Advanced Computation:
Computational Electromagnetics

Slice Absorption Method (SAM)

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Outline

- Three-Dimensional FDFD
- Matrix Ordering
- Slice Absorption Method
- Plane Wave Source
- Transparent Boundary Condition
- Field Solution
- Fourier-Space SAM
- Example Simulations
- Dispersion Analysis Using the SAM

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Three-Dimensional FDFD

Matrix Form of Maxwell's Equations

$$\frac{\partial}{\partial y'}E_z - \frac{\partial}{\partial z'}E_y = \mu_{xx}\tilde{H}_x \qquad \frac{E_z^{i,j+1,k} - E_z^{i,j,k}}{\Delta y'} - \frac{E_y^{i,j,k+1} - E_y^{i,j,k}}{\Delta z'} = \mu_{xx}^{i,j,k}\tilde{H}_x^{i,j,k} \qquad \mathbf{D}_{y'}^{e}\mathbf{e}_z - \mathbf{D}_{z'}^{e}\mathbf{e}_y = \boldsymbol{\mu}_{xx}\tilde{\mathbf{h}}_x$$

$$\frac{\partial}{\partial z'}E_x - \frac{\partial}{\partial x'}E_z = \mu_{yy}\tilde{H}_y \;\Rightarrow\; \frac{E_x^{i,j,k+1} - E_x^{i,j,k}}{\Delta z'} - \frac{E_z^{i+1,j,k} - E_z^{i,j,k}}{\Delta x'} = \mu_{yy}^{i,j,k}\tilde{H}_y^{i,j,k} \;\Rightarrow\; \mathbf{D}_{z'}^{e}\mathbf{e}_x - \mathbf{D}_{x'}^{e}\mathbf{e}_z = \boldsymbol{\mu}_{yy}\tilde{\mathbf{h}}_y$$

$$\frac{\partial}{\partial x'}E_y - \frac{\partial}{\partial y'}E_x = \mu_{zz}\tilde{H}_z \qquad \frac{E_y^{i+1,j,k} - E_y^{i,j,k}}{\Delta x'} - \frac{E_x^{i,j+1,k} - E_x^{i,j,k}}{\Delta y'} = \mu_{zz}^{i,j,k}\tilde{H}_z^{i,j,k} \qquad \mathbf{D}_{x'}^{e}\mathbf{e}_y - \mathbf{D}_{y'}^{e}\mathbf{e}_x = \boldsymbol{\mu}_{zz}\tilde{\mathbf{h}}_z$$

$$\frac{\partial}{\partial y'}\tilde{H}_z - \frac{\partial}{\partial z'}\tilde{H}_y = \varepsilon_{xx}E_x \qquad \frac{\tilde{H}_z^{i,j,k} - \tilde{H}_z^{i,j-1,k}}{\Delta y'} - \frac{\tilde{H}_y^{i,j,k} - \tilde{H}_y^{i,j,k-1}}{\Delta z'} = \varepsilon_{xx}^{i,j,k}E_x^{i,j,k} \qquad \mathbf{D}_{y'}^{h}\tilde{\mathbf{h}}_z - \mathbf{D}_{z'}^{h}\tilde{\mathbf{h}}_y = \boldsymbol{\varepsilon}_{xx}\mathbf{e}_x$$

$$\frac{\partial}{\partial z'}\tilde{H}_x - \frac{\partial}{\partial x'}\tilde{H}_z = \varepsilon_{yy}E_y \;\Rightarrow\; \frac{\tilde{H}_x^{i,j,k} - \tilde{H}_x^{i,j,k-1}}{\Delta z'} - \frac{\tilde{H}_z^{i,j,k} - \tilde{H}_z^{i-1,j,k}}{\Delta x'} = \varepsilon_{yy}^{i,j,k}E_y^{i,j,k} \;\Rightarrow\; \mathbf{D}_{z'}^{h}\tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^{h}\tilde{\mathbf{h}}_z = \boldsymbol{\varepsilon}_{yy}\mathbf{e}_y$$

