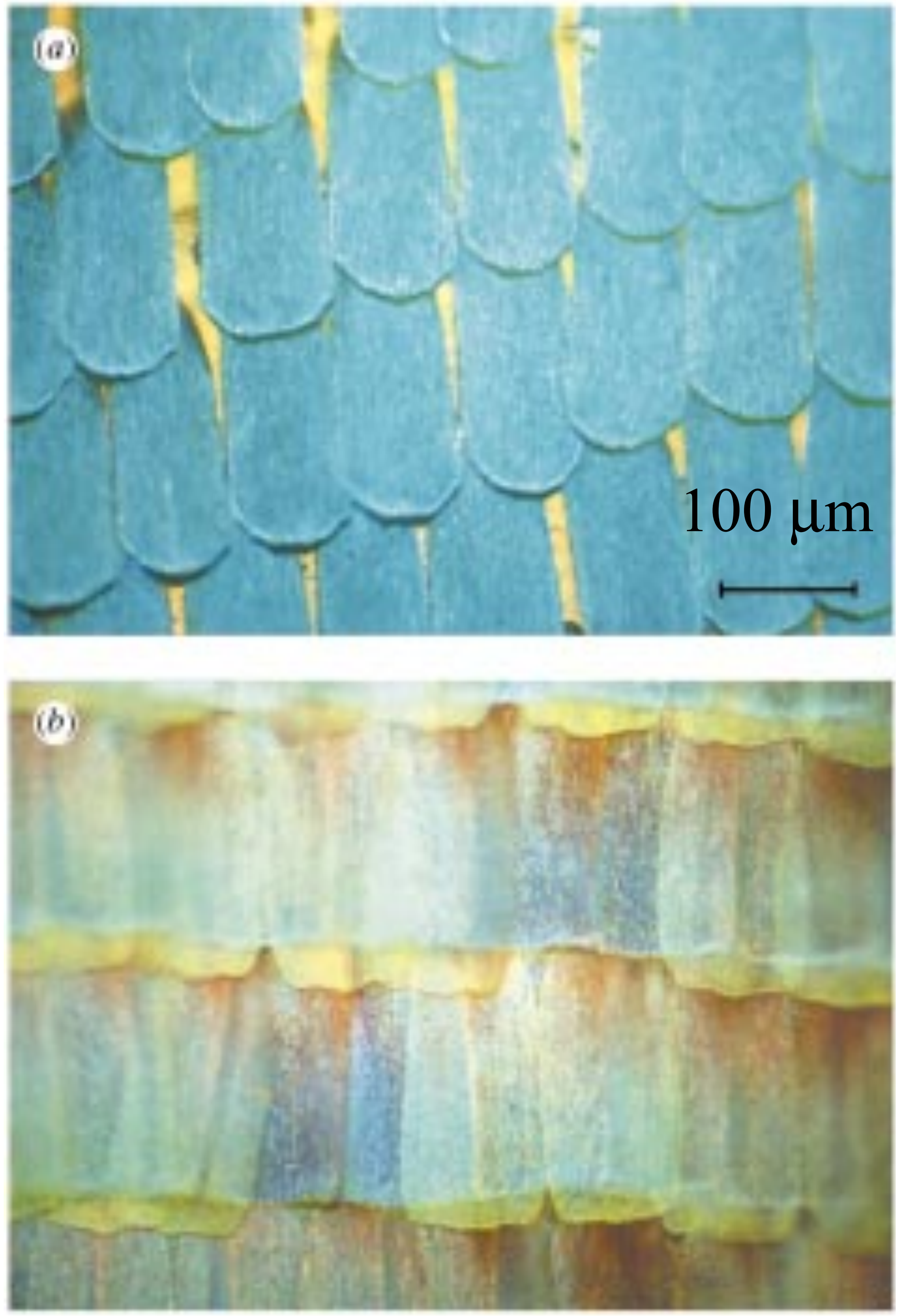
The Nanophotonics Challenge: Simulating Bioinspired Nanophotonic Structures

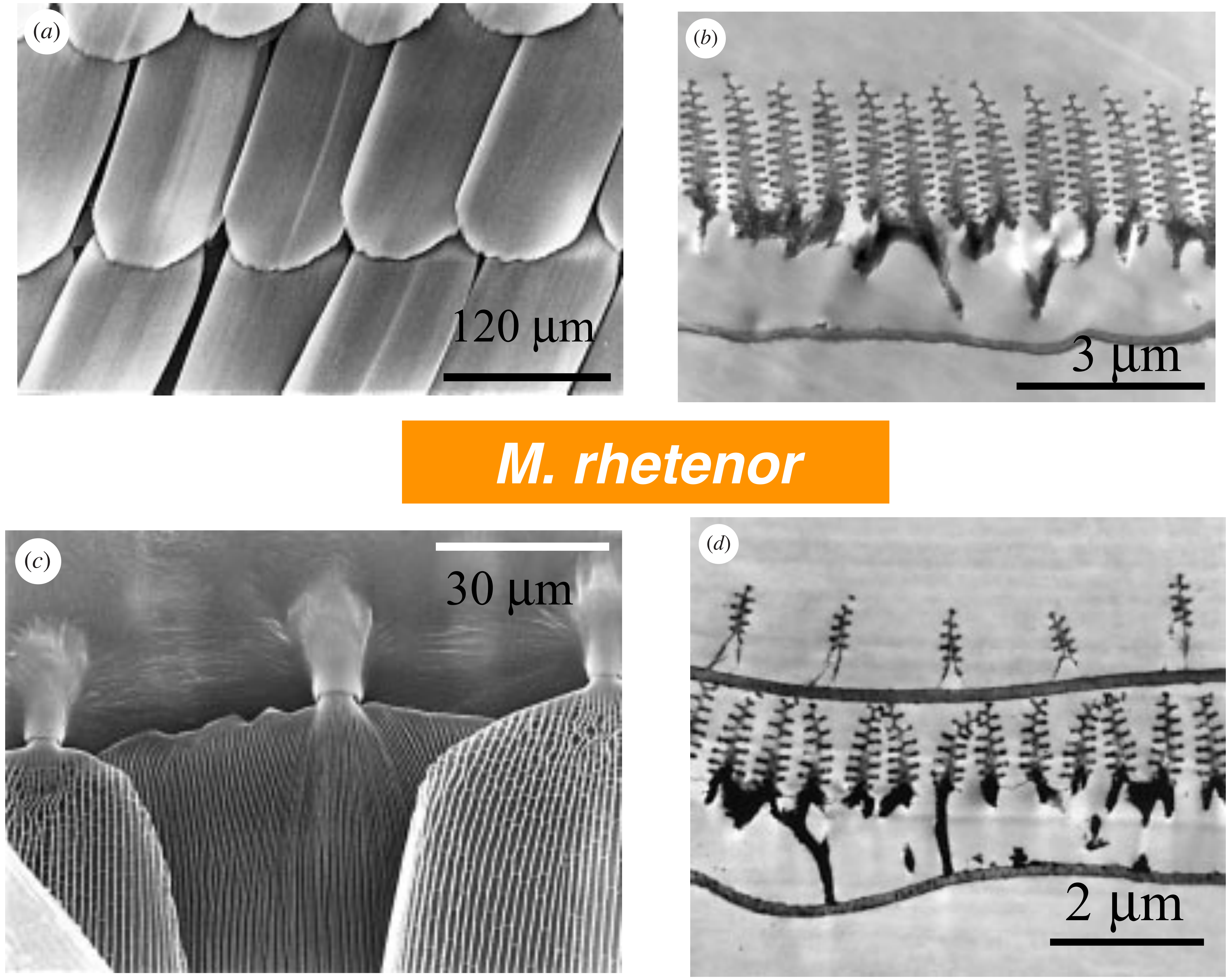
Enas Sakr, Jie Zhu, and Peter Bermel

What Gives the Morpho Butterfly Its Magnificent Blue?

