



Advanced Computation:
Computational Electromagnetics

The Method of Lines (MoL)

1

Outline

- Formulation of 3D method of lines
- Formulation of 2D method of lines
- Multilayer devices using scattering matrices
- Comparison to RCWA

2

Definition of Method of Lines

The method of lines was developed by mathematicians to solve partial differential equations (PDEs).

All but one independent variables are discretized.

This leads to a large set of coupled ordinary differential equations (ODEs).

The system of ODEs are solved analytically.

In electromagnetics, the independent variables are usually x , y , and z .

We typically discretize x and y and leave z analytical.

Any method can be used to discretize the independent variables. This includes Fourier transform, finite-differences, finite-elements, etc.

In electromagnetics, the “method of lines” implies that finite-differences are used to discretize x and y .

RCWA is the method of lines, but uses a Fourier transform instead of finite-differences to discretize x and y .

Sign Convention

This formulation of the method of lines uses the following sign convention for waves travelling in the $+z$ direction.

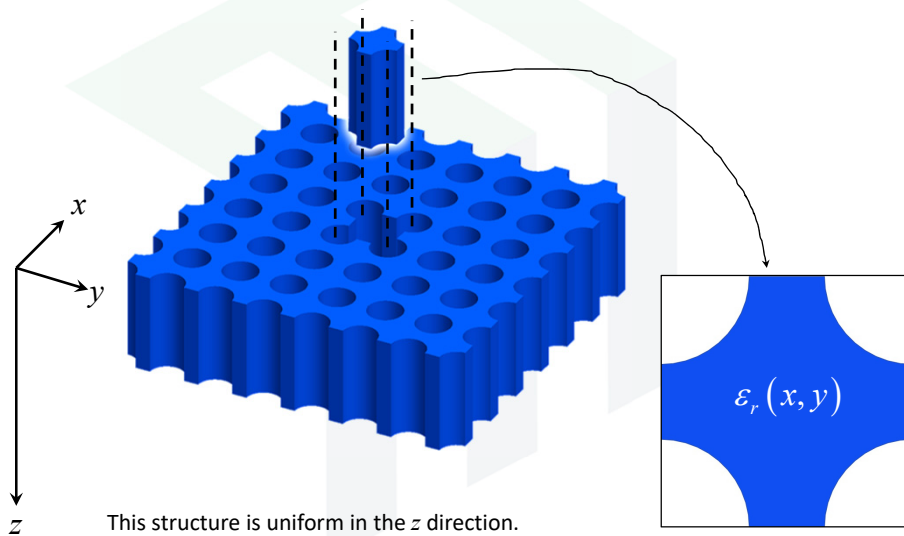
$$e^{-jkz}$$

Formulation of 3D Method of Lines

Slide 5

5

The 2D Unit Cell



EMPossible

Slide 6

6

Starting Point for MOL

We start with Maxwell's equations in the following form...

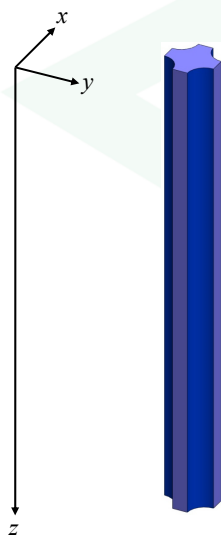
$$\begin{aligned} \frac{\partial E_z}{\partial y'} - \frac{\partial E_y}{\partial z'} &= \mu_r \tilde{H}_x & \frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} &= \varepsilon_r E_x \\ \frac{\partial E_x}{\partial z'} - \frac{\partial E_z}{\partial x'} &= \mu_r \tilde{H}_y & \frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} &= \varepsilon_r E_y \\ \frac{\partial E_y}{\partial x'} - \frac{\partial E_x}{\partial y'} &= \mu_r \tilde{H}_z & \frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'} &= \varepsilon_r E_z \end{aligned}$$

Recall that we normalized the magnetic field and grid according to

$$\tilde{H} = -j \sqrt{\frac{\mu_0}{\varepsilon_0}} \vec{H} \quad x' = k_0 x \quad y' = k_0 y \quad z' = k_0 z$$

7

z-Uniform Media



We are going to consider Maxwell's equations inside a media that is uniform in the z direction.

The media may be inhomogeneous in the x - y plane, but it must be uniform in the z direction.

8

Semi-Analytical Matrix Form of Maxwell's Equations

We can go straight to matrix form using the concept of matrix derivative operators. We keep the z direction analytical.

$$\frac{\partial E_z}{\partial y'} - \frac{\partial E_y}{\partial z'} = \mu \tilde{H}_x$$

$$\frac{\partial E_x}{\partial z'} - \frac{\partial E_z}{\partial x'} = \mu \tilde{H}_y$$

$$\frac{\partial E_y}{\partial x'} - \frac{\partial E_x}{\partial y'} = \mu \tilde{H}_z$$



$$\mathbf{D}_{y'}^e \mathbf{e}_z - \frac{d}{dz'} \mathbf{e}_y = \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z = \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x = \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z$$

$$\frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} = \epsilon_x E_x$$

$$\frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} = \epsilon_x E_y$$

$$\frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'} = \epsilon_x E_z$$



$$\mathbf{D}_{y'}^h \tilde{\mathbf{h}}_z - \frac{d}{dz'} \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z = \boldsymbol{\epsilon}_{yy} \mathbf{e}_y$$

$$\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x = \boldsymbol{\epsilon}_{zz} \mathbf{e}_z$$

