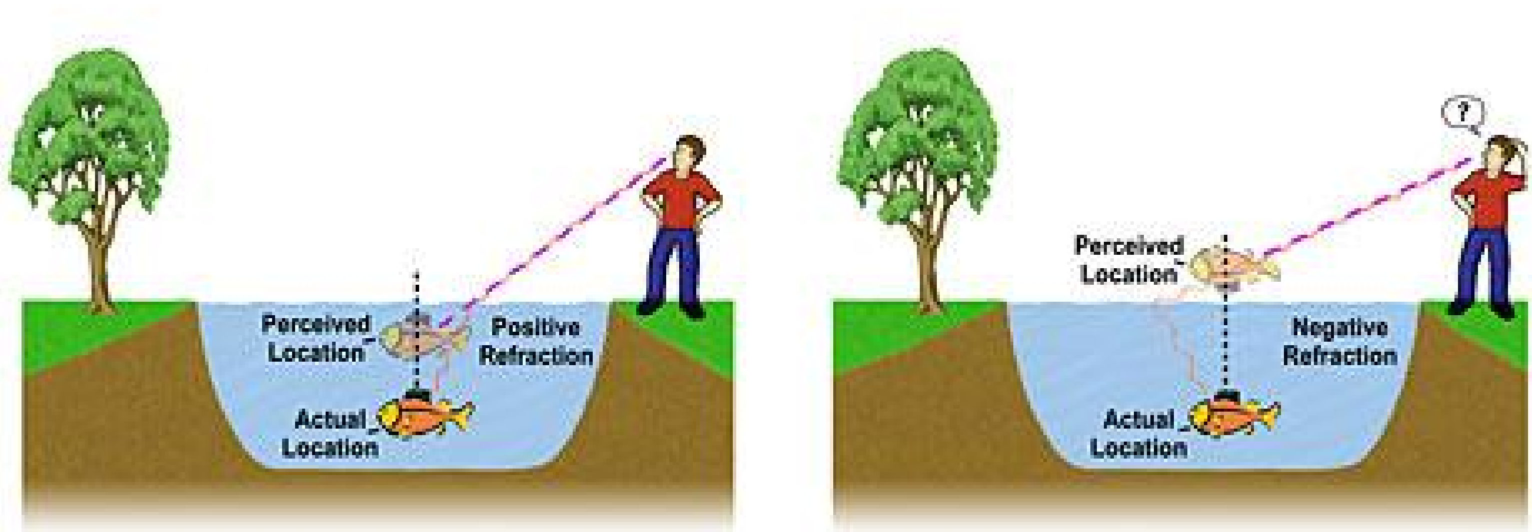
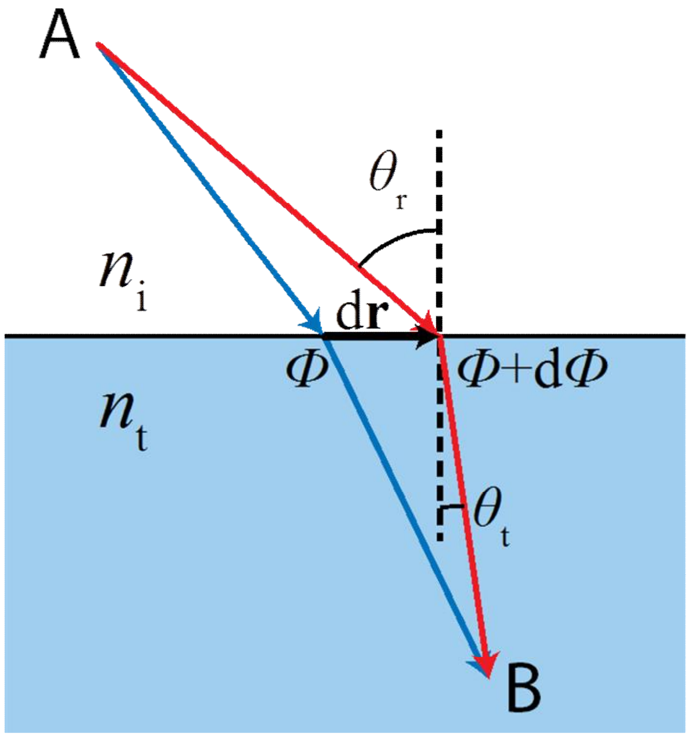