https://www.youtube.com/watch?v=29Ts7CsJDpg

Morpho wing scales



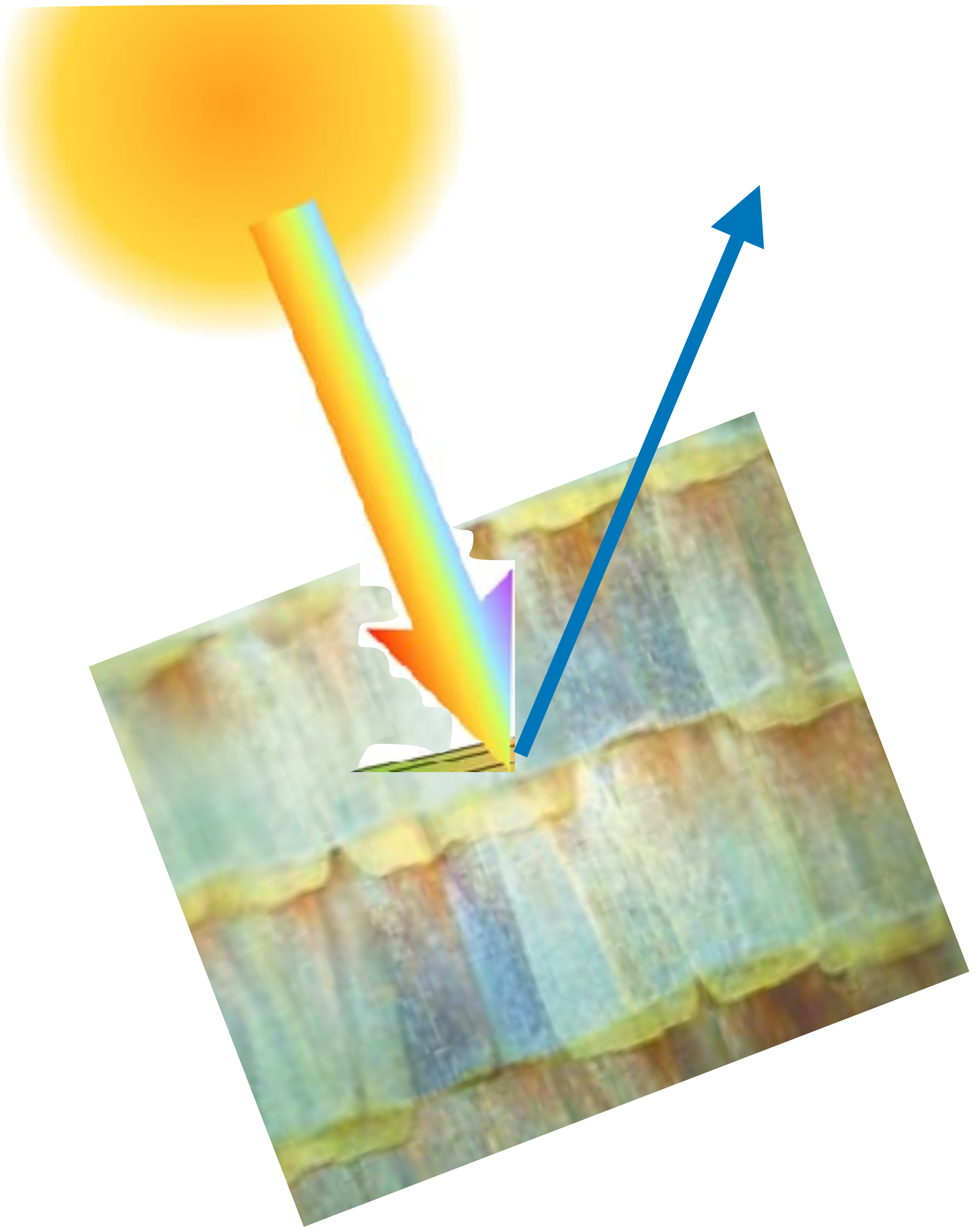


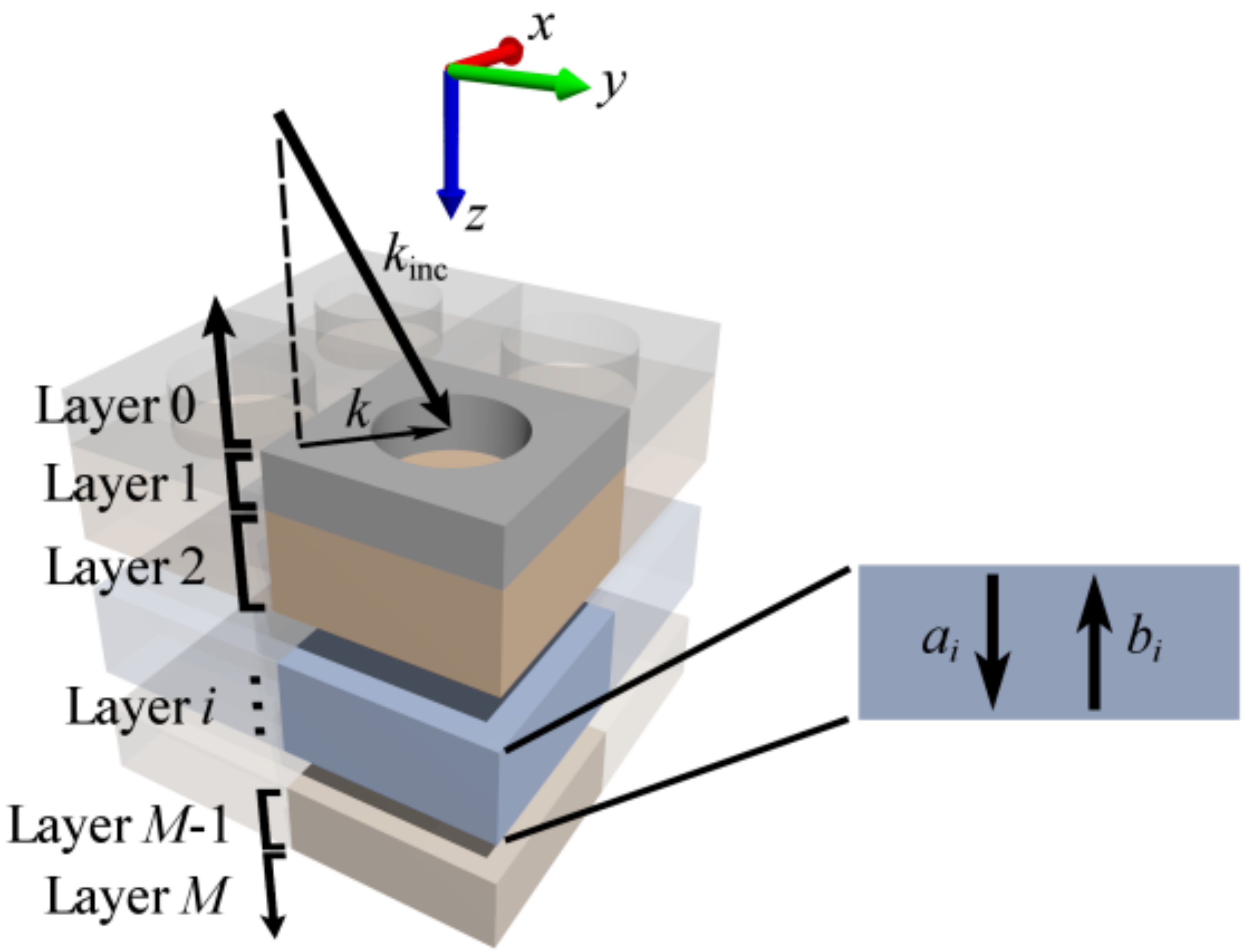
M. rhetenor

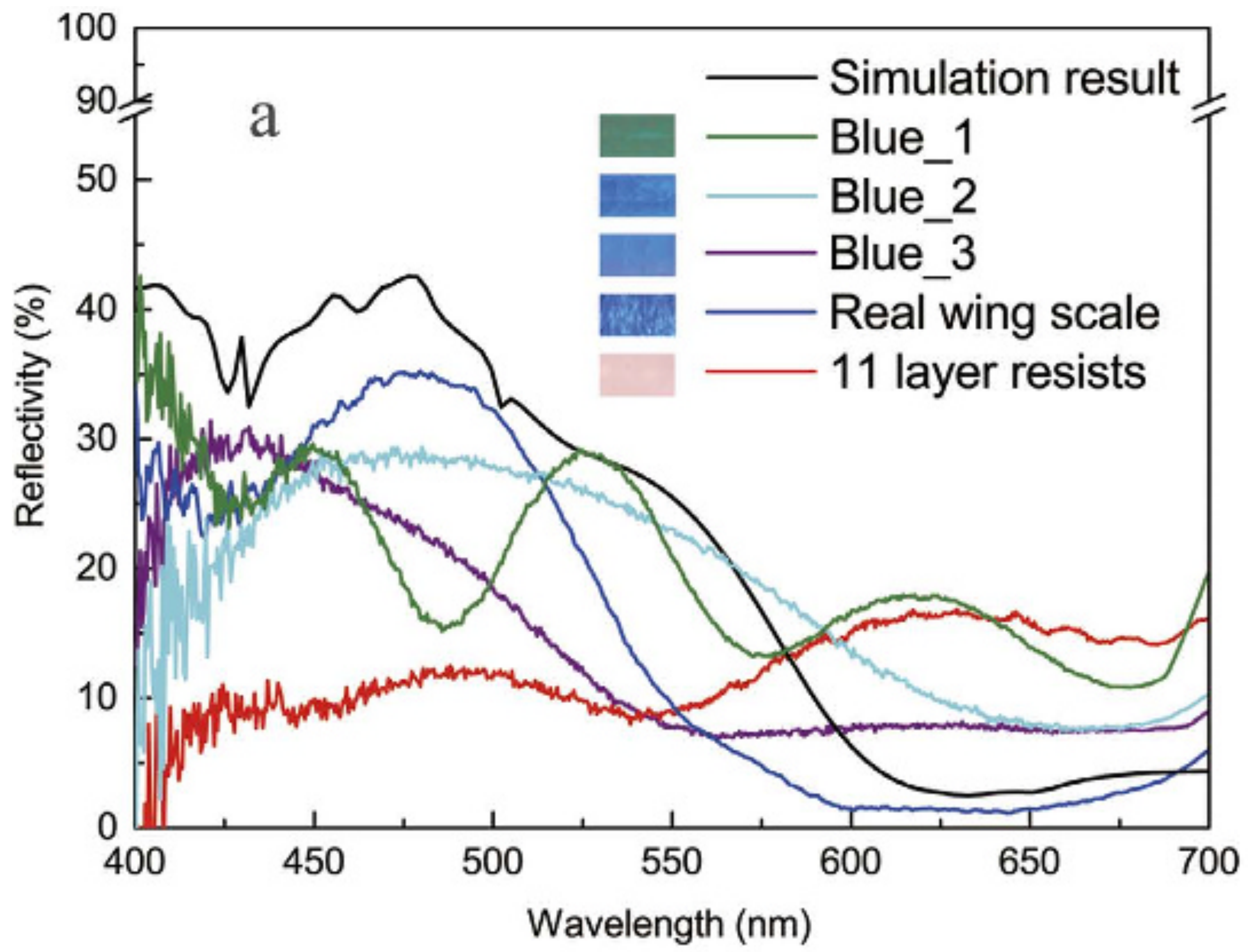
M. didius

Vucusic, P., *et al.* 1999, Proc. R. Soc. Lond. B.2661403–1411.

The Challenge: Can we reproduce the effect using simulations?

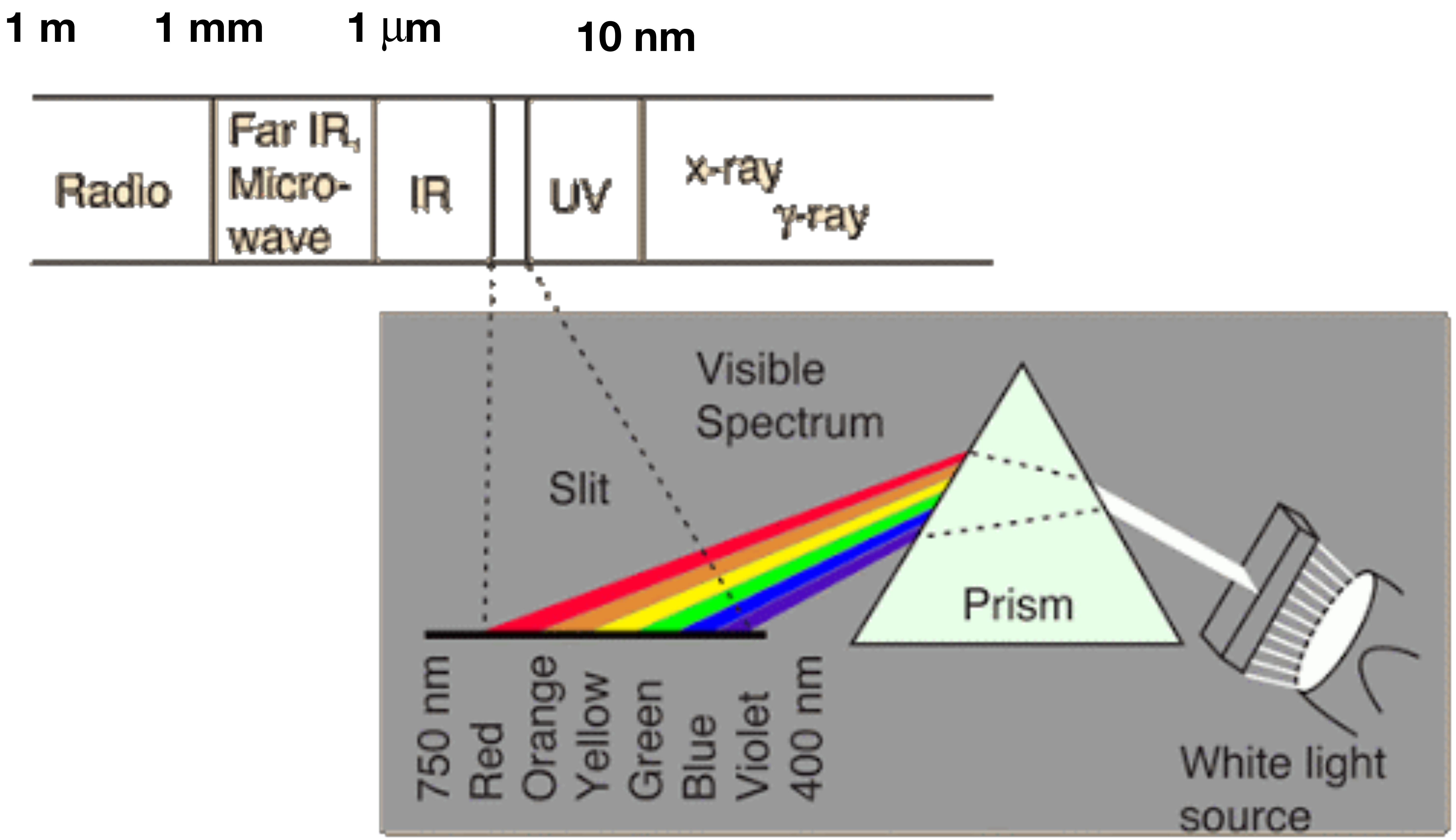






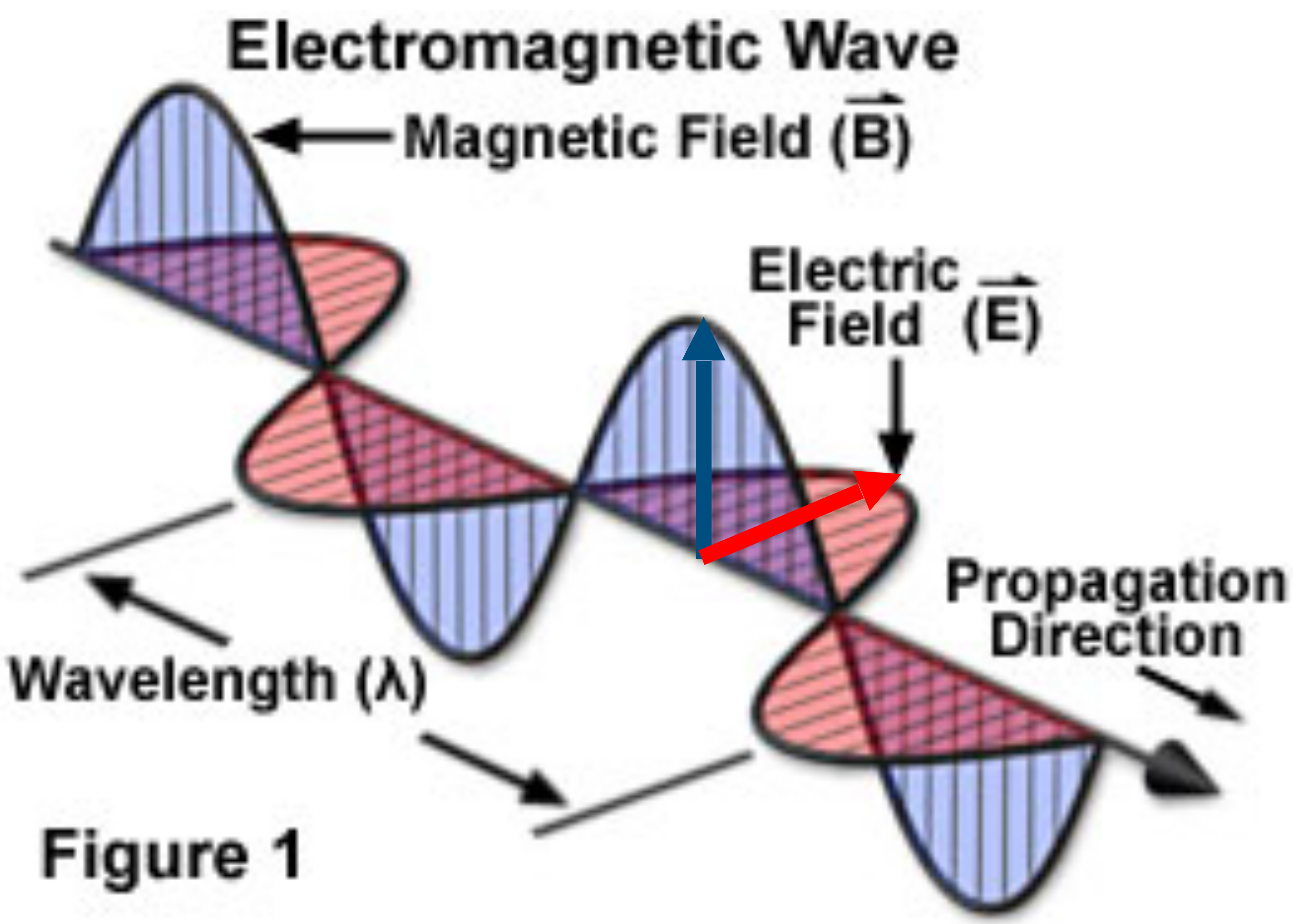
Electromagnetic (EM) simulations

Understanding light waves
The electromagnetic spectrum



http://hyperphysics.phy-astr.gsu.edu/hbase/ems3.html

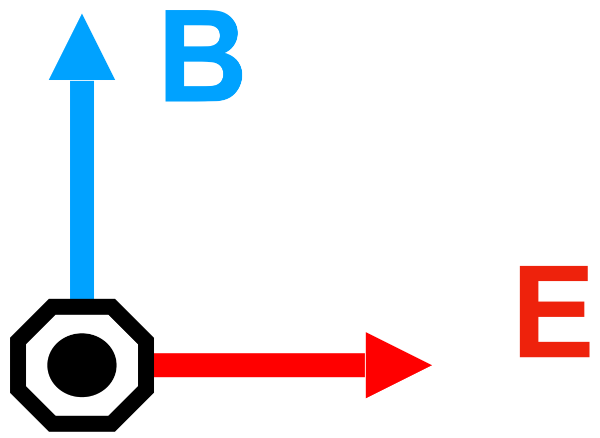
Understanding light waves



https://micro.magnet.fsu.edu/primer/java/electromagnetic/index.html

EM-optics governed by Maxwell's equations

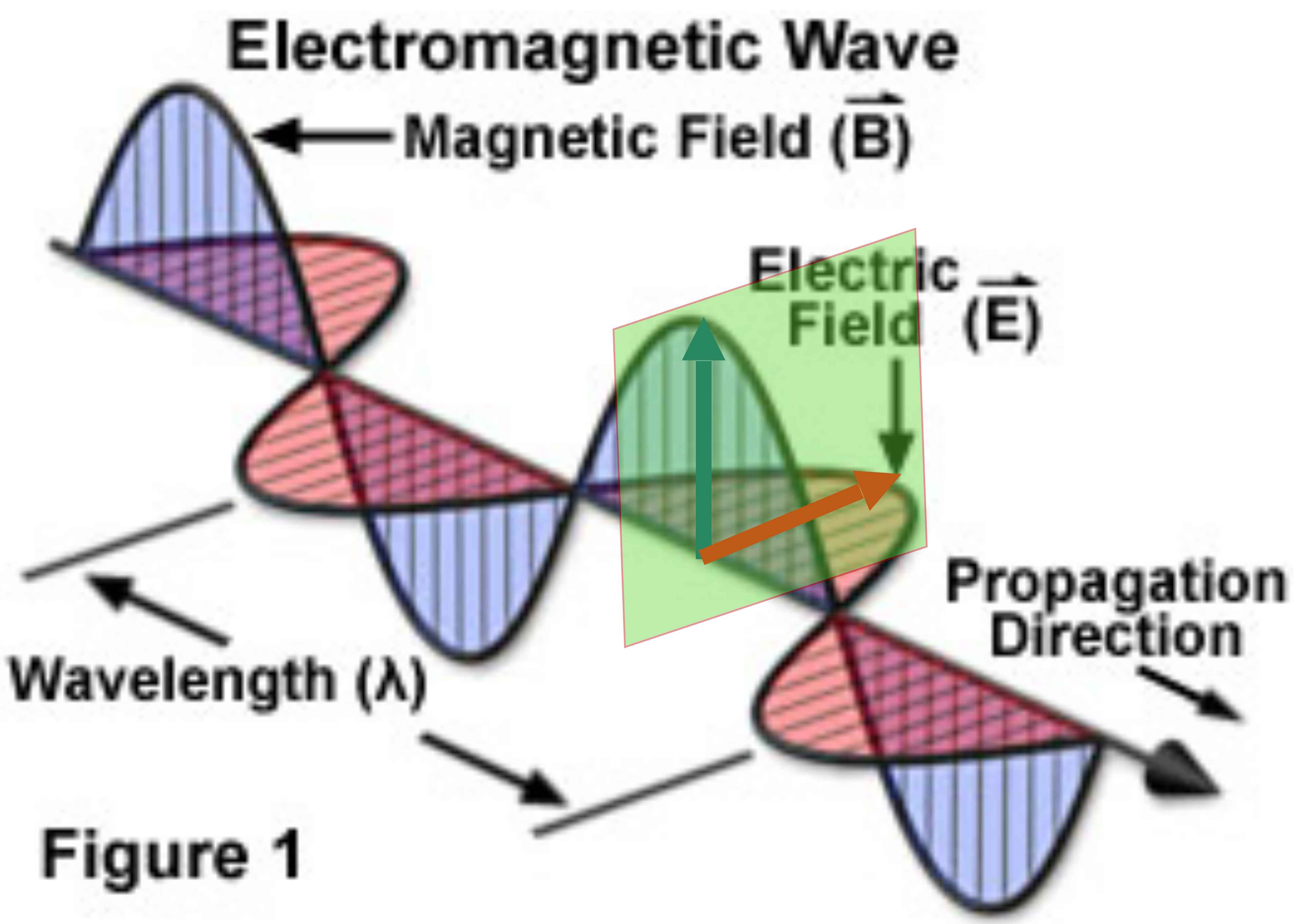
A collection of equations describing relations between time-varying electric fields and magnetic fields and their behavior at interfaces