Eliminate Longitudinal Field Components

We solve the third and sixth equation for \mathbf{e}_z and \mathbf{h}_z and substitute these back into the remaining four equations.

$$\mathbf{D}_{y'}^e \mathbf{e}_z - \frac{d}{dz'} \mathbf{e}_y = \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x \quad \rightarrow \quad \frac{d}{dz'} \mathbf{e}_x = -\mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x + (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \tilde{\mathbf{h}}_y$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z = \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y \quad \rightarrow \quad \frac{d}{dz'} \mathbf{e}_y = -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) \tilde{\mathbf{h}}_x + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x = \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z \quad \rightarrow \quad \tilde{\mathbf{h}}_z = \boldsymbol{\mu}_{zz}^{-1} (\mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x)$$

$$\mathbf{D}_{y'}^h \tilde{\mathbf{h}}_z - \frac{d}{dz'} \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{xx} \mathbf{e}_x \quad \rightarrow \quad \frac{d}{dz'} \tilde{\mathbf{h}}_x = -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e \mathbf{e}_x + (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \mathbf{e}_y$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z = \boldsymbol{\epsilon}_{yy} \mathbf{e}_y \quad \rightarrow \quad \frac{d}{dz'} \tilde{\mathbf{h}}_y = -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) \mathbf{e}_x + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y$$

$$\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x = \boldsymbol{\epsilon}_{zz} \mathbf{e}_z \quad \rightarrow \quad \mathbf{e}_z = \boldsymbol{\epsilon}_{zz}^{-1} (\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x)$$

Block Matrix Form

We write the remaining four equations in block matrix form as

$$\begin{aligned} \frac{d}{dz'} \mathbf{e}_y &= -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) \tilde{\mathbf{h}}_x + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y \\ \frac{d}{dz'} \mathbf{e}_x &= -\mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x + (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \tilde{\mathbf{h}}_y \end{aligned}$$

$$\frac{d}{dz'} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \begin{bmatrix} -\mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h & (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \\ -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) & \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix}$$

$$\begin{aligned} \frac{d}{dz'} \tilde{\mathbf{h}}_x &= -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e \mathbf{e}_x + (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \mathbf{e}_y \\ \frac{d}{dz'} \tilde{\mathbf{h}}_y &= -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) \mathbf{e}_x + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y \end{aligned}$$

$$\frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} = \begin{bmatrix} -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e & (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \\ -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) & \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \end{bmatrix} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix}$$

Standard PQ Form

We can now write our two equations in the “standard” **P** and **Q** form.

$$\frac{d}{dz'} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \mathbf{P} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} \quad \mathbf{P} = \begin{bmatrix} -\mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h & (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \\ -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) & \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \end{bmatrix}$$

$$\frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} = \mathbf{Q} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e & (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \\ -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) & \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \end{bmatrix}$$

Matrix Wave Equation

We differentiate the “P” equation with respect to z' and substitute the “Q” equation into the result to derive the matrix wave equation.

$$\begin{aligned} \frac{d}{dz'} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{P} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} & \frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} &= \mathbf{Q} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \\ \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{P} \cdot \frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} \\ \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{PQ} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \\ \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} - \mathbf{PQ} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} - \mathbf{\Omega}^2 \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{0} \\ \mathbf{\Omega}^2 &= \mathbf{PQ} \end{aligned}$$

Solution to the Wave Equation

The solution to the wave equation is written the same as in RCWA and TMM.

$$\begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \mathbf{W} e^{-\lambda z'} \mathbf{c}^+ + \mathbf{W} e^{\lambda z'} \mathbf{c}^- \quad \text{where } \mathbf{W} \text{ and } \lambda^2 \text{ are the eigen-vectors} \\ \text{and eigen-values of } \mathbf{\Omega}^2$$

The overall solution is then

$$\Psi(\tilde{z}) = \begin{bmatrix} \mathbf{e}_x(\tilde{z}) \\ \mathbf{e}_y(\tilde{z}) \\ \tilde{\mathbf{h}}_x(\tilde{z}) \\ \tilde{\mathbf{h}}_y(\tilde{z}) \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ -\mathbf{V} & \mathbf{V} \end{bmatrix} \begin{bmatrix} e^{-\lambda \tilde{z}} & \mathbf{0} \\ \mathbf{0} & e^{\lambda \tilde{z}} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix} \quad \mathbf{V} = \mathbf{QW}\lambda^{-1}$$

Based on previous lectures, you know the rest of this story!

Interpretation of the Solution

$$\boldsymbol{\psi}(\tilde{z}) = \mathbf{W} e^{\lambda \tilde{z}} \mathbf{c}$$

$\boldsymbol{\psi}(z)$ – Overall solution which is the sum of all the modes at plane z' .