$$\frac{\partial}{\partial x'}\tilde{H}_y - \frac{\partial}{\partial y'}\tilde{H}_x = \varepsilon_{zz}E_z \qquad \frac{\tilde{H}_y^{i,j,k} - \tilde{H}_y^{i-1,j,k}}{\Delta x'} - \frac{\tilde{H}_x^{i,j,k} - \tilde{H}_x^{i,j-1,k}}{\Delta y'} = \varepsilon_{zz}^{i,j,k}E_z^{i,j,k} \qquad \mathbf{D}_{x'}^{h}\tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^{h}\tilde{\mathbf{h}}_x = \boldsymbol{\varepsilon}_{zz}\mathbf{e}_z$$

Block Matrix Form

We can write our matrix equations in block matrix form.

$$\begin{aligned}\mathbf{D}^e_{y'}\mathbf{e}_z - \mathbf{D}^e_{z'}\mathbf{e}_y &= \boldsymbol{\mu}_{xx}\tilde{\mathbf{h}}_x\\ \mathbf{D}^e_{z'}\mathbf{e}_x - \mathbf{D}^e_{x'}\mathbf{e}_z &= \boldsymbol{\mu}_{yy}\tilde{\mathbf{h}}_y\\ \mathbf{D}^e_{x'}\mathbf{e}_y - \mathbf{D}^e_{y'}\mathbf{e}_x &= \boldsymbol{\mu}_{zz}\tilde{\mathbf{h}}_z\end{aligned} \;\Rightarrow\; \begin{bmatrix}\mathbf{0} & -\mathbf{D}^e_{z'} & \mathbf{D}^e_{y'}\\ \mathbf{D}^e_{z'} & \mathbf{0} & -\mathbf{D}^e_{x'}\\ -\mathbf{D}^e_{y'} & \mathbf{D}^e_{x'} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{e}_x\\ \mathbf{e}_y\\ \mathbf{e}_z\end{bmatrix} = \begin{bmatrix}\boldsymbol{\mu}_{xx} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\mu}_{yy} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \boldsymbol{\mu}_{zz}\end{bmatrix}\begin{bmatrix}\tilde{\mathbf{h}}_x\\ \tilde{\mathbf{h}}_y\\ \tilde{\mathbf{h}}_z\end{bmatrix}$$

$$\nabla' \times \vec{E} = [\mu]\vec{\tilde{H}} \rightarrow \mathbf{C}^e\vec{\mathbf{e}} = [\boldsymbol{\mu}]\vec{\tilde{\mathbf{h}}}$$

$$\begin{aligned}\mathbf{D}^h_{y'}\tilde{\mathbf{h}}_z - \mathbf{D}^h_{z'}\tilde{\mathbf{h}}_y &= \boldsymbol{\varepsilon}_{xx}\mathbf{e}_x\\ \mathbf{D}^h_{z'}\tilde{\mathbf{h}}_x - \mathbf{D}^h_{x'}\tilde{\mathbf{h}}_z &= \boldsymbol{\varepsilon}_{yy}\mathbf{e}_y\\ \mathbf{D}^h_{x'}\tilde{\mathbf{h}}_y - \mathbf{D}^h_{y'}\tilde{\mathbf{h}}_x &= \boldsymbol{\varepsilon}_{zz}\mathbf{e}_z\end{aligned} \;\Rightarrow\; \begin{bmatrix}\mathbf{0} & -\mathbf{D}^h_{z'} & \mathbf{D}^h_{y'}\\ \mathbf{D}^h_{z'} & \mathbf{0} & -\mathbf{D}^h_{x'}\\ -\mathbf{D}^h_{y'} & \mathbf{D}^h_{x'} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\tilde{\mathbf{h}}_x\\ \tilde{\mathbf{h}}_y\\ \tilde{\mathbf{h}}_z\end{bmatrix} = \begin{bmatrix}\boldsymbol{\varepsilon}_{xx} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\varepsilon}_{yy} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \boldsymbol{\varepsilon}_{zz}\end{bmatrix}\begin{bmatrix}\mathbf{e}_x\\ \mathbf{e}_y\\ \mathbf{e}_z\end{bmatrix}$$

$$\nabla' \times \vec{\tilde{H}} = [\varepsilon]\vec{E} \rightarrow \mathbf{C}^h\vec{\tilde{\mathbf{h}}} = [\boldsymbol{\varepsilon}]\vec{\mathbf{e}}$$