Propagation direction

James Clerk Maxwell (1831-1879)
Scottish physicist & mathematician

Understanding light waves



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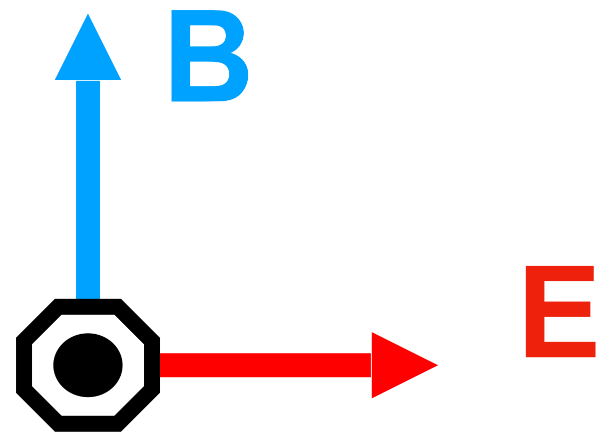

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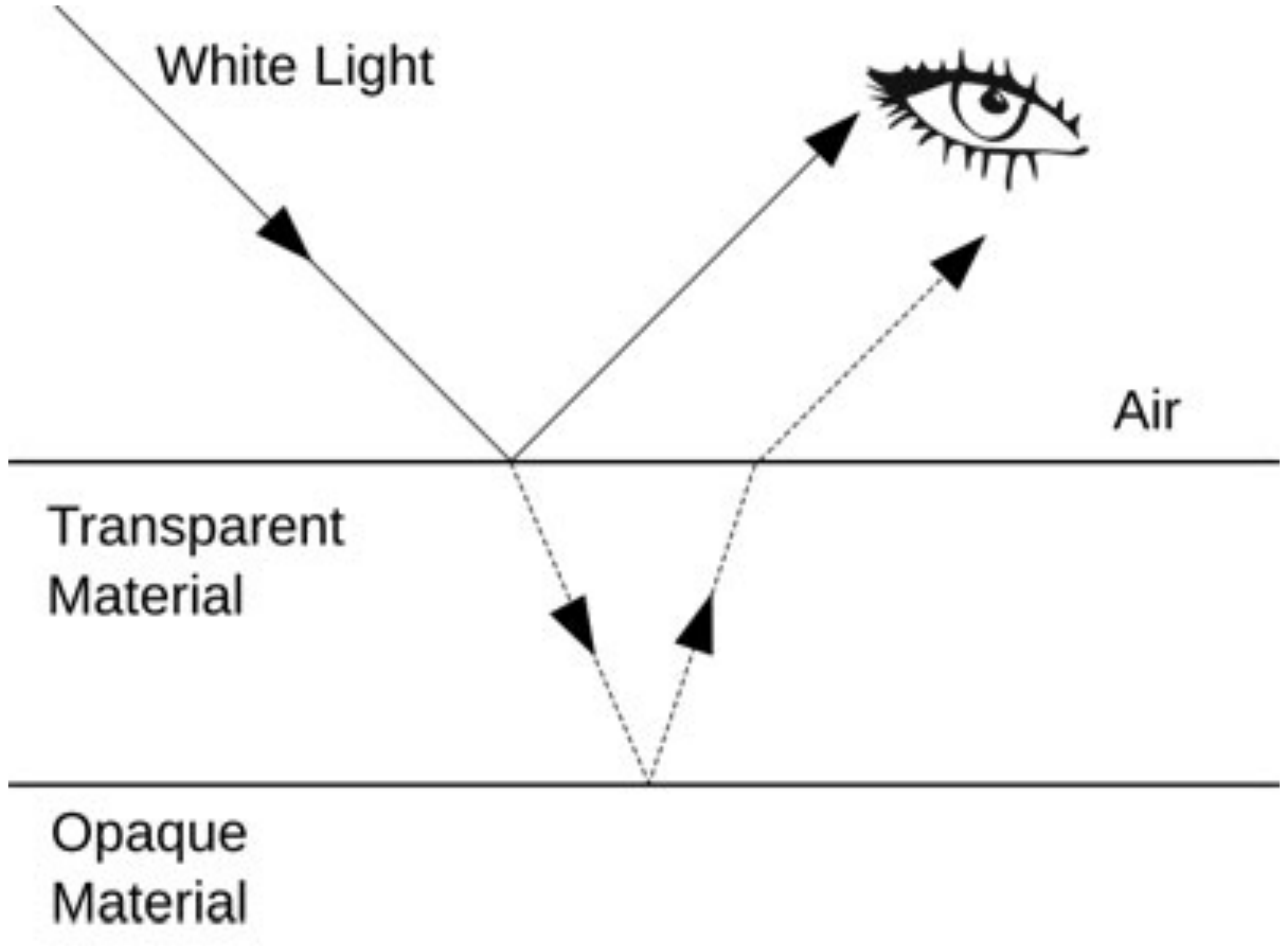
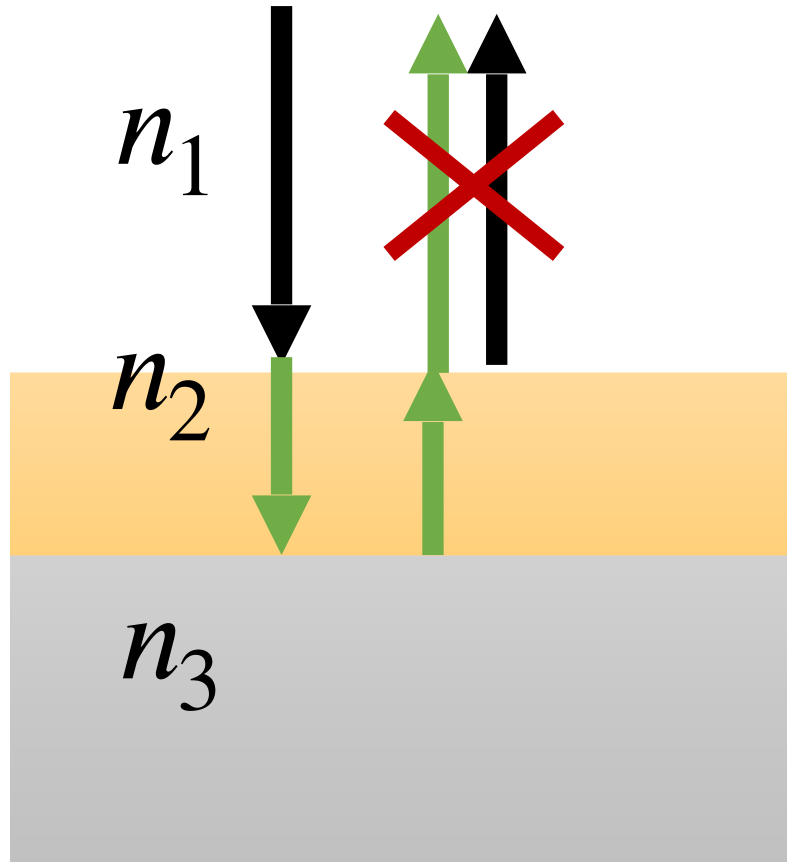
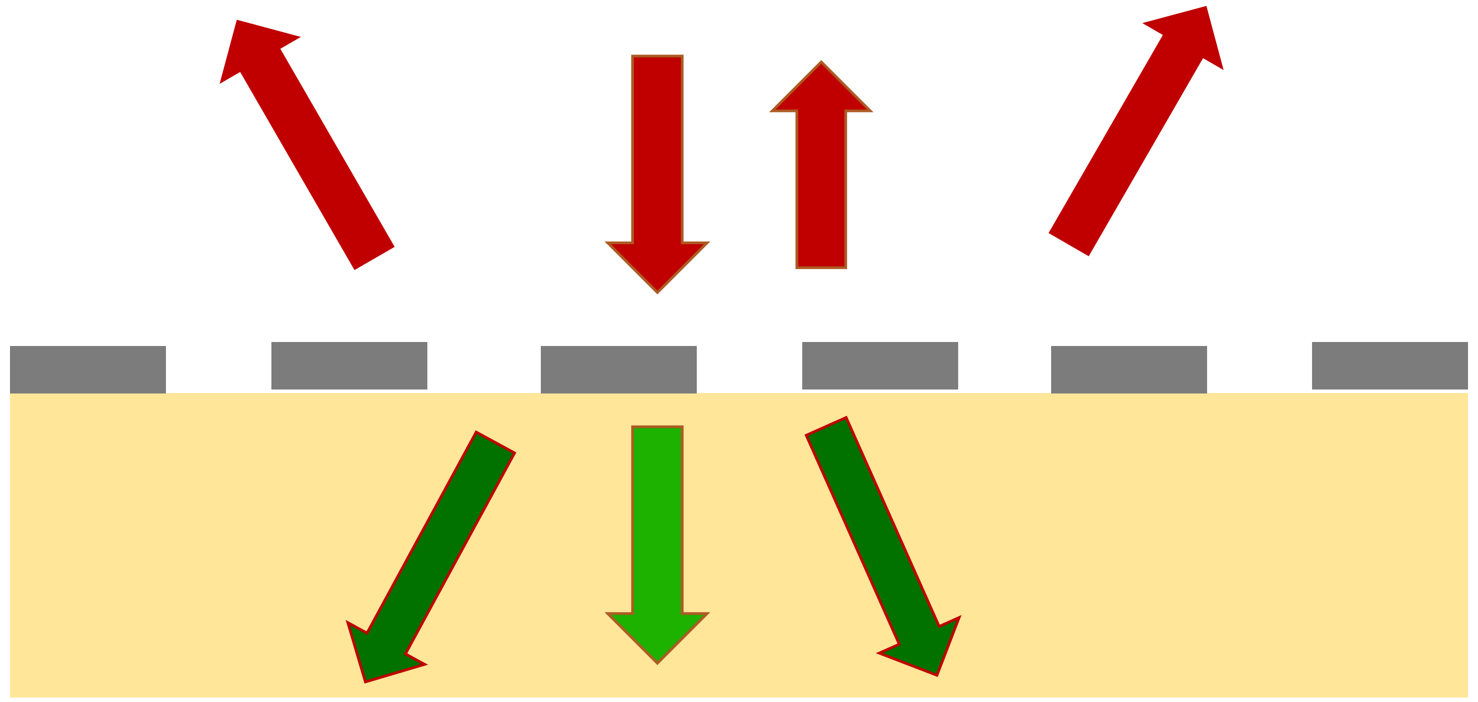






Reflection and refraction

Constructive and destructive interference

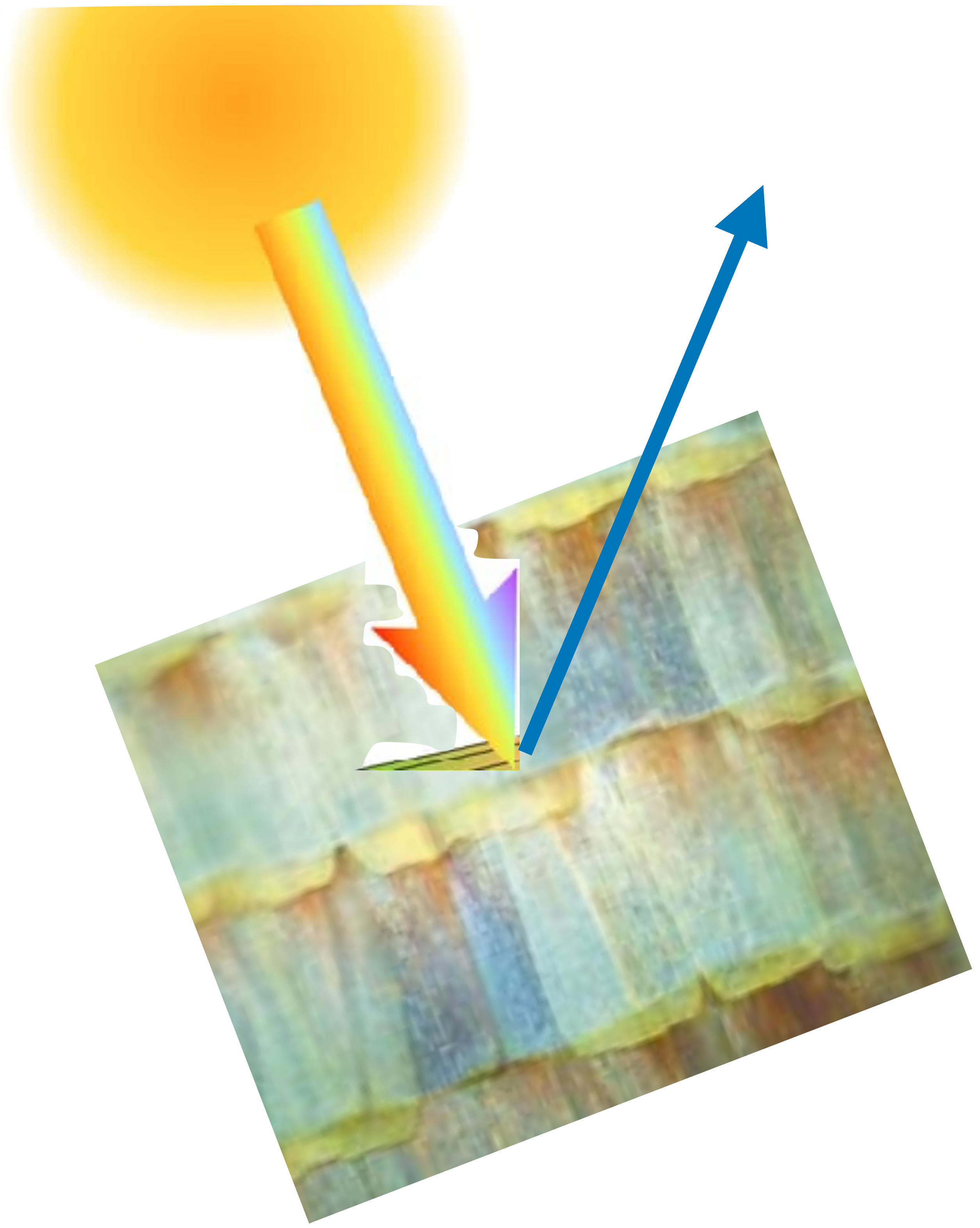
Diffraction

http://www.differencebetween.net/science/difference-between-reflection-and-refraction/

EM Simulation

Do I have to solve Maxwell's equations?!

Yes and No!



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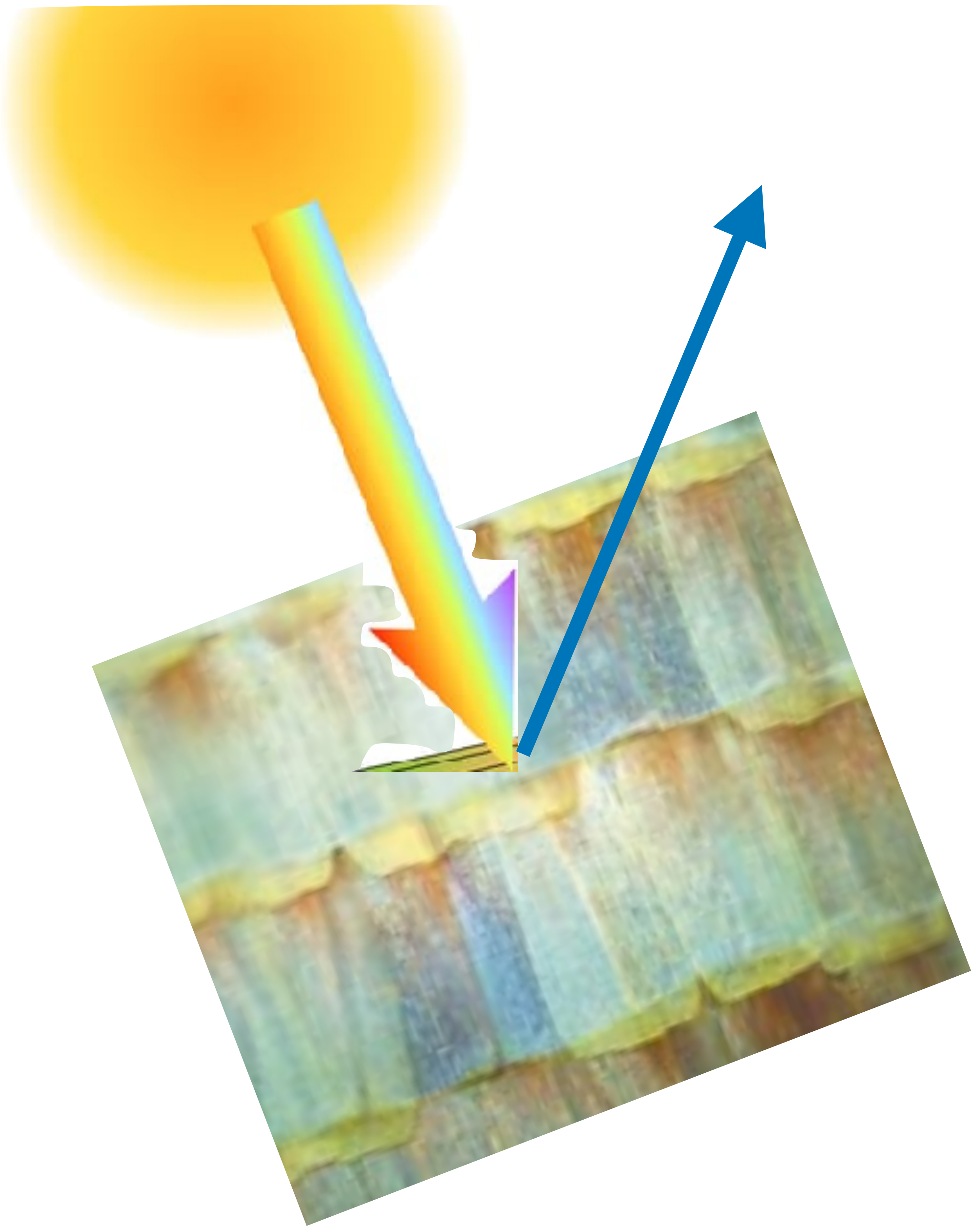

- With a solver you can!
- Define your structure's dimensions and involved materials.
- Define your incident wave parameters.
- Use an EM simulation tool to solve Maxwell's equations in your structure. Define all simulation parameters.

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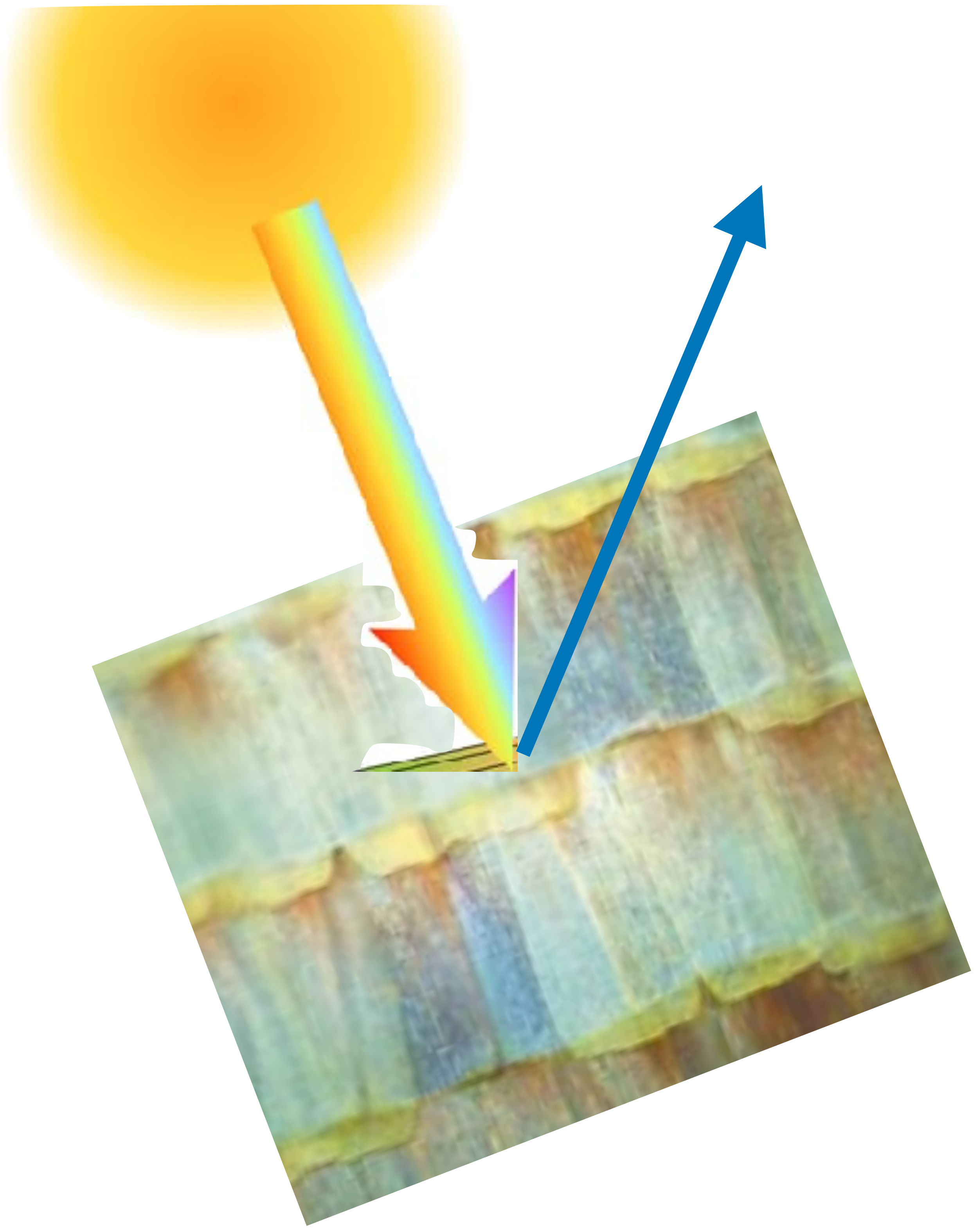

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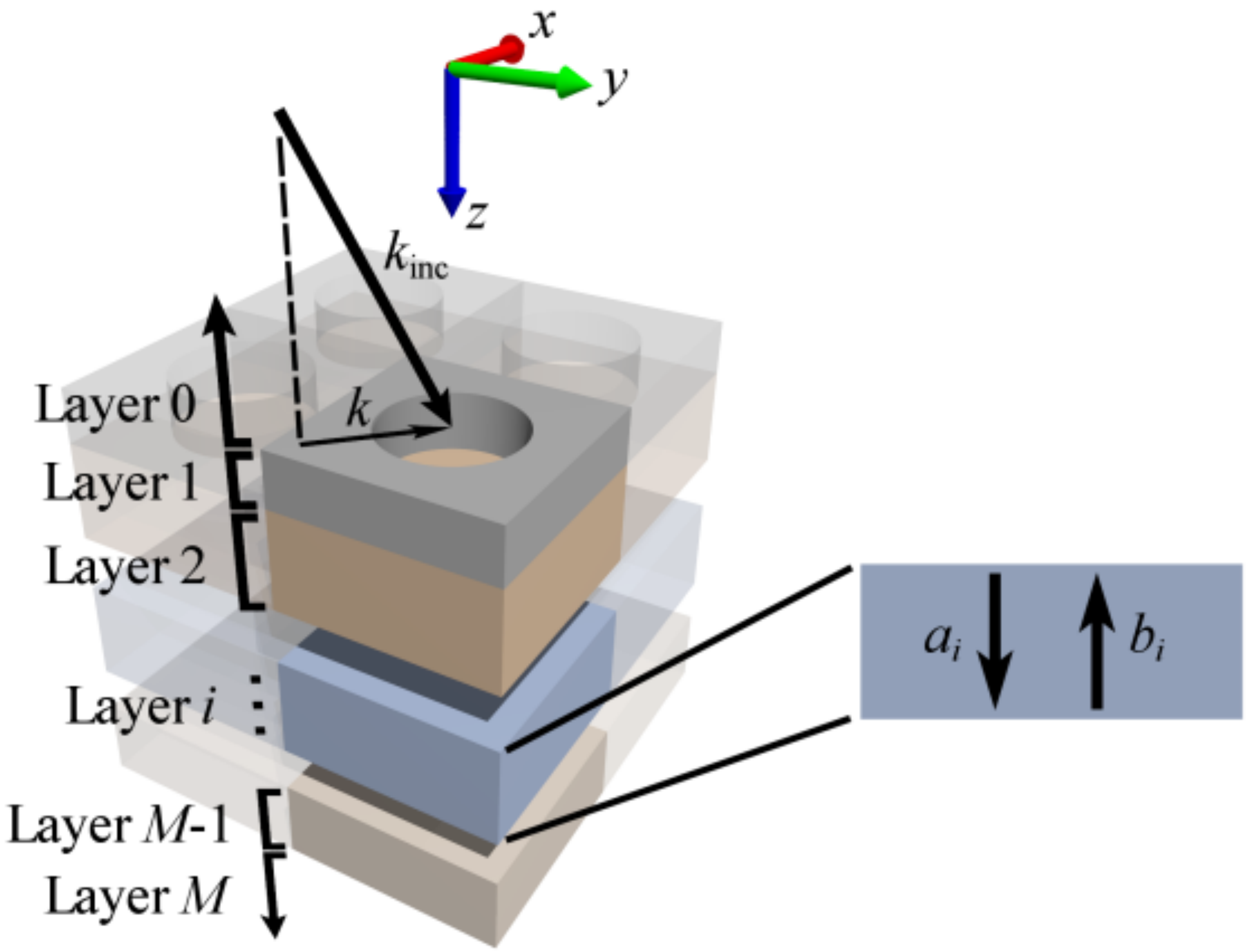

EM optics: Maxwell's equations

I. Gauss' law for electricity $\nabla \cdot \mathbf{D} = \rho$ **(Divergence)**

$\mathbf{D}=\varepsilon_0\mathbf{E}$ *Free space*

$\mathbf{D}=\varepsilon\mathbf{E}$ *Isotropic linear dielectric*

II. Gauss' law for magnetism $\nabla \cdot \mathbf{B} = 0$

III. Faraday's law of induction $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ **(Curl)**

IV. Ampere's law $\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$

$\mathbf{B}=\mu_0\mathbf{H}$ *Free space*

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1. Diverging $\mathbf{E}$-fields relate to charges (bound and free) ρ
   $\mathbf{D}$: Electric displacement vector
   $\mathbf{E}$: Electric field vector

Free-space electric permitvitty

$$\varepsilon_0 = \frac{10^{-9}}{36\pi} \text{ F/m}$$

Free-space magnetic permeability

$$\mu_0 = 4\pi \times 10^{-7} \text{ H/m}$$

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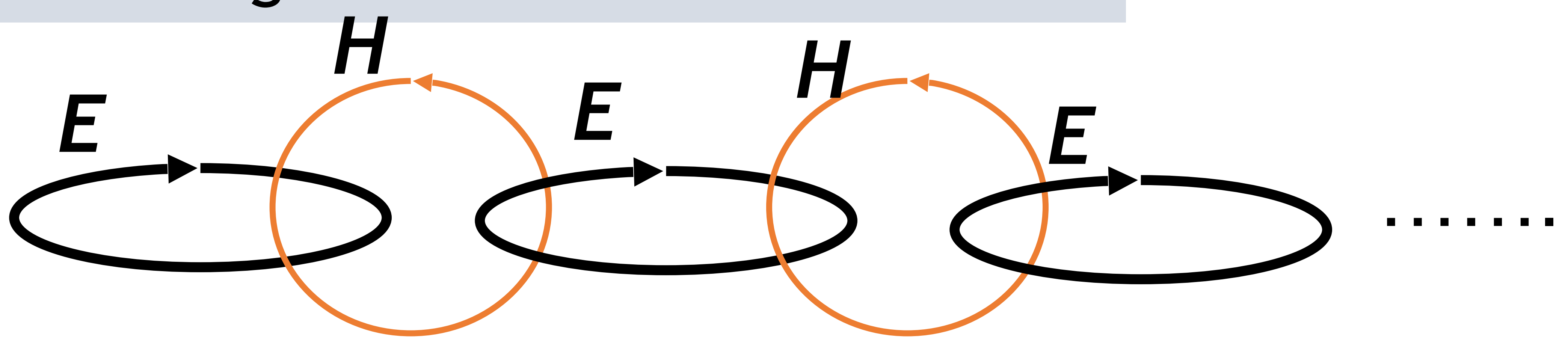

The Wave Equation

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}$$

$$\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t}$$

$$\nabla^2 \mathbf{E} = \mu\varepsilon \frac{\partial^2 \mathbf{E}}{\partial^2 t}$$

Ellingson, Steven. *Electromagnetics Volume 1*. Virginia Tech Libraries, 2018

The Wave Equation

In a source free medium: Combining Equations (III) and (IV), playing around with some vector calculus and substituting by Equation (I) $\left(\rho \text{ and } \mathbf{J} = 0\right)$

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Laplacian operator

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SOLUTION:

Waves propagating with a (phase) velocity $v = \frac{1}{\sqrt{\mu\varepsilon}}$

$$\mathbf{E}(\boldsymbol{r}, t) = \mathrm{Re}\left\{\mathbf{E_0}(\boldsymbol{r})\exp(-j\omega t)\right\}$$

Position

Time harmonic dependence

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Phasor representation

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Uniform plane waves

Homogeneous vector Helmholtz equation

$$\nabla^2 \mathbf{E}_0(\boldsymbol{r}) + \frac{\omega^2}{v^2}\mathbf{E}_0(\boldsymbol{r}) = 0$$

Refractive index $n = \frac{c}{v}$

Constant vectors

$$\mathbf{E}_0(\boldsymbol{r}) = \mathbf{E}_0^+ e^{-j\boldsymbol{k}\cdot\boldsymbol{r}} + \mathbf{E}_0^- e^{j\boldsymbol{k}\cdot\boldsymbol{r}}$$

Forward wave Backward wave

Propagation constant

$$k = \frac{\omega}{v} = \omega\sqrt{\mu\varepsilon} = \frac{\omega}{c}n$$

3×10^8 m/s

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Forward wave   Backward wave

E_o, H_o and k form a right-hand triplet and

$$\mathbf{H}_o = \frac{n}{\eta_o}\hat{k} \times \mathbf{E}_o \qquad \eta_o = \sqrt{\mu_o / \varepsilon_o}$$

Intrinsic impedance

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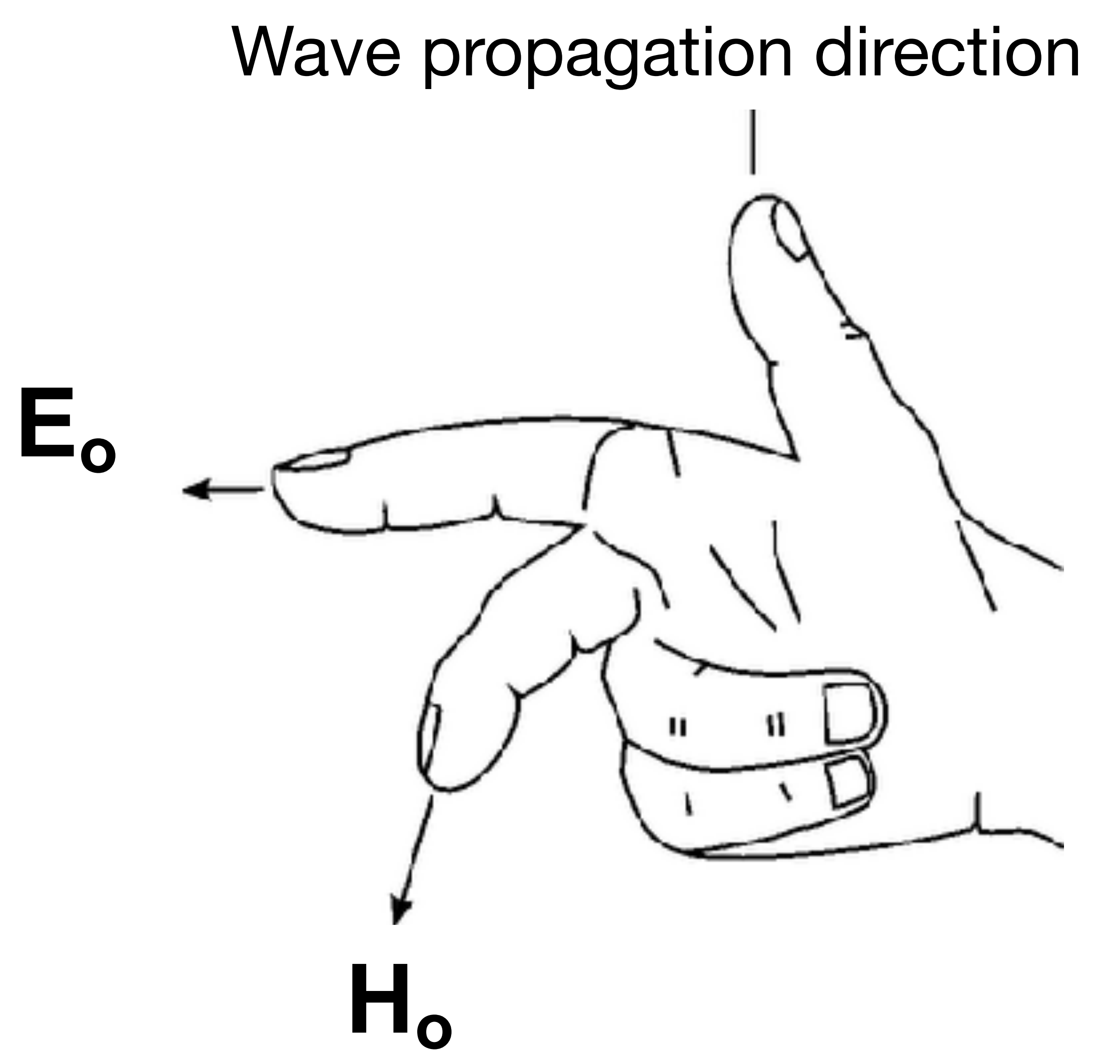
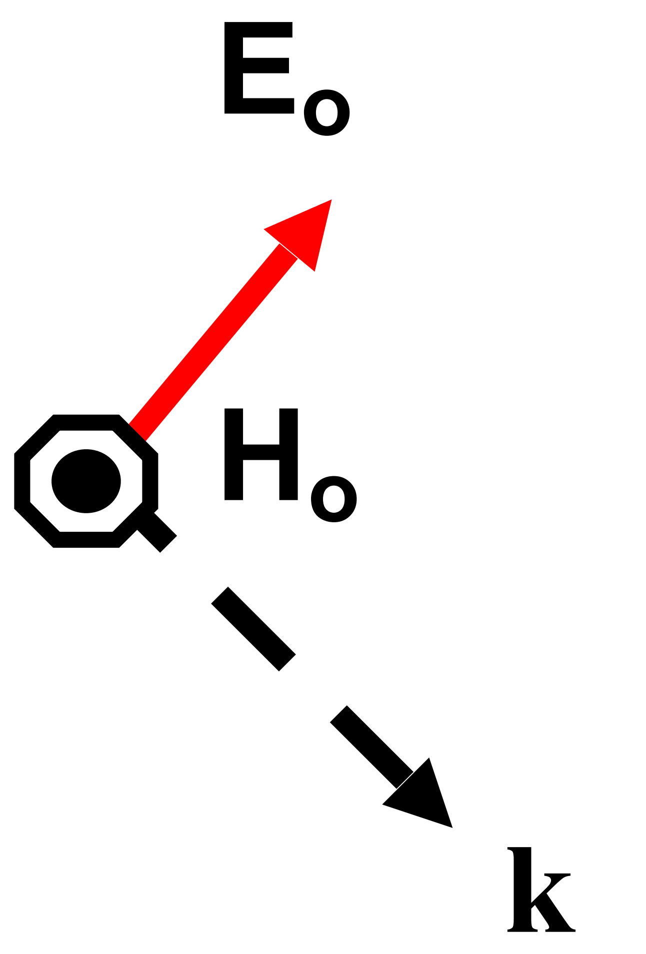
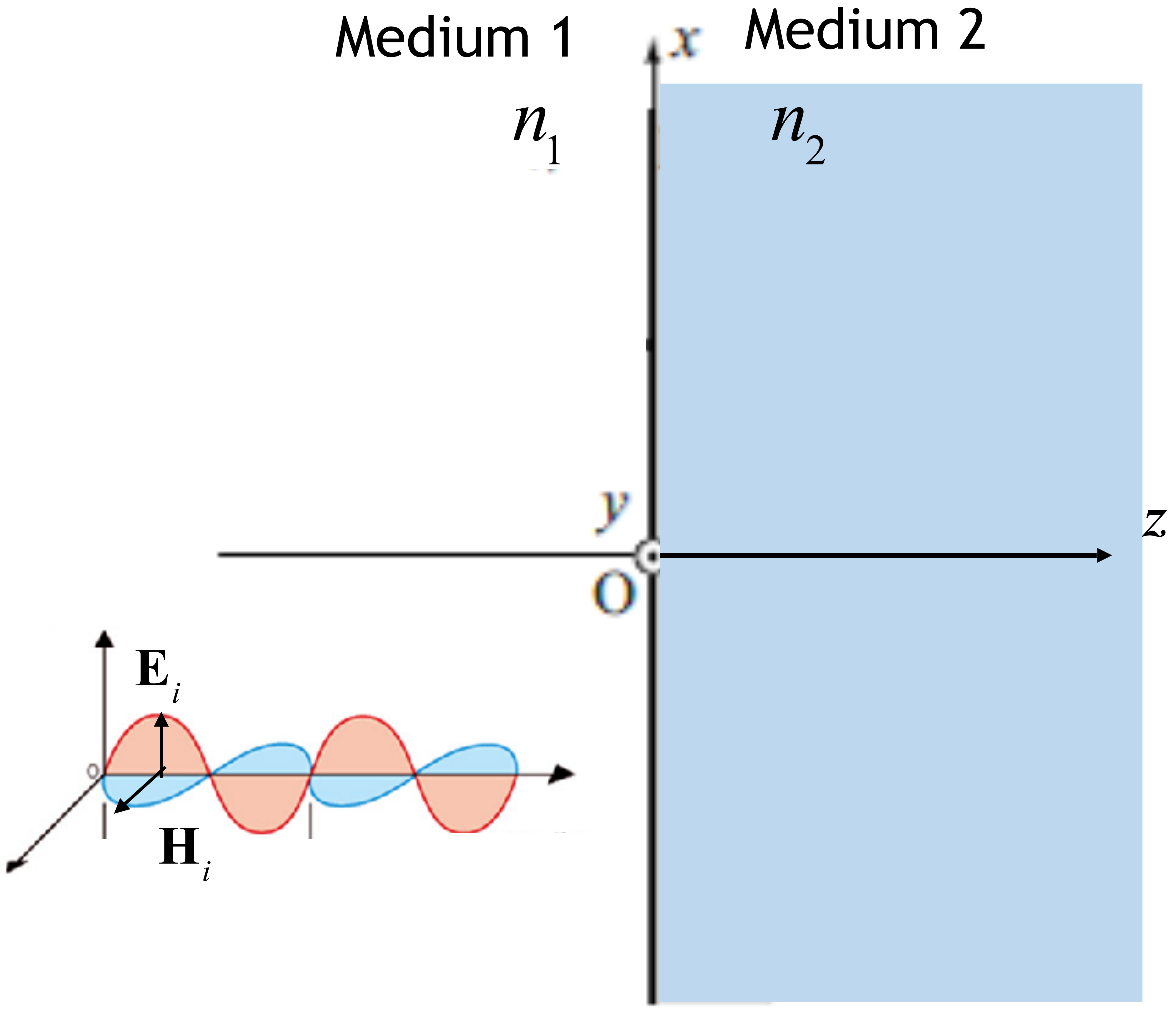




Simple problem:
Normal incidence at a dielectric interface



Solving boundary conditions at the interface

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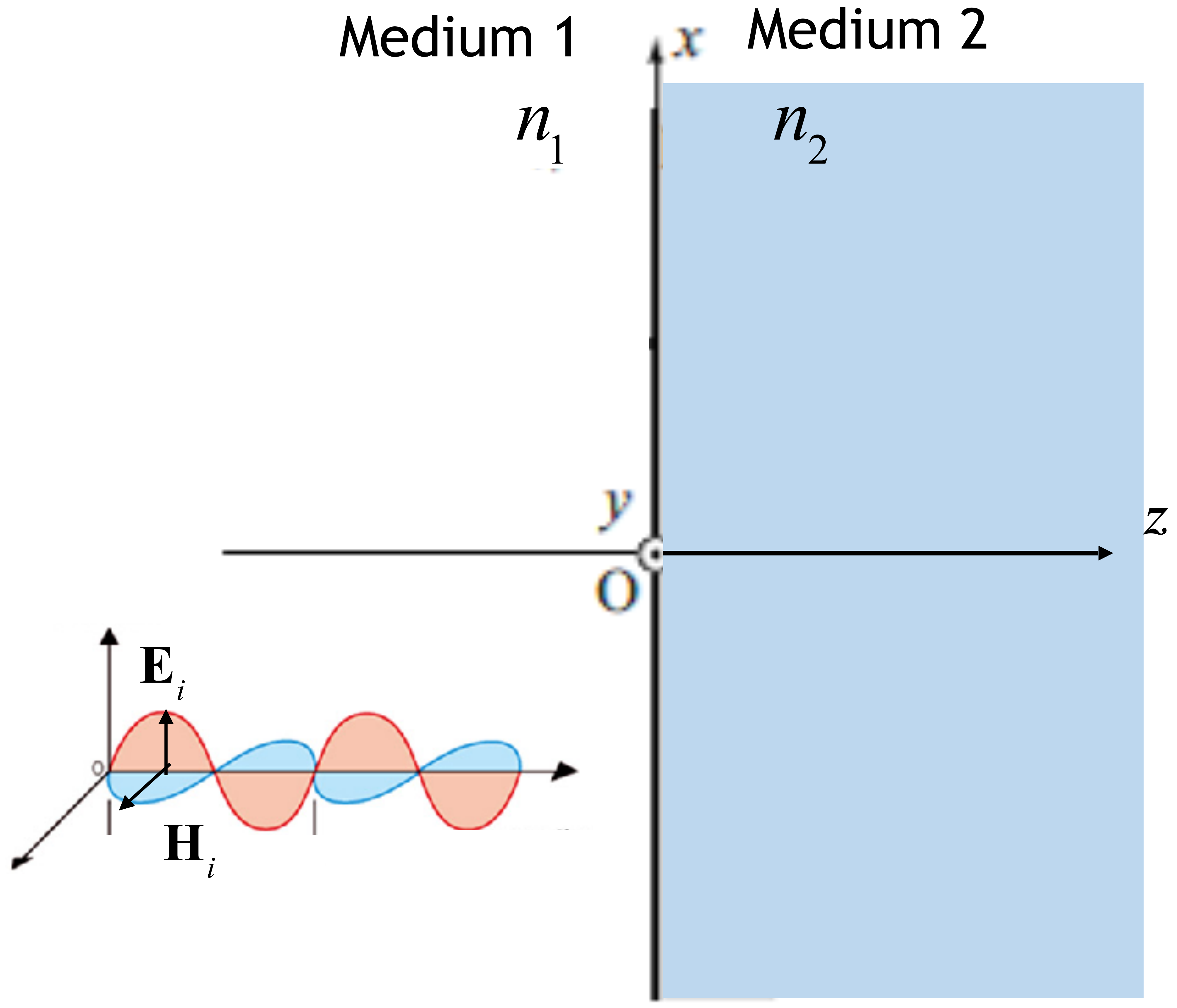

Incident wave

$$\mathbf{E}_i = \hat{x} E_{i0} e^{jk_1 z}$$

$$\mathbf{H}_i = \hat{y} \frac{E_{i0}}{\eta_1} e^{jk_1 z}$$

Solving boundary conditions at the interface

Simple problem:
Normal incidence at a dielectric interface

Reflected wave

$$\mathbf{E}_r = \hat{x} E_{r0} e^{jk_1 z}$$

$$\mathbf{H}_r = -\hat{y} \frac{E_{r0}}{\eta_1} e^{jk_1 z}$$

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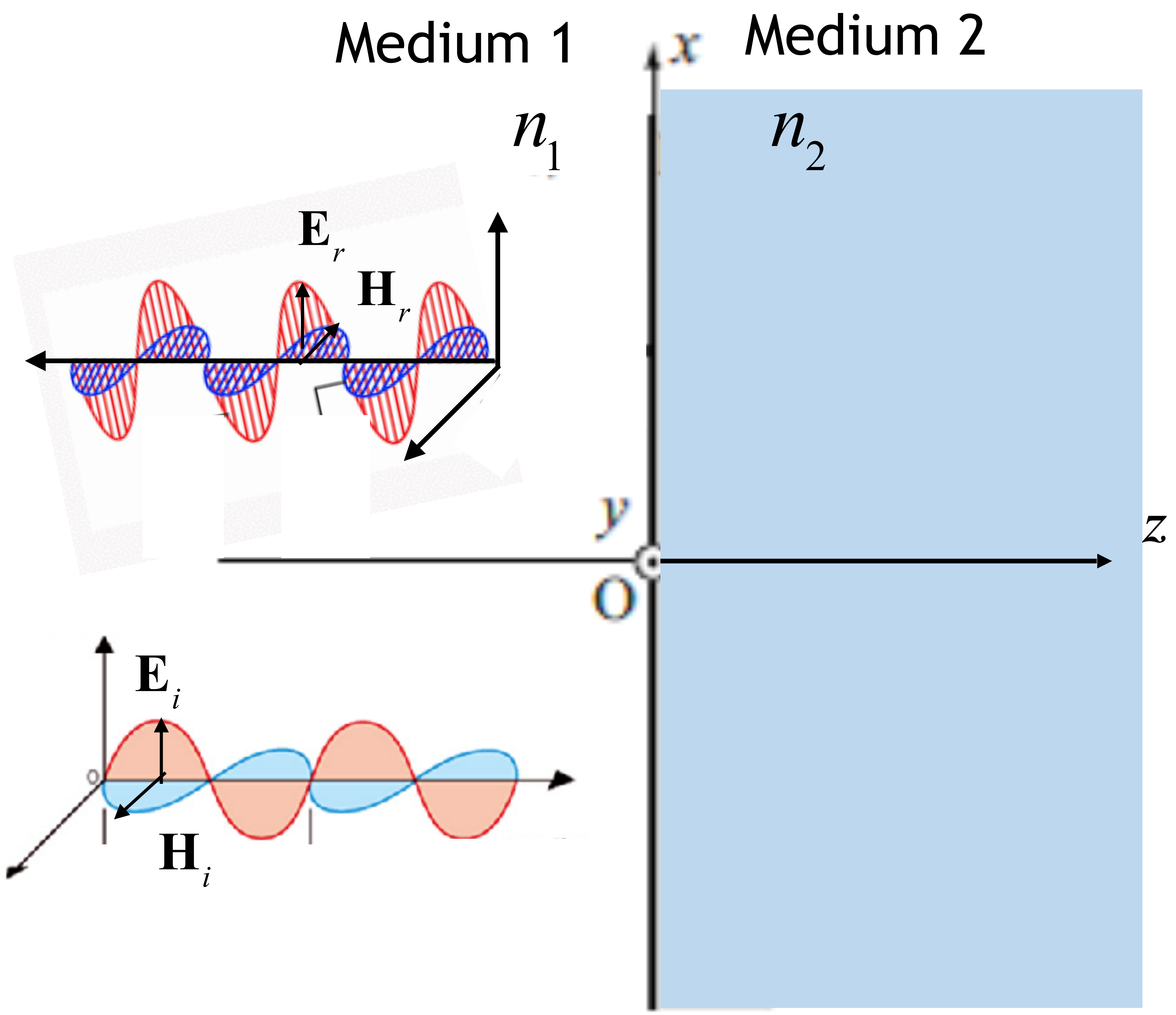

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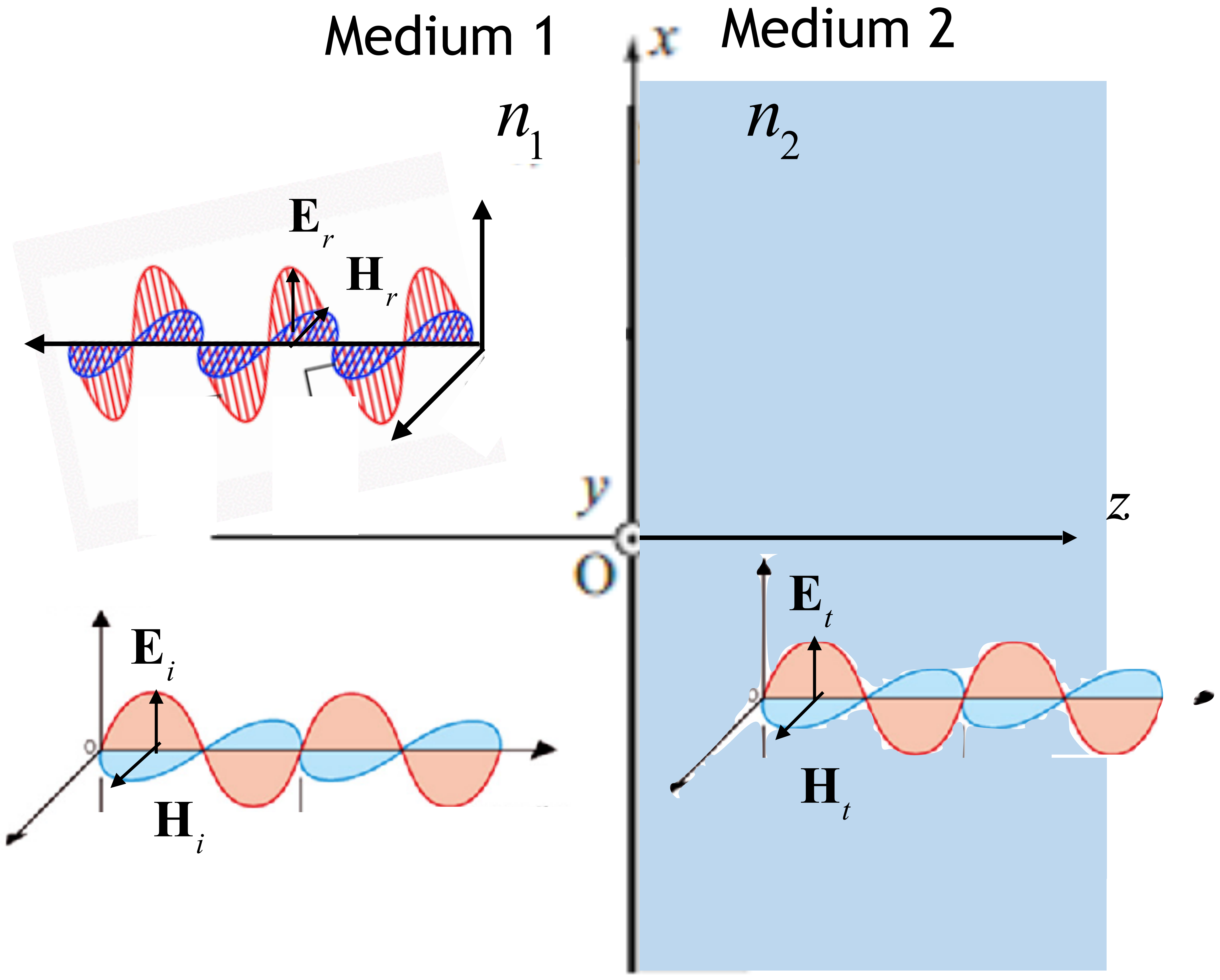

Transmitted wave

$$\mathbf{E}_t = \hat{x} E_{t0} e^{jk_2 z}$$

$$\mathbf{H}_t = \hat{y} \frac{E_{t0}}{\eta_2} e^{jk_2 z}$$

Solving boundary conditions at the interface

Simple problem:
Normal incidence at a dielectric interface

Define reflection and transmission coefficients (Quantities solved for in S4)

Reflected wave

$$\mathbf{E}_r = \hat{x} E_{r0} e^{jk_1 z}$$

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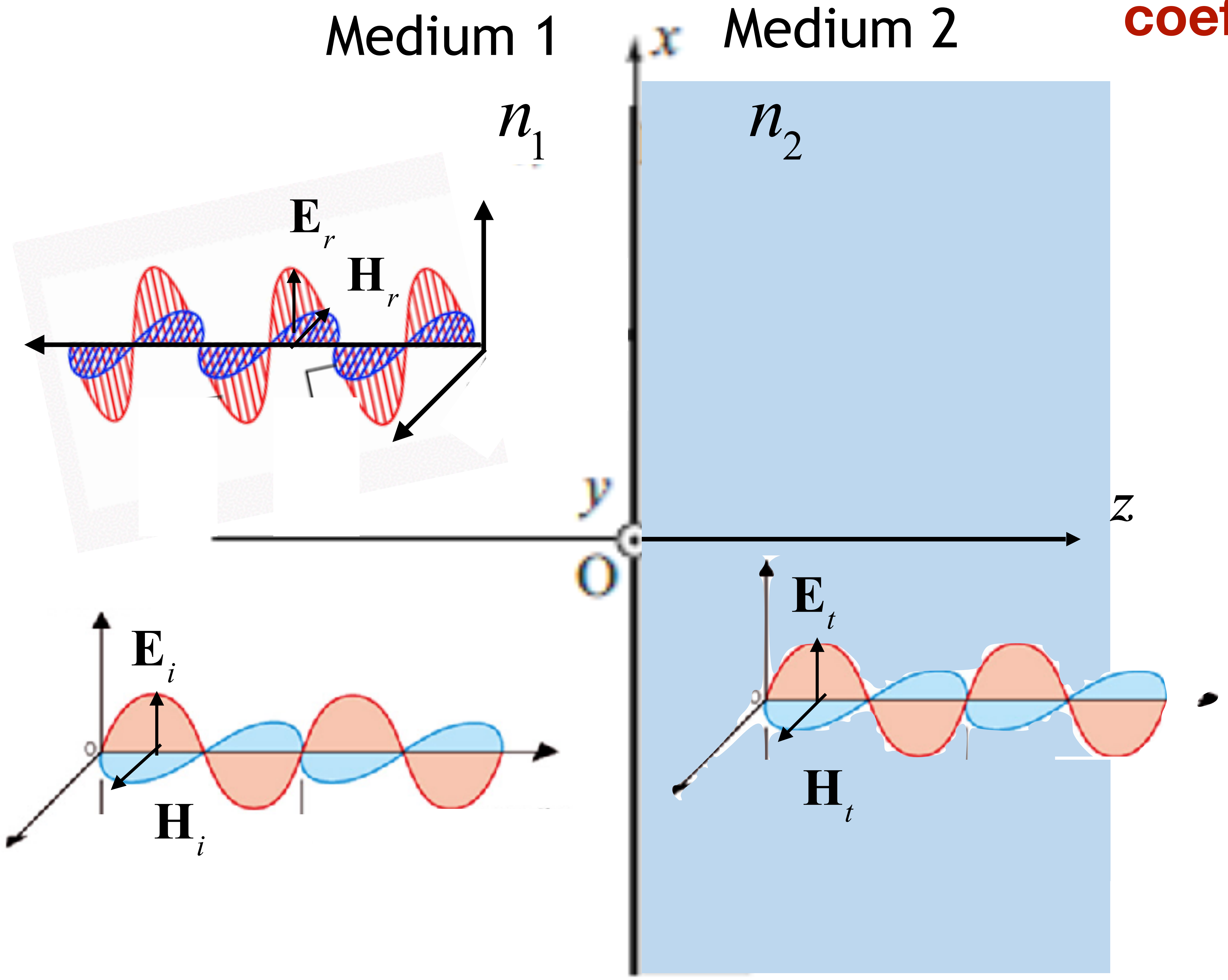

$$r = \left| \frac{E_{r0}}{E_{i0}} \right|^2 \qquad t = 1 - r$$

$$r = \left(\frac{n_1 - n_2}{n_1 + n_2} \right)^2 \qquad t = \frac{4 n_1 n_2}{\left(n_1 + n_2 \right)^2}$$

For normal incidence

Transmitted wave

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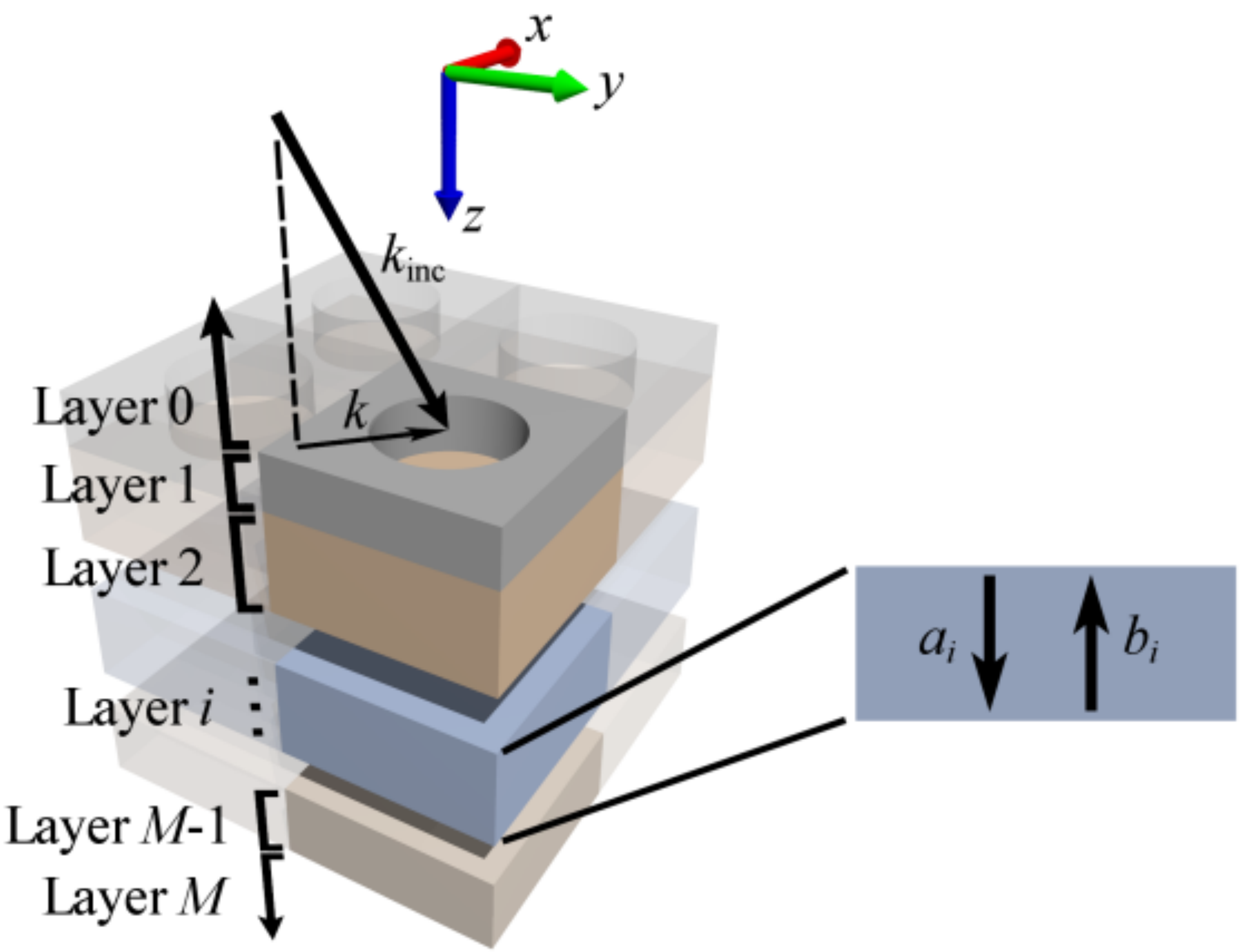
Solving boundary conditions at the interface

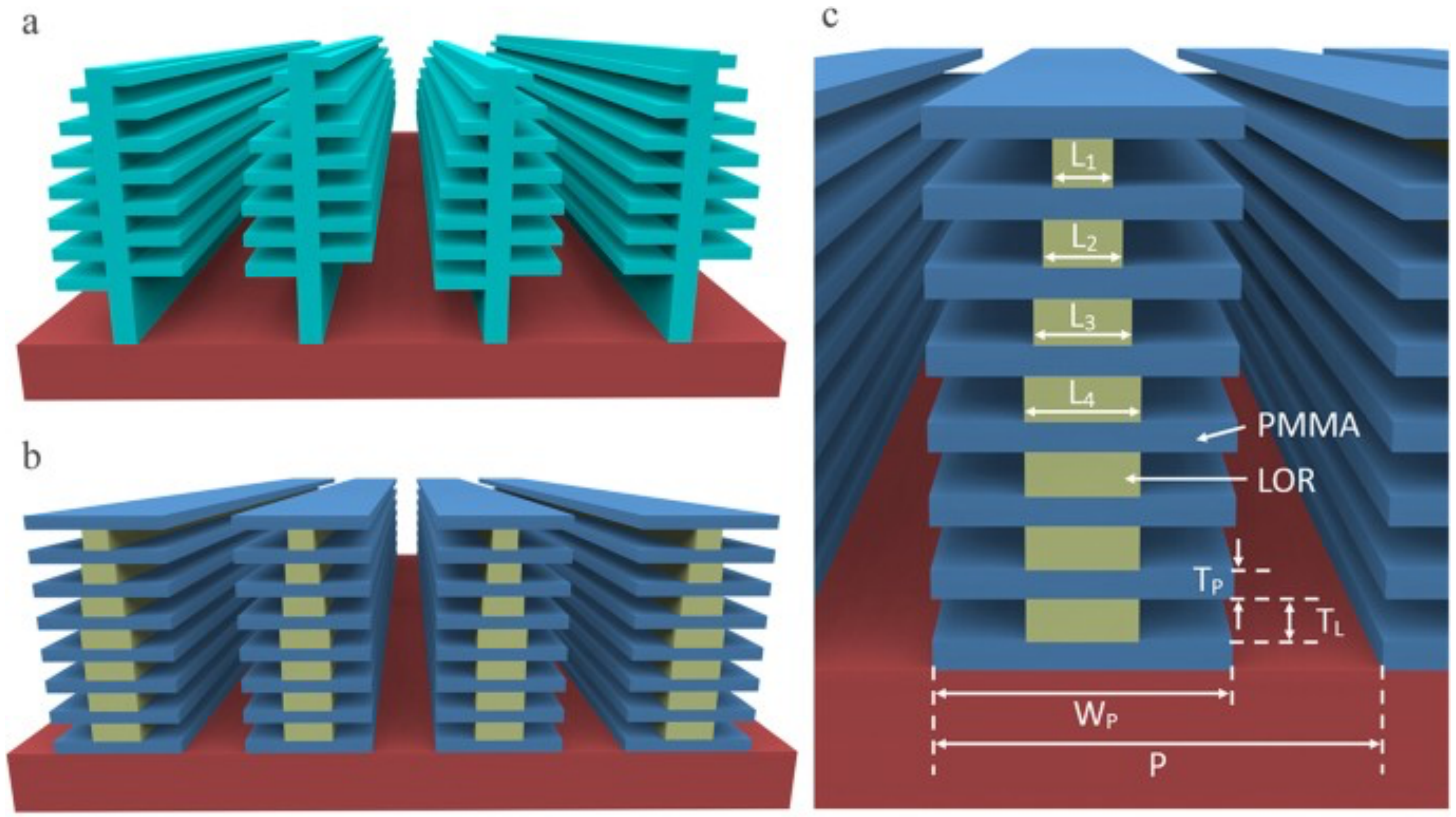
Stanford Stratified Structure Solver (S4)

- A frequency domain code to solve the linear Maxwell's equations in layered periodic structures.
- Implemented using Lua frontend scripting
- Computes transmission, reflection, or absorption spectra of structures composed of periodic, patterned, planar layers.
- We will follow up by a tutorial.



Liu, V., and Fan, S., Computer Physics Communications **183**, 2233-2244 (2012)

The challenge: Reproducing the blue morpho butterfly optical effect



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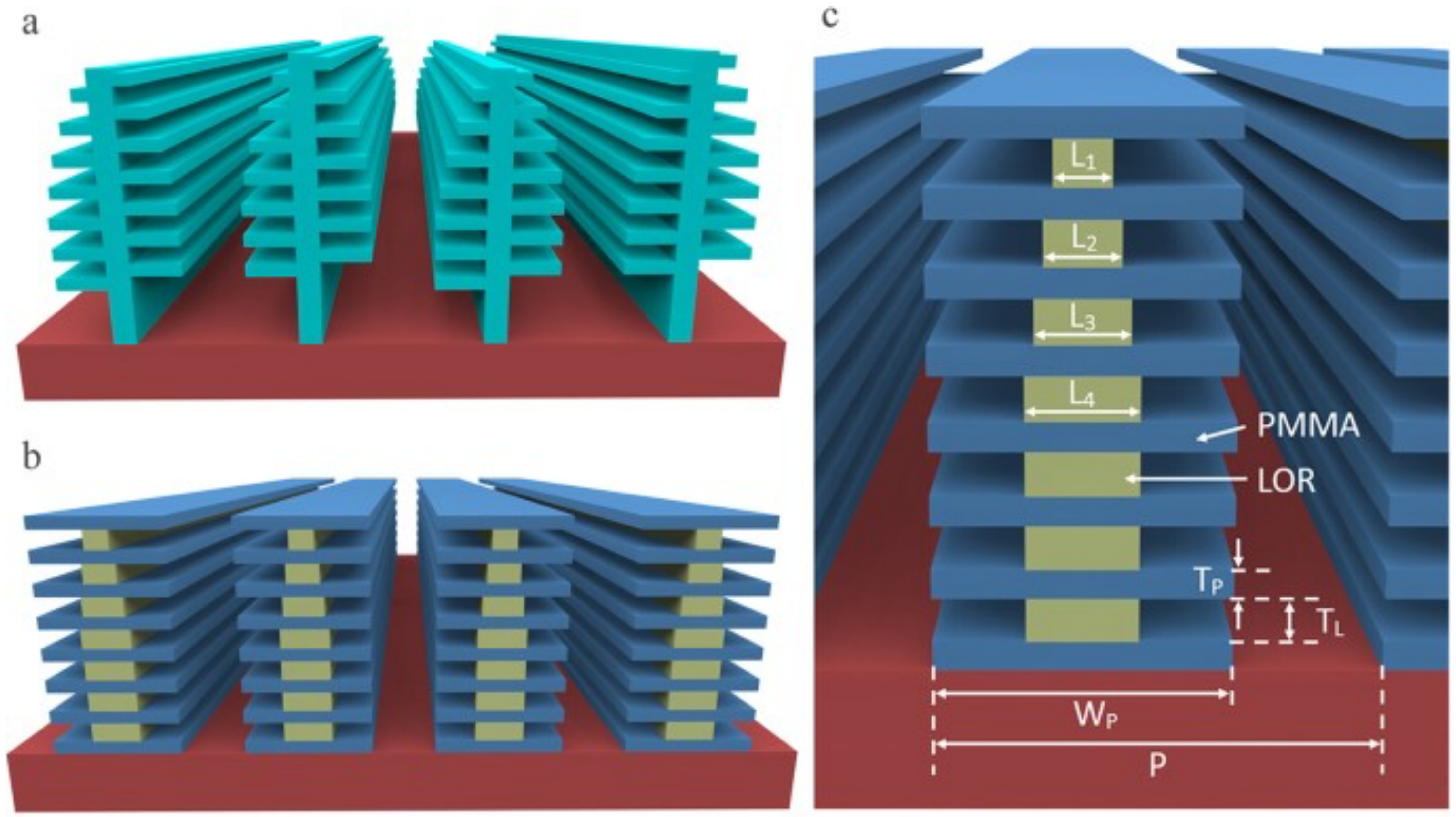

- Benchmark a refractive semi-infinite plane

$$r = \left(\frac{n_1 - n_2}{n_1 + n_2} \right)^2 .$$

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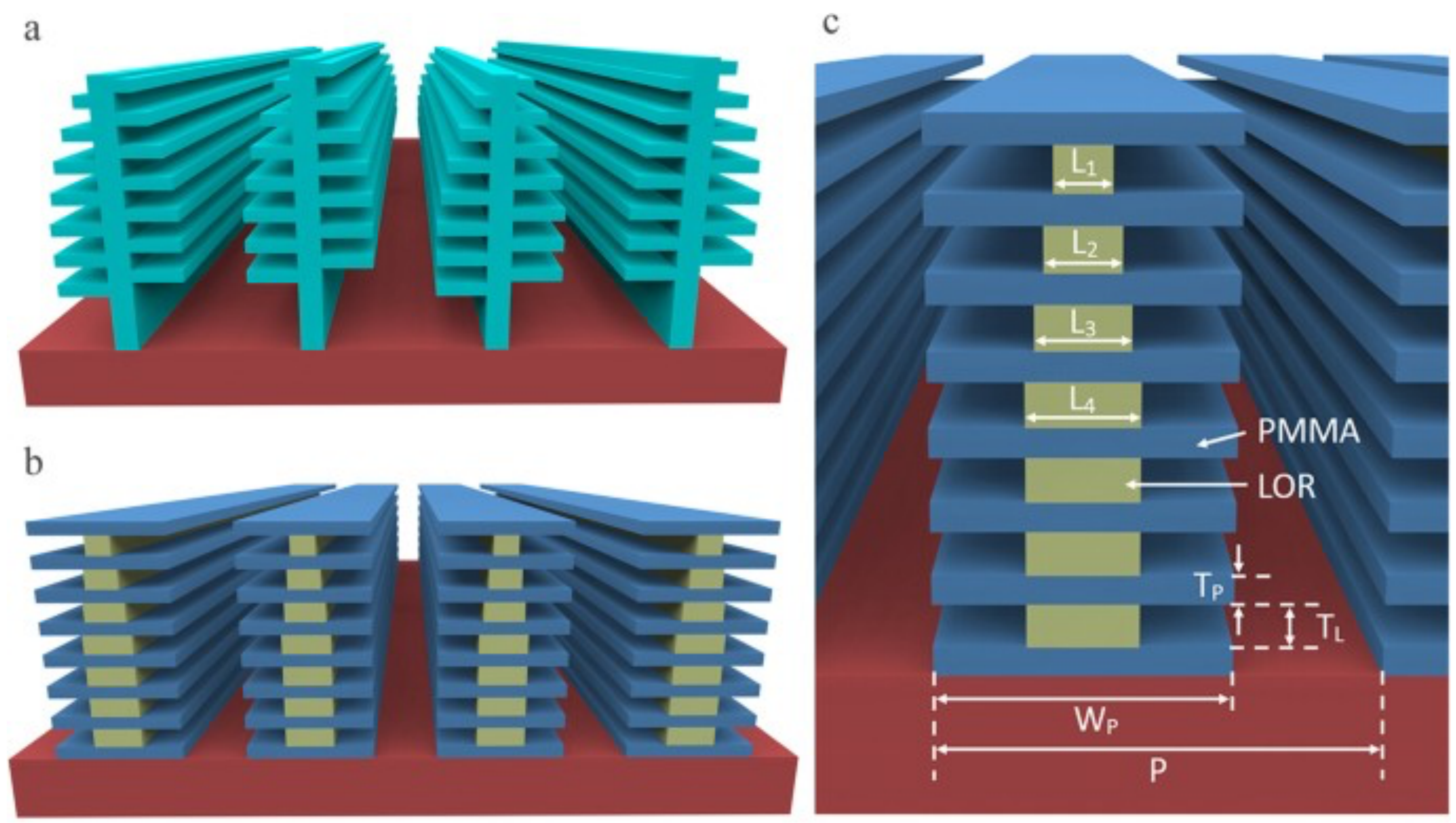

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- Build upon your substrate: What could be a simple multilayer structure to represent the blue morph butterfly?

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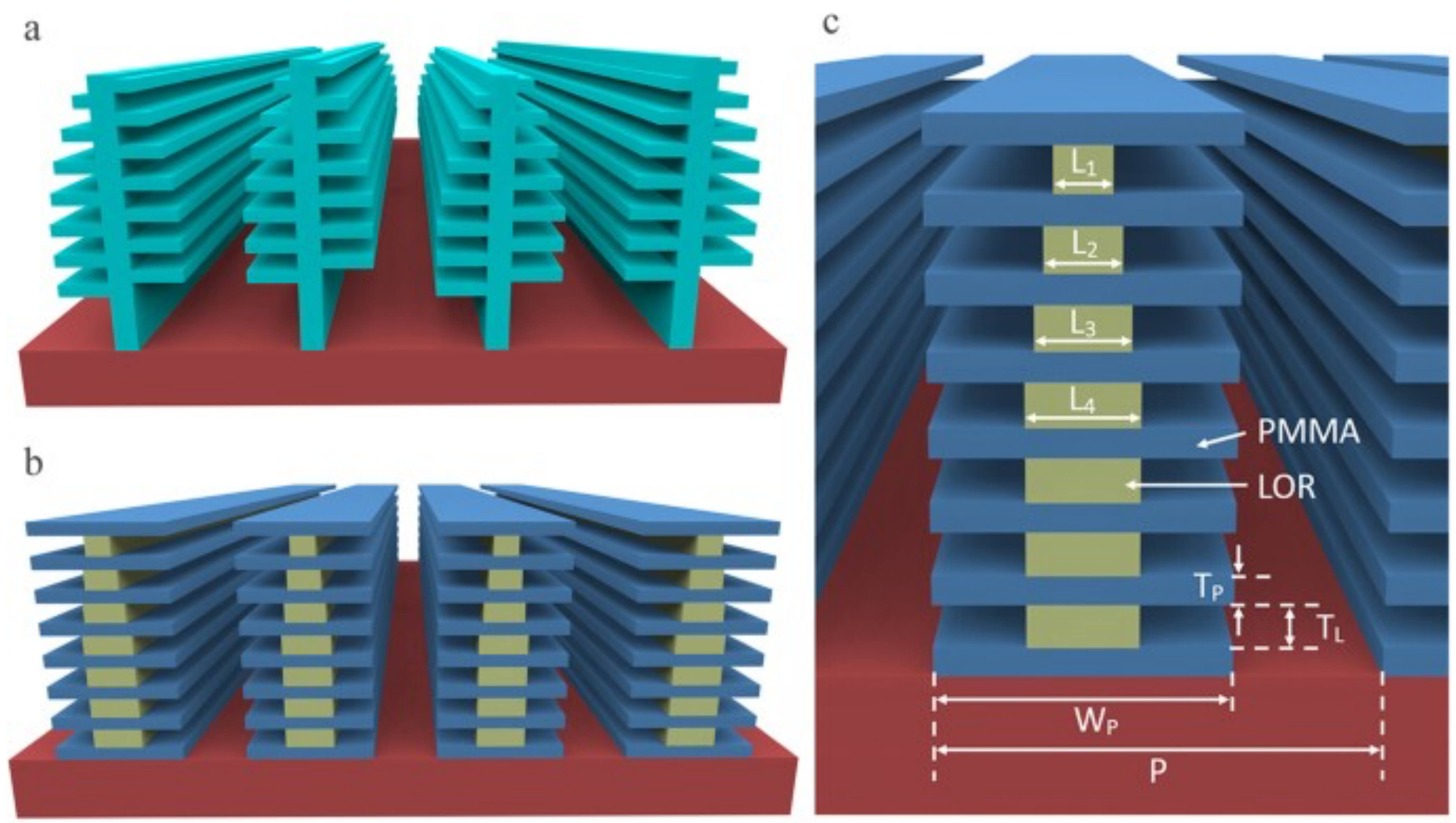

- Benchmark a refractive semi-infinite plane

$$r = \left(\frac{n_1 - n_2}{n_1 + n_2} \right)^2 .$$

- Build upon your substrate: What could be a simple multilayer structure to represent the blue morph butterfly?

- Add more details to your tree structure and compare.

Â Zhang, S., Chen, Y. **Nanofabrication and coloration study of artificial *Morpho* butterfly wings with aligned lamellae layers**. *Sci Rep* 5, 16637 (2015).

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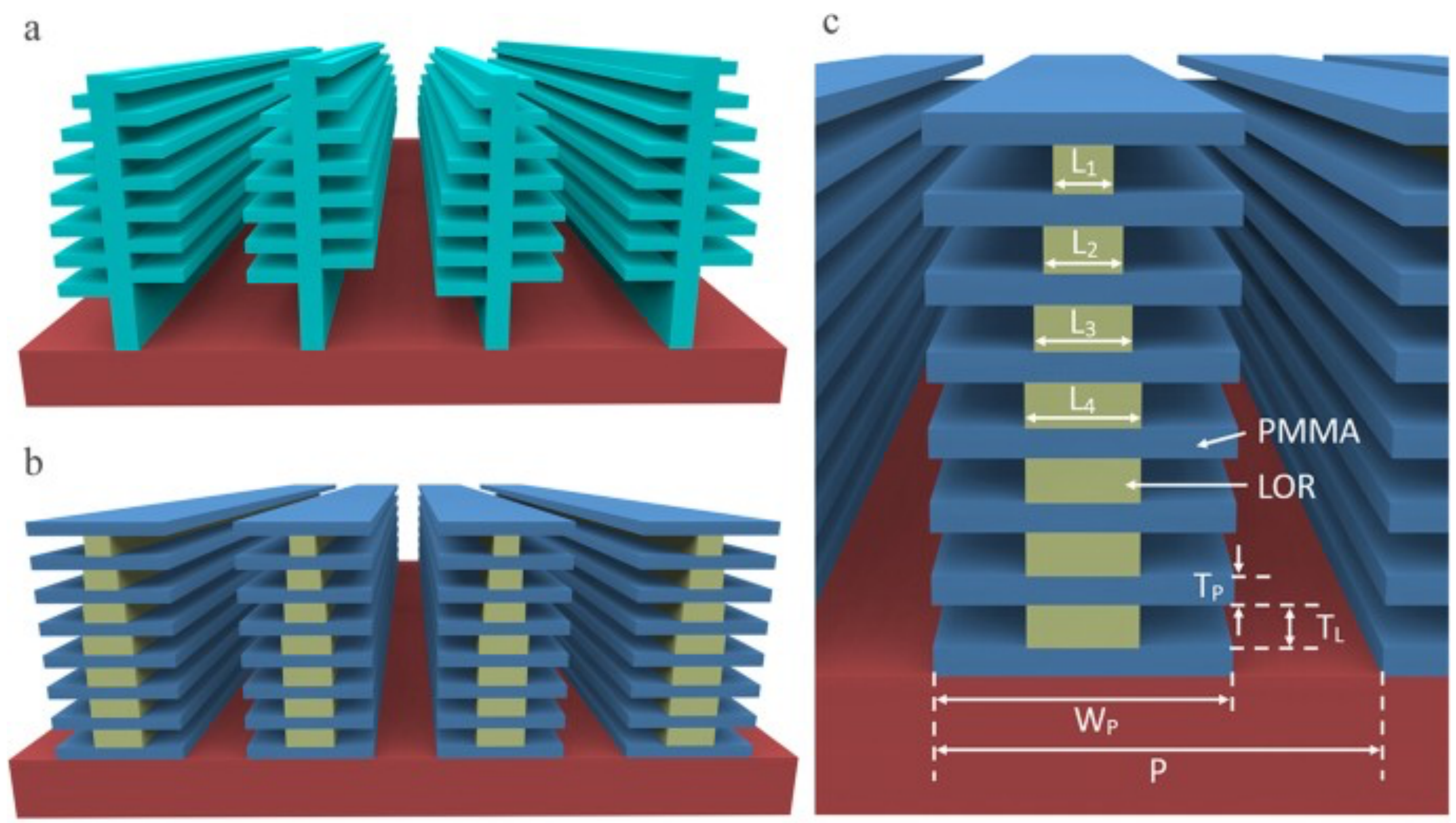

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- What do you conclude from your results? What variables could control wavelength dependence or angular dependence?

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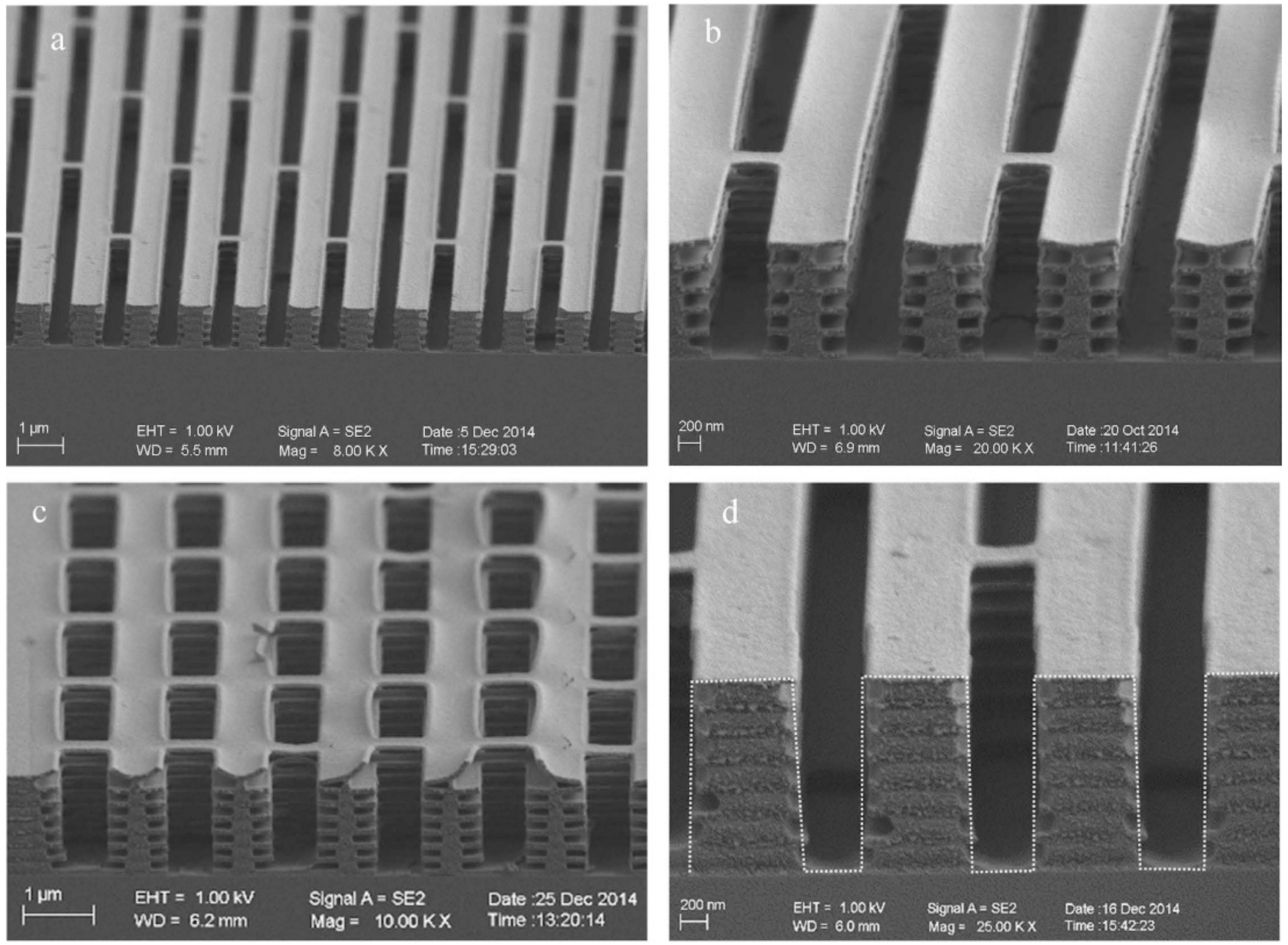
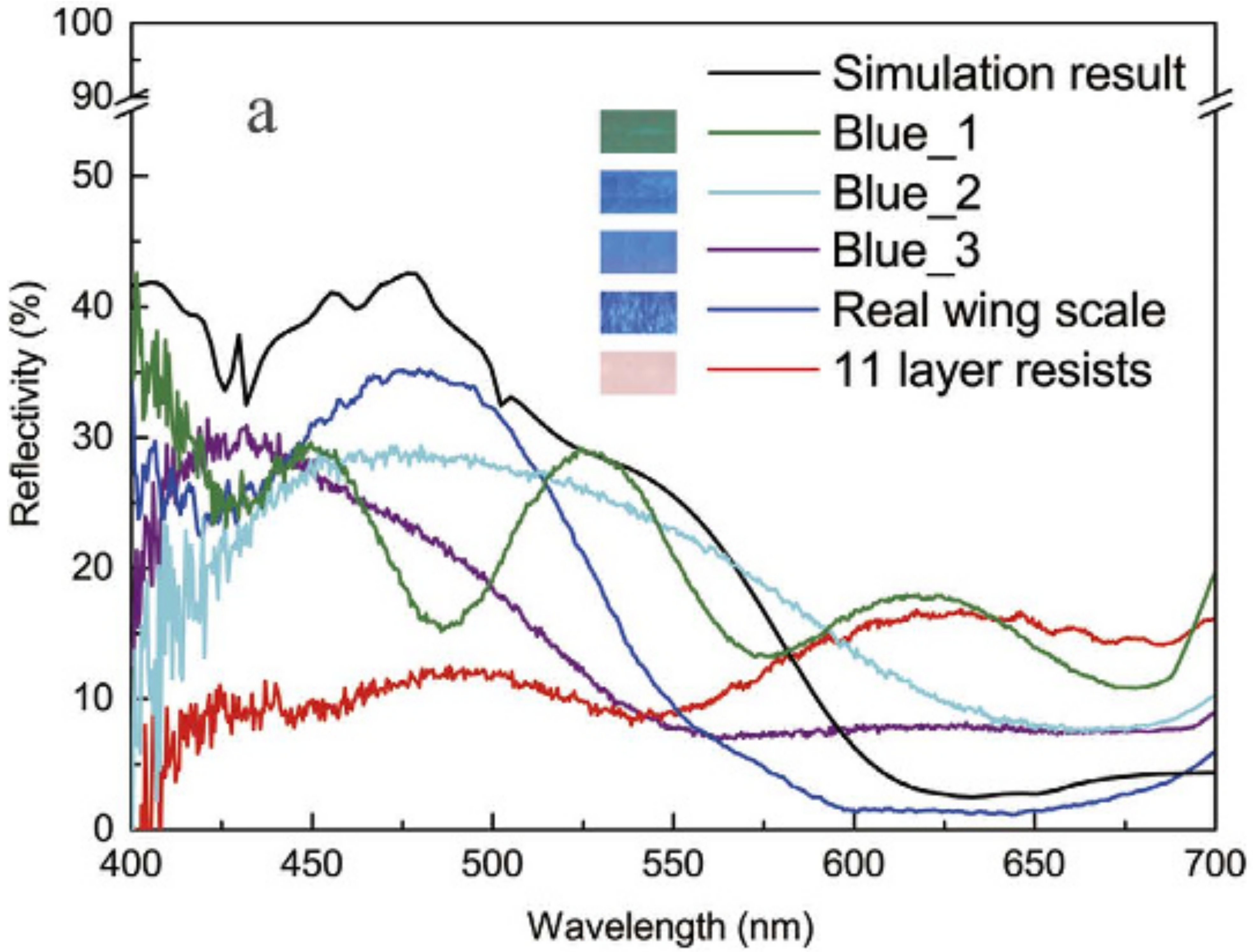
Bioinspired micro grating





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Conclusion

- The morpho butterfly is an example of structural coloring.
- The wing scale of the morpho butterfly inspired artificial structure with added tunability and selectivity.
- Electromagnetic simulation is a powerful technique to understand, analyze and tune many optical effects in nanostructures.

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THANK YOU

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The nanoHUB team