\mathbf{W} – Square matrix whose column vectors describe the “modes” that can exist in the material. These are essentially pictures of the modes which quantify the relative amplitudes of $E_x, E_y, H_x,$ and H_y .

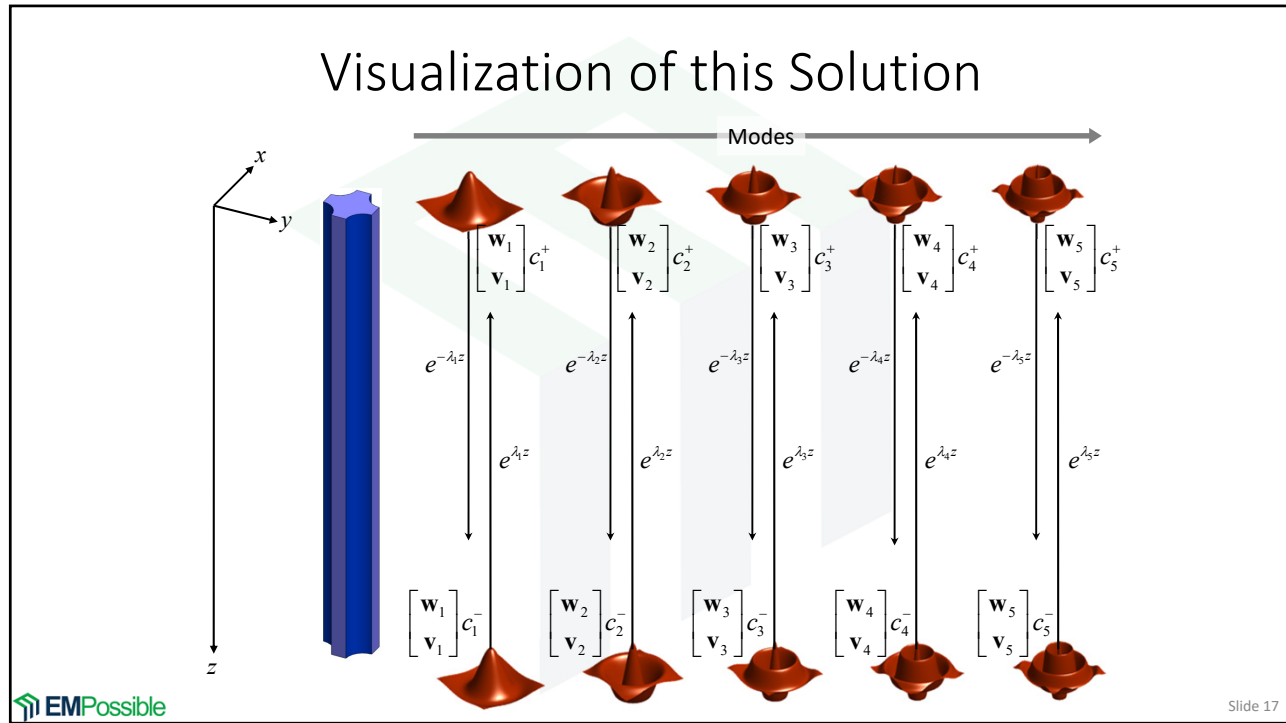
\mathbf{c} – Column vector containing the amplitude coefficient of each of the modes. This quantifies how much energy is in each mode.

$e^{\lambda z'}$ – Diagonal matrix describing how the modes propagate. This includes accumulation of phase as well as decaying (loss) or growing (gain) amplitude.