Illustration: UC Berkeley

Generalized Snell's Law



Principle of least action → The momenta difference between blue and red path is zero

$$(n_i \mathbf{k}_0 \sin\theta_i + \nabla\Phi) \mathrm{d}\mathbf{r}$$

$$-(n_t \mathbf{k}_0 \sin\theta_t) \mathrm{d}\mathbf{r} = 0$$

since $\mathbf{k} = \nabla\Phi$ †

For reflection

$$\sin\theta_r - \sin\theta_i = n_i^{-1} k_0^{-1} \nabla\Phi$$

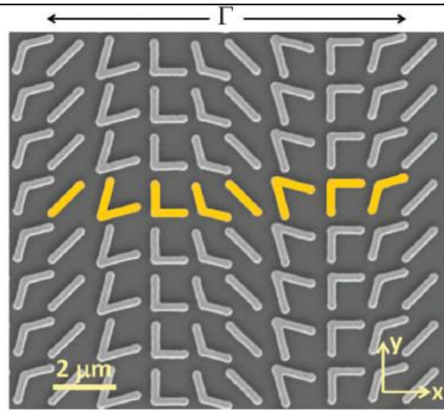
For refraction

$$n_t \sin\theta_t - n_i \sin\theta_i = k_0^{-1} \nabla\Phi$$

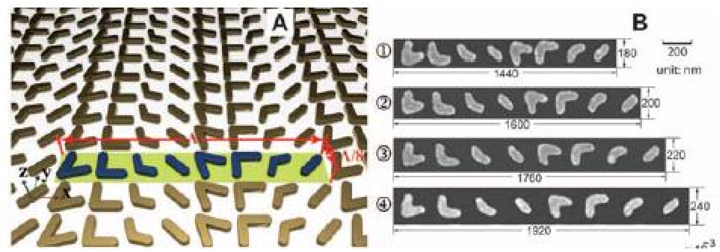
† Landau and Lifshitz, The Classical Theory of Fields (4 ed.)

In essence, momentum conservation!

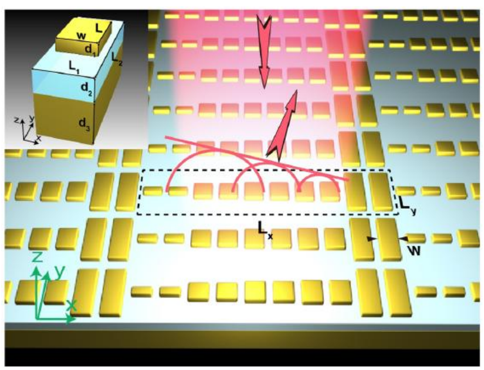
Generalized Snell's Law: Recent Work



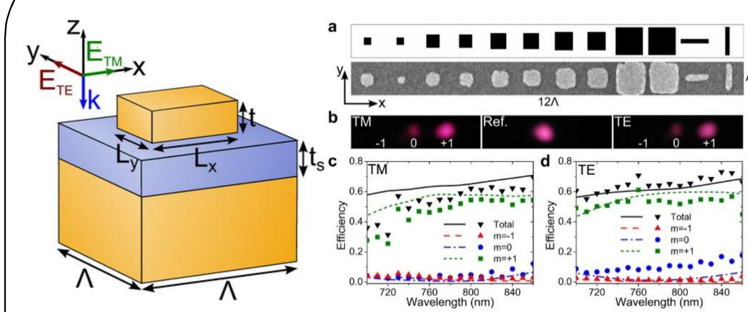
Nanfang Yu *et al.*, *Science* **334**, 333 (2011).



Xingjie Ni *et al.*, *Science* **335**, 427 (2012).

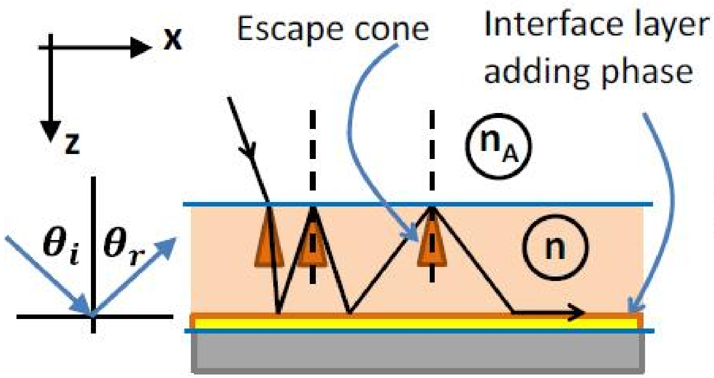


Shulin Sun *et al.*, *Nano Lett.* **12**, 6263 (2012).

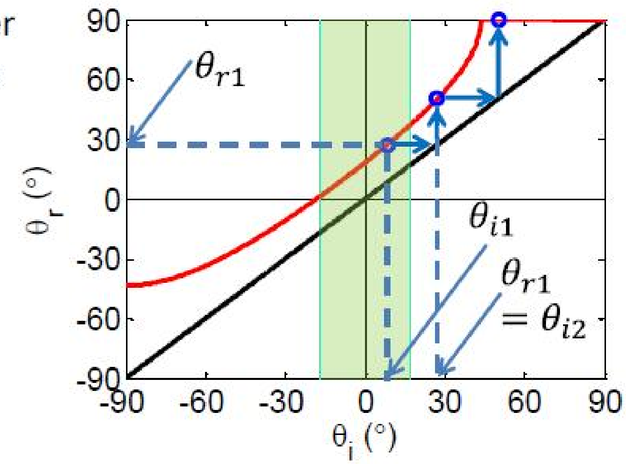


Anders Pors *et al.*, *Sci. Rep.* **3**, 2155 (2013).

Ultra-thin Metasurface Absorbers/Emitters

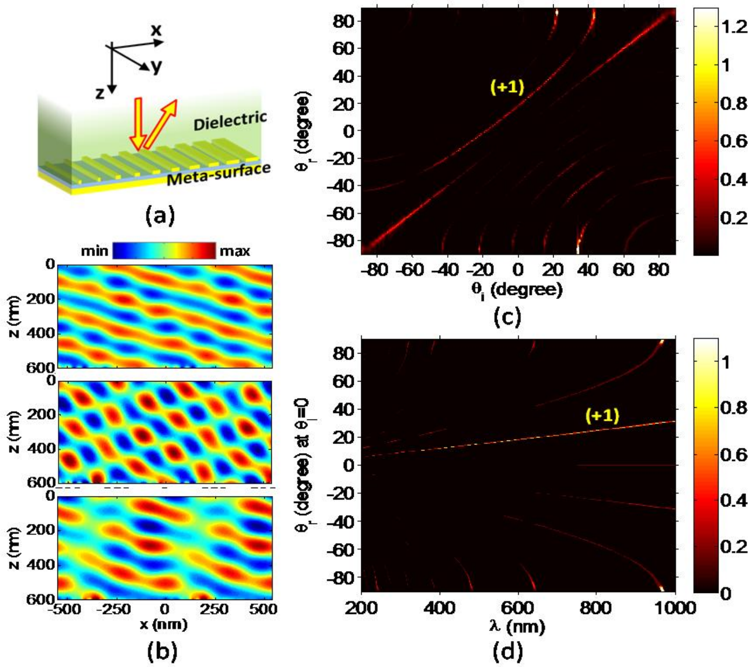


Metasurface bends light at each reflection



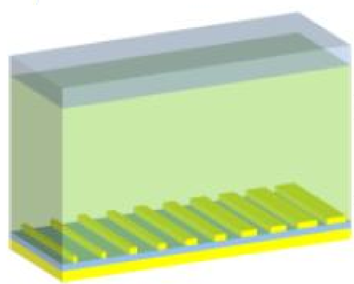
Complete coupling with external radiation in ultrathin layers

S4Sim Example: Xylophone Metasurface for Light Deflection

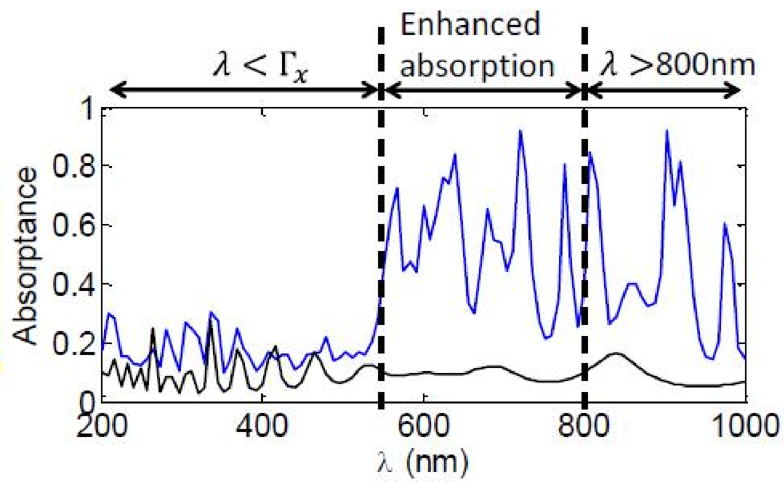


M. Ryyan Khan, Xufeng Wang, Peter Bermel, and Muhammad A. Alam, "Enhanced light trapping in solar cells with a meta-mirror following Generalized Snell's law," *Opt. Express* **22**, A973-A985 (2014).

Xylophone Metasurface: Absorption Enhancement



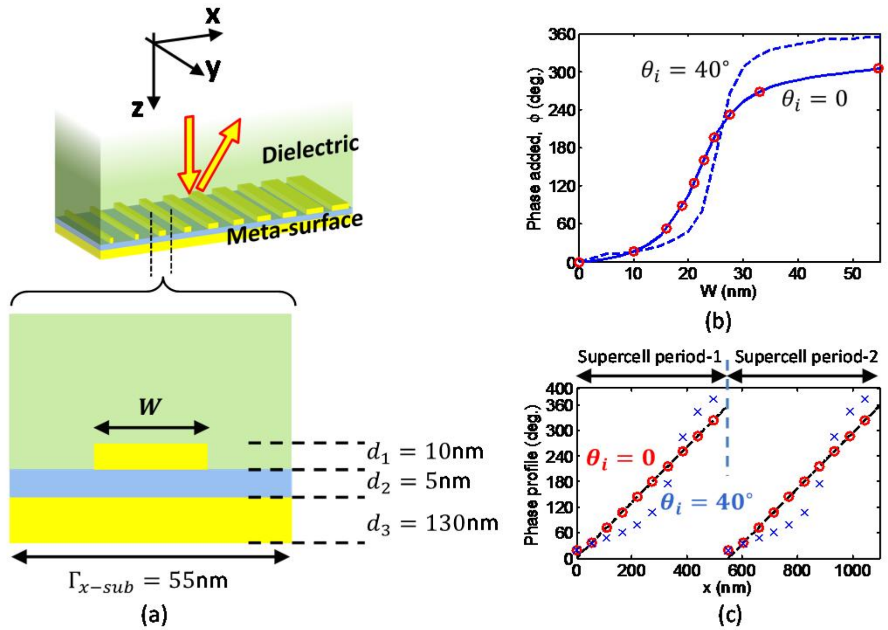
Simulated xylophone metasurface



Typical absorption in ultrathin layer (black) strong enhanced by metasurface (blue)

M. Ryyan Khan, Xufeng Wang, Peter Bermel, and Muhammad A. Alam, "Enhanced light trapping in solar cells with a meta-mirror following Generalized Snell's law," *Opt. Express* **22**, A973-A985 (2014).

Tailoring Metamirror Response for All Angles



W (nm)	0	10	16.05	18.88	21.09	22.84	24.74	27.56	33.04	55
Φ (deg.)	0	16.64	52.64	88.64	124.64	160.64	196.64	232.64	268.64	305.2

M. Ryyan Khan, Xufeng Wang, Peter Bermel, and Muhammad A. Alam, "Enhanced light trapping in solar cells with a meta-mirror following Generalized Snell's law," *Opt. Express* **22**, A973-A985 (2014).

Next Class

- Is Monday, Mar. 6
- Next time, we will continue with transfer matrix models, focusing on CAMFR