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Three-Dimensional FDFD

Block Matrix Form

$$\mathbf{C}^e\vec{\mathbf{e}} = [\boldsymbol{\mu}]\vec{\tilde{\mathbf{h}}}$$

$$\mathbf{C}^h\vec{\tilde{\mathbf{h}}} = [\boldsymbol{\varepsilon}]\vec{\mathbf{e}}$$

$$\vec{\tilde{\mathbf{h}}} = \begin{bmatrix}\tilde{\mathbf{h}}_x\\ \tilde{\mathbf{h}}_y\\ \tilde{\mathbf{h}}_z\end{bmatrix} \qquad \vec{\mathbf{e}} = \begin{bmatrix}\mathbf{e}_x\\ \mathbf{e}_y\\ \mathbf{e}_z\end{bmatrix}$$

$$[\boldsymbol{\mu}] = \begin{bmatrix}\boldsymbol{\mu}_{xx} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\mu}_{yy} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \boldsymbol{\mu}_{zz}\end{bmatrix} \qquad [\boldsymbol{\varepsilon}] = \begin{bmatrix}\boldsymbol{\varepsilon}_{xx} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\varepsilon}_{yy} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \boldsymbol{\varepsilon}_{zz}\end{bmatrix}$$

$$\mathbf{C}^h = \begin{bmatrix}\mathbf{0} & -\mathbf{D}^h_{z'} & \mathbf{D}^h_{y'}\\ \mathbf{D}^h_{z'} & \mathbf{0} & -\mathbf{D}^h_{x'}\\ -\mathbf{D}^h_{y'} & \mathbf{D}^h_{x'} & \mathbf{0}\end{bmatrix} \qquad \mathbf{C}^e = \begin{bmatrix}\mathbf{0} & -\mathbf{D}^e_{z'} & \mathbf{D}^e_{y'}\\ \mathbf{D}^e_{z'} & \mathbf{0} & -\mathbf{D}^e_{x'}\\ -\mathbf{D}^e_{y'} & \mathbf{D}^e_{x'} & \mathbf{0}\end{bmatrix}$$

Matrix Wave Equations

$$\left(\mathbf{C}^e[\boldsymbol{\varepsilon}]^{-1}\mathbf{C}^h - [\boldsymbol{\mu}]\right)\vec{\tilde{\mathbf{h}}} = \mathbf{0}$$

$$\left(\mathbf{C}^h[\boldsymbol{\mu}]^{-1}\mathbf{C}^e - [\boldsymbol{\varepsilon}]\right)\vec{\mathbf{e}} = \mathbf{0}$$

$$\boxed{\boldsymbol{\Omega}\vec{\mathbf{e}} = \mathbf{0}}$$

For 3D analysis, $\boldsymbol{\Omega}$ is usually too big to solve by simple means.

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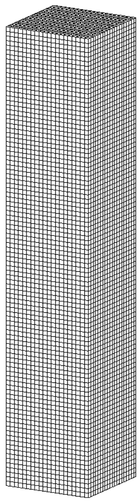
Grid to Matrix Scaling & Memory

Typical grid required to model a 3D device.



$N_x = 20$
$N_y = 20$
$N_z = 100$

Number of points in grid:	40,000 points
Complex #'s for $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$:	120,000 complex #'s
Real #'s for $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$:	240,000 real floating-point #'s
Size of matrix $\mathbf{\Omega}$:	120k × 120k complex #'s
Number of complex elements:	14.4 billion complex #'s
Number of real elements:	28.8 billion real #'s
Memory to store full $\mathbf{\Omega}$:	214.6 Gb
Size of $\mathbf{e}_x$:	40k complex numbers
Memory for $\mathbf{e}_x$:	625 kb
Size of full $\mathbf{D}_x$:	40k × 40k complex numbers
Memory for full $\mathbf{D}_x$:	23.8 Gb
Density of $\mathbf{D}_x$:	0.005% non zero elements
Memory for sparse $\mathbf{D}_x$:	1.5 Mb
Size of full $\mathbf{C}^e$:	120k × 120k complex numbers
Memory for full $\mathbf{C}^e$:	214.6 Gb
Density of $\mathbf{C}^e$:	0.0033% non zero elements
Memory for Sparse $\mathbf{C}^e$:	8.2 Mb
Memory for direct solution:	110 Gb

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Matrix Ordering

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Standard FDFD Order

Matrix Wave Equation

$$\mathbf{\Omega}\vec{\mathbf{e}} = \mathbf{0}$$

$$\mathbf{\Omega} = \mathbf{C}^h [\boldsymbol{\mu}]^{-1} \mathbf{C}^e - [\boldsymbol{\varepsilon}]$$

Matrix Order

$$\begin{bmatrix} \mathbf{\Omega}_{xx} & \mathbf{\Omega}_{xy} & \mathbf{\Omega}_{xz} \\ \mathbf{\Omega}_{yx} & \mathbf{\Omega}_{yy} & \mathbf{\Omega}_{yz} \\ \mathbf{\Omega}_{zx} & \mathbf{\Omega}_{zy} & \mathbf{\Omega}_{zz} \end{bmatrix} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \\ \mathbf{e}_z \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

$$\mathbf{e}_x = \begin{bmatrix} E_x^{1,1,1} \\ E_x^{2,1,1} \\ \vdots \\ E_x^{N_x,1,1} \\ E_x^{1,2,1} \\ E_x^{2,2,1} \\ \vdots \\ E_x^{N_x,2,1} \\ \vdots \\ E_x^{N_x,N_y,1} \\ E_x^{1,1,2} \\ \vdots \\ E_x^{N_x,N_y,N_z} \end{bmatrix} \quad \mathbf{e}_y = \begin{bmatrix} E_y^{1,1,1} \\ E_y^{2,1,1} \\ \vdots \\ E_y^{N_x,1,1} \\ E_y^{1,2,1} \\ E_y^{2,2,1} \\ \vdots \\ E_y^{N_x,2,1} \\ \vdots \\ E_y^{N_x,N_y,1} \\ E_y^{1,1,2} \\ \vdots \\ E_y^{N_x,N_y,N_z} \end{bmatrix} \quad \mathbf{e}_z = \begin{bmatrix} E_z^{1,1,1} \\ E_z^{2,1,1} \\ \vdots \\ E_z^{N_x,1,1} \\ E_z^{1,2,1} \\ E_z^{2,2,1} \\ \vdots \\ E_z^{N_x,2,1} \\ \vdots \\ E_z^{N_x,N_y,1} \\ E_z^{1,1,2} \\ \vdots \\ E_z^{N_x,N_y,N_z} \end{bmatrix}$$

Raster first along x, then y, and then z.

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Reorder Operation

The matrix equation is reordered in a manner that groups all fields located within the same slices into adjacent rows and/or columns.

$$\tilde{\mathbf{\Omega}}\tilde{\mathbf{e}} = \mathbf{0}$$

$$\tilde{\mathbf{\Omega}} = \text{reorder}(\mathbf{\Omega})$$

$$\tilde{\mathbf{e}} = \text{reorder}(\vec{\mathbf{e}})$$

$$\langle \tilde{\mathbf{\Omega}} \rangle_{\tilde{p}\tilde{q}} = \langle \mathbf{\Omega} \rangle_{pq}$$

$$p = 1