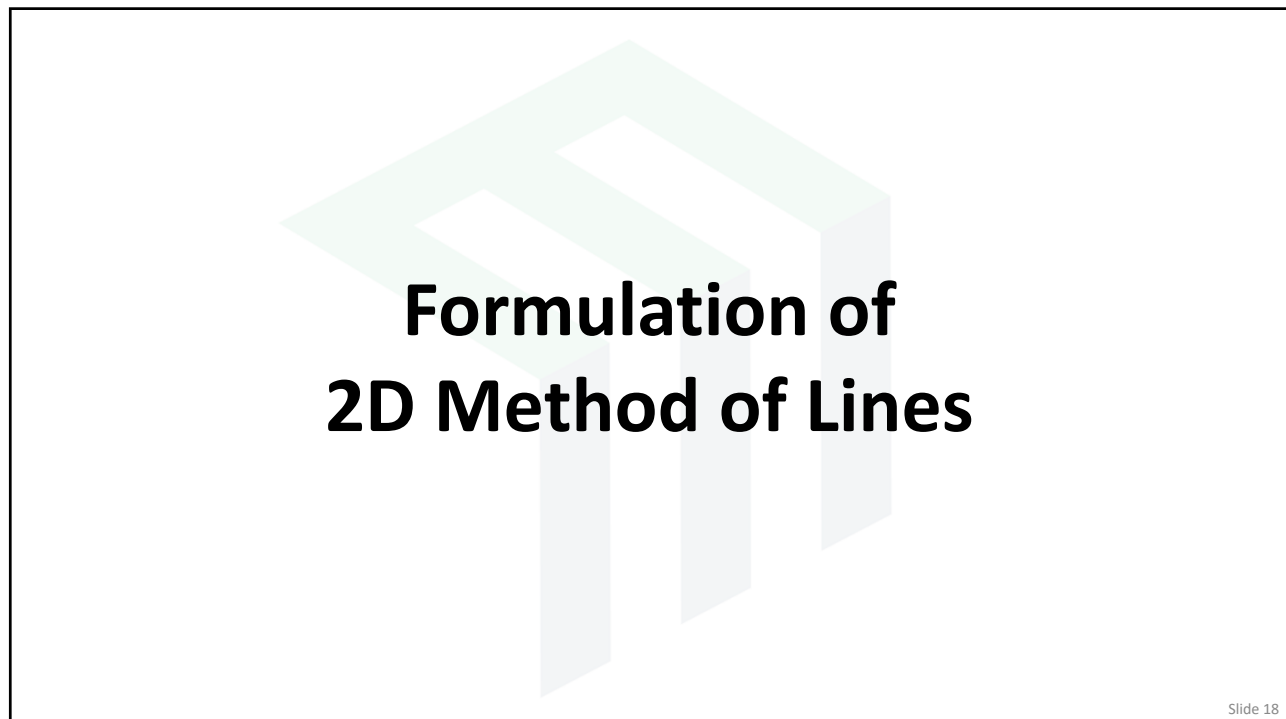
Solution in a Homogeneous Layer

In a homogeneous layer, the \mathbf{P} and \mathbf{Q} matrices are

$$\mathbf{P} = \frac{1}{\epsilon_r} \begin{bmatrix} -\mathbf{D}_x^e \mathbf{D}_y^h & (\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_x^e \mathbf{D}_x^h) \\ -(\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_y^e \mathbf{D}_y^h) & \mathbf{D}_y^e \mathbf{D}_x^h \end{bmatrix} \quad \mathbf{Q} = \frac{1}{\mu_r} \begin{bmatrix} -\mathbf{D}_x^h \mathbf{D}_y^e & (\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_x^h \mathbf{D}_x^e) \\ -(\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_y^h \mathbf{D}_y^e) & \mathbf{D}_y^h \mathbf{D}_x^e \end{bmatrix}$$



17



18

Starting Point

We will start with Maxwell's equations in real-space and in matrix form as derived earlier this lecture.

$$\frac{\partial E_z}{\partial y'} - \frac{\partial E_y}{\partial z'} = \mu_1 \tilde{H}_x$$

$$\frac{\partial E_x}{\partial z'} - \frac{\partial E_z}{\partial x'} = \mu_1 \tilde{H}_y$$

$$\frac{\partial E_y}{\partial x'} - \frac{\partial E_x}{\partial y'} = \mu_1 \tilde{H}_z$$



$$\mathbf{D}_{y'}^e \mathbf{e}_z - \frac{d}{dz'} \mathbf{e}_y = \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z = \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x = \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z$$

$$\frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} = \epsilon_1 E_x$$

$$\frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} = \epsilon_1 E_y$$

$$\frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'} = \epsilon_1 E_z$$



$$\mathbf{D}_{y'}^h \tilde{\mathbf{h}}_z - \frac{d}{dz'} \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z = \boldsymbol{\epsilon}_{yy} \mathbf{e}_y$$

$$\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x = \boldsymbol{\epsilon}_{zz} \mathbf{e}_z$$

Reduction to Two Dimensions

For diagonally anisotropic devices that are uniform in the y direction and when there is no wave propagation in the y direction, we have

$$\mathbf{D}_{y'}^e = \mathbf{D}_{y'}^h = \mathbf{0}$$

Maxwell's equations reduce to

$$-\frac{d}{dz'} \mathbf{e}_y = \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z = \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_{x'}^e \mathbf{e}_y = \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z = \boldsymbol{\epsilon}_{yy} \mathbf{e}_y$$

$$\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{zz} \mathbf{e}_z$$

Two Independent Modes

Maxwell's equations have decoupled into two independent modes.

$$-\frac{d}{dz'} \mathbf{e}_y = \mu_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_x^e \mathbf{e}_z = \mu_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_x^e \mathbf{e}_y = \mu_{zz} \tilde{\mathbf{h}}_z$$

E Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_x^h \tilde{\mathbf{h}}_z = \epsilon_{yy} \mathbf{e}_y$$

$$-\frac{d}{dz'} \mathbf{e}_y = \mu_{xx} \tilde{\mathbf{h}}_x$$

$$\mathbf{D}_x^e \mathbf{e}_y = \mu_{zz} \tilde{\mathbf{h}}_z$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \epsilon_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_x^h \tilde{\mathbf{h}}_z = \epsilon_{yy} \mathbf{e}_y$$

$$\mathbf{D}_x^h \tilde{\mathbf{h}}_y = \epsilon_{zz} \mathbf{e}_z$$

H Mode

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_x^e \mathbf{e}_z = \mu_{yy} \tilde{\mathbf{h}}_y$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \epsilon_{xx} \mathbf{e}_x$$

$$\mathbf{D}_x^h \tilde{\mathbf{h}}_y = \epsilon_{zz} \mathbf{e}_z$$

Apply Dielectric Smoothing

To improve convergence, we can incorporate dielectric smoothing as follows:

E Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_x^h \tilde{\mathbf{h}}_z = \langle \epsilon_{yy} \rangle \mathbf{e}_y$$

$$-\frac{d}{dz'} \mathbf{e}_y = \langle \mu_{xx}^{-1} \rangle^{-1} \tilde{\mathbf{h}}_x$$

$$\mathbf{D}_x^e \mathbf{e}_y = \langle \mu_{zz} \rangle \tilde{\mathbf{h}}_z$$

H Mode

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_x^e \mathbf{e}_z = \langle \mu_{yy} \rangle \tilde{\mathbf{h}}_y$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \langle \epsilon_{xx}^{-1} \rangle^{-1} \mathbf{e}_x$$

$$\mathbf{D}_x^h \tilde{\mathbf{h}}_y = \langle \epsilon_{zz} \rangle \mathbf{e}_z$$

Eliminate Longitudinal Components

We solve for the longitudinal components

$$\tilde{\mathbf{h}}_z = \langle \boldsymbol{\mu}_{zz} \rangle^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y$$

$$\mathbf{e}_z = \langle \boldsymbol{\epsilon}_{zz} \rangle^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y$$

and substitute these expressions into the remaining equations.

E Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x = \langle \boldsymbol{\epsilon}_{yy} \rangle \mathbf{e}_y + \mathbf{D}_{x'}^h \langle \boldsymbol{\mu}_{zz} \rangle^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y$$

$$\frac{d}{dz'} \mathbf{e}_y = -\langle \boldsymbol{\mu}_{xx}^{-1} \rangle^{-1} \tilde{\mathbf{h}}_x$$

H Mode

$$\frac{d}{dz'} \mathbf{e}_x = \langle \boldsymbol{\mu}_{yy} \rangle \tilde{\mathbf{h}}_y + \mathbf{D}_{x'}^e \langle \boldsymbol{\epsilon}_{zz} \rangle^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_y = -\langle \boldsymbol{\epsilon}_{xx}^{-1} \rangle^{-1} \mathbf{e}_x$$

Standard P and Q Form

We write our matrix equations in the standard **PQ** form.

E Mode

$$\frac{d}{dz'} \mathbf{e}_y = \mathbf{P} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x = \mathbf{Q} \mathbf{e}_y$$

$$\mathbf{P} = -\langle \boldsymbol{\mu}_{xx}^{-1} \rangle^{-1}$$

$$\mathbf{Q} = \langle \boldsymbol{\epsilon}_{yy} \rangle + \mathbf{D}_{x'}^h \langle \boldsymbol{\mu}_{zz} \rangle^{-1} \mathbf{D}_{x'}^e$$

H Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_y = \mathbf{P} \mathbf{e}_x$$

$$\frac{d}{dz'} \mathbf{e}_x = \mathbf{Q} \tilde{\mathbf{h}}_y$$

$$\mathbf{P} = -\langle \boldsymbol{\epsilon}_{xx}^{-1} \rangle^{-1}$$

$$\mathbf{Q} = \langle \boldsymbol{\mu}_{yy} \rangle + \mathbf{D}_{x'}^e \langle \boldsymbol{\epsilon}_{zz} \rangle^{-1} \mathbf{D}_{x'}^h$$

...and now you know the rest of the story.

Multilayer Devices Using Scattering Matrices

R. C. Rumpf, "Improved formulation of scattering matrices for semi-analytical methods that is consistent with convention," PIERS B, Vol. 35, 241-261, 2011.

Slide 25

25

Eigen System in Each Layer

Boundary conditions required that all layers have the same K_x and K_y matrices.

$$P_1 = \begin{bmatrix} -D_y^0 \epsilon_{zz}^1 D_y^0 & (\mu_{xy} + D_y^0 \epsilon_{zz}^1 D_y^0) \\ -(\mu_{xz} + D_y^0 \epsilon_{zz}^1 D_y^0) & D_y^0 \epsilon_{zz}^1 D_y^0 \end{bmatrix}$$

$$Q_1 = \begin{bmatrix} -D_y^0 \mu_{zz}^1 D_y^0 & (\epsilon_{xy} + D_y^0 \mu_{zz}^1 D_y^0) \\ -(\epsilon_{xz} + D_y^0 \mu_{zz}^1 D_y^0) & D_y^0 \mu_{zz}^1 D_y^0 \end{bmatrix}$$

$$\Omega_1^2 = P_1 Q_1 \rightarrow W_1, \lambda_1 \rightarrow V_1 \quad c_1^+, c_1^-$$

$$P_2 = \begin{bmatrix} -D_y^1 \epsilon_{zz}^2 D_y^1 & (\mu_{xy} + D_y^1 \epsilon_{zz}^2 D_y^1) \\ -(\mu_{xz} + D_y^1 \epsilon_{zz}^2 D_y^1) & D_y^1 \epsilon_{zz}^2 D_y^1 \end{bmatrix}$$

$$Q_2 = \begin{bmatrix} -D_y^1 \mu_{zz}^2 D_y^1 & (\epsilon_{xy} + D_y^1 \mu_{zz}^2 D_y^1) \\ -(\epsilon_{xz} + D_y^1 \mu_{zz}^2 D_y^1) & D_y^1 \mu_{zz}^2 D_y^1 \end{bmatrix}$$

$$\Omega_2^2 = P_2 Q_2 \rightarrow W_2, \lambda_2 \rightarrow V_2 \quad c_2^+, c_2^-$$

$$P_3 = \begin{bmatrix} -D_y^2 \epsilon_{zz}^3 D_y^2 & (\mu_{xy} + D_y^2 \epsilon_{zz}^3 D_y^2) \\ -(\mu_{xz} + D_y^2 \epsilon_{zz}^3 D_y^2) & D_y^2 \epsilon_{zz}^3 D_y^2 \end{bmatrix}$$

$$Q_3 = \begin{bmatrix} -D_y^2 \mu_{zz}^3 D_y^2 & (\epsilon_{xy} + D_y^2 \mu_{zz}^3 D_y^2) \\ -(\epsilon_{xz} + D_y^2 \mu_{zz}^3 D_y^2) & D_y^2 \mu_{zz}^3 D_y^2 \end{bmatrix}$$

$$\Omega_3^2 = P_3 Q_3 \rightarrow W_3, \lambda_3 \rightarrow V_3 \quad c_3^+, c_3^-$$

Slide 26

26

Field Relations & Boundary Conditions

Field inside the i^{th} layer:

$$\Psi_i(\tilde{z}) = \begin{bmatrix} \mathbf{e}_x(\tilde{z}) \\ \mathbf{e}_y(\tilde{z}) \\ \tilde{\mathbf{h}}_x(\tilde{z}) \\ \tilde{\mathbf{h}}_y(\tilde{z}) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\lambda_i \tilde{z}} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i \tilde{z}} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Boundary conditions at the first interface:

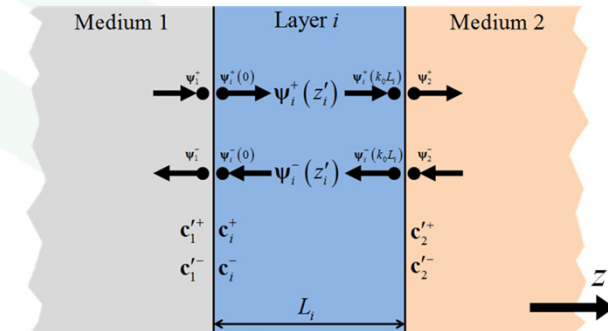
$$\Psi_1 = \Psi_i(0)$$

$$\begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ -\mathbf{V}_1 & \mathbf{V}_1 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1^+ \\ \mathbf{c}_1^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Boundary conditions at the second interface:

$$\Psi_i(k_0 L_i) = \Psi_2$$

$$\begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\lambda_i k_0 L_i} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i k_0 L_i} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_2 & \mathbf{W}_2 \\ -\mathbf{V}_2 & \mathbf{V}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{bmatrix}$$



Note: k_0 has been incorporated to normalize L_i .

27

Adopt the Symmetric S-Matrix Approach

The scattering matrix \mathbf{S}_i of the i^{th} layer is still defined as:

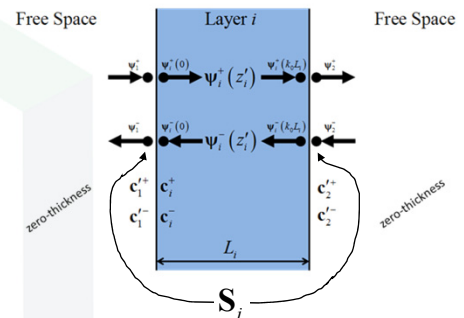
$$\begin{bmatrix} \mathbf{c}_1'^- \\ \mathbf{c}_2'^+ \end{bmatrix} = \mathbf{S}^{(i)} \begin{bmatrix} \mathbf{c}_1'^+ \\ \mathbf{c}_2'^- \end{bmatrix} \quad \mathbf{S}^{(i)} = \begin{bmatrix} \mathbf{S}_{11}^{(i)} & \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{21}^{(i)} & \mathbf{S}_{22}^{(i)} \end{bmatrix}$$

But the elements are calculated as

$$\mathbf{S}_{11}^{(i)} = (\mathbf{A}_i - \mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{B}_i)^{-1} (\mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{A}_i - \mathbf{B}_i)$$

$$\mathbf{S}_{12}^{(i)} = (\mathbf{A}_i - \mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{B}_i)^{-1} \mathbf{X}_i (\mathbf{A}_i - \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{B}_i)$$

$$\left. \begin{aligned} \mathbf{S}_{21}^{(i)} &= \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{22}^{(i)} &= \mathbf{S}_{11}^{(i)} \end{aligned} \right\} \begin{aligned} &\bullet \text{Layers are symmetric so the scattering matrix elements have redundancy.} \\ &\bullet \text{Scattering matrix equations are simplified.} \\ &\bullet \text{Fewer calculations.} \\ &\bullet \text{Less memory storage.} \end{aligned}$$



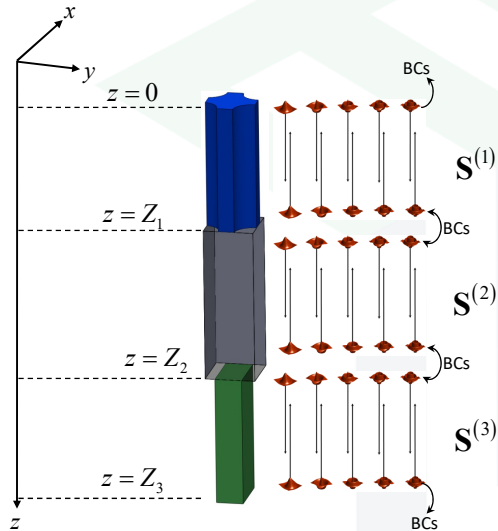
$$\mathbf{A}_i = \mathbf{W}_i^{-1} \mathbf{W}_0 + \mathbf{V}_i^{-1} \mathbf{V}_0$$

$$\mathbf{B}_i = \mathbf{W}_i^{-1} \mathbf{W}_0 - \mathbf{V}_i^{-1} \mathbf{V}_0$$

$$\mathbf{X}_i = e^{-\lambda_i k_0 L_i}$$

28

Global Scattering Matrix



Scattering matrix for all layers.

$$\mathbf{S}^{(\text{device})} = \mathbf{S}^{(1)} \otimes \mathbf{S}^{(2)} \otimes \mathbf{S}^{(3)}$$

Connection to outside regions

$$\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{ref})} \otimes \mathbf{S}^{(\text{device})} \otimes \mathbf{S}^{(\text{tm})}$$

Recall this procedure from Lecture 5.

Reflection/Transmission Side Scattering Matrices

The reflection-side scattering matrix is

$$\mathbf{S}_{11}^{(\text{ref})} = -\mathbf{A}_{\text{ref}}^{-1} \mathbf{B}_{\text{ref}}$$

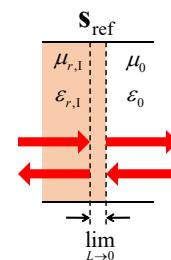
$$\mathbf{S}_{12}^{(\text{ref})} = 2\mathbf{A}_{\text{ref}}^{-1}$$

$$\mathbf{S}_{21}^{(\text{ref})} = 0.5(\mathbf{A}_{\text{ref}} - \mathbf{B}_{\text{ref}} \mathbf{A}_{\text{ref}}^{-1} \mathbf{B}_{\text{ref}})$$

$$\mathbf{S}_{22}^{(\text{ref})} = \mathbf{B}_{\text{ref}} \mathbf{A}_{\text{ref}}^{-1}$$

$$\mathbf{A}_{\text{ref}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}$$

$$\mathbf{B}_{\text{ref}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}$$



The transmission-side scattering matrix is

$$\mathbf{S}_{11}^{(\text{tm})} = \mathbf{B}_{\text{tm}} \mathbf{A}_{\text{tm}}^{-1}$$

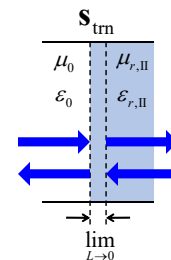
$$\mathbf{S}_{12}^{(\text{tm})} = 0.5(\mathbf{A}_{\text{tm}} - \mathbf{B}_{\text{tm}} \mathbf{A}_{\text{tm}}^{-1} \mathbf{B}_{\text{tm}})$$

$$\mathbf{S}_{21}^{(\text{tm})} = 2\mathbf{A}_{\text{tm}}^{-1}$$

$$\mathbf{S}_{22}^{(\text{tm})} = -\mathbf{A}_{\text{tm}}^{-1} \mathbf{B}_{\text{tm}}$$

$$\mathbf{A}_{\text{tm}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{tm}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{tm}}$$

$$\mathbf{B}_{\text{tm}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{tm}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{tm}}$$



Calculating the Transmitted and Reflected Fields

The electric field source is calculated as

$$\mathbf{c}_{\text{inc}} = \mathbf{W}_{\text{ref}}^{-1} \bar{\mathbf{e}}_{xy}^{\text{inc}} \quad \bar{\mathbf{e}}_{xy}^{\text{inc}} = \begin{bmatrix} p_x e^{-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)} \\ p_y e^{-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)} \end{bmatrix}$$

\mathbf{x} and \mathbf{y} are column vectors containing the coordinates of the points in the cross section.

Recall calculating the polarization components p_x and p_y in TMM.
 $|\bar{\mathbf{p}}| = 1$

Given the global scattering matrix, the coefficients for the reflected and transmitted fields are

$$\mathbf{c}_{\text{ref}} = \mathbf{S}_{11} \mathbf{c}_{\text{inc}} \quad \mathbf{c}_{\text{tm}} = \mathbf{S}_{21} \mathbf{c}_{\text{inc}}$$

The transverse components of the reflected and transmitted fields are then

$$\bar{\mathbf{e}}_{xy}^{\text{ref}} = \mathbf{W}_{\text{ref}} \mathbf{c}_{\text{ref}} = \mathbf{W}_{\text{ref}} \mathbf{S}_{11} \mathbf{c}_{\text{inc}} = \begin{bmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{bmatrix}$$

$$\bar{\mathbf{e}}_{xy}^{\text{tm}} = \mathbf{W}_{\text{tm}} \mathbf{c}_{\text{tm}} = \mathbf{W}_{\text{tm}} \mathbf{S}_{21} \mathbf{c}_{\text{inc}} = \begin{bmatrix} \mathbf{t}_x \\ \mathbf{t}_y \end{bmatrix}$$

31

Calculate the Amplitudes of the Spatial Harmonics

Remove the phase tilt

$$A_{x,\text{ref}}(x, y) = r_x(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

$$A_{y,\text{ref}}(x, y) = r_y(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

$$A_{x,\text{tm}}(x, y) = t_x(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

$$A_{y,\text{tm}}(x, y) = t_y(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

Calculate amplitudes of the spatial harmonics

$$\mathbf{r}_x = \text{FFT}_{2D} \{A_{x,\text{ref}}(x, y)\}$$

$$\mathbf{r}_y = \text{FFT}_{2D} \{A_{y,\text{ref}}(x, y)\}$$

$$\mathbf{t}_x = \text{FFT}_{2D} \{A_{x,\text{tm}}(x, y)\}$$

$$\mathbf{t}_y = \text{FFT}_{2D} \{A_{y,\text{tm}}(x, y)\}$$

32

Calculating the Longitudinal Components

The longitudinal field components are calculated from the transverse components using the divergence equation.

$$\mathbf{r}_z = -\mathbf{K}_{z,\text{ref}}^{-1} \left(\mathbf{K}_x \mathbf{r}_x + \mathbf{K}_y \mathbf{r}_y \right)$$

$$\mathbf{t}_z = -\mathbf{K}_{z,\text{tm}}^{-1} \left(\mathbf{K}_x \mathbf{t}_x + \mathbf{K}_y \mathbf{t}_y \right)$$

Note, the \mathbf{K} matrices are not normalized.

Calculating the Diffraction Efficiencies

The diffraction efficiencies \mathbf{R} and \mathbf{T} are calculated as

$$|\vec{\mathbf{r}}|^2 = |\mathbf{r}_x|^2 + |\mathbf{r}_y|^2 + |\mathbf{r}_z|^2$$

$$|\vec{\mathbf{t}}|^2 = |\mathbf{t}_x|^2 + |\mathbf{t}_y|^2 + |\mathbf{t}_z|^2$$

$$\mathbf{R} = \frac{\text{Re} \left[-\mathbf{K}_{z,\text{ref}} / \mu_{r,\text{inc}} \right]}{\text{Re} \left[k_z^{\text{inc}} / \mu_{r,\text{inc}} \right]} |\vec{\mathbf{r}}|^2$$

$$\mathbf{T} = \frac{\text{Re} \left[\mathbf{K}_{z,\text{tm}} / \mu_{r,\text{tm}} \right]}{\text{Re} \left[k_z^{\text{inc}} / \mu_{r,\text{inc}} \right]} |\vec{\mathbf{t}}|^2$$

Remember that these equations assume the source was given unit amplitude.

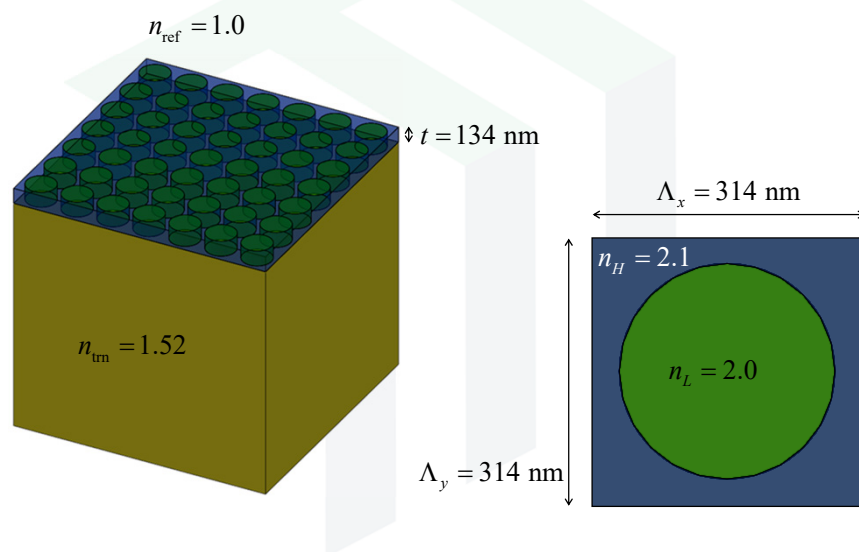
Note, the \mathbf{K} matrices are not normalized here.

Comparison to RCWA

Slide 35

35

Dielectric Device Comparison



EMPossible

Slide 36

36

Comparison of Model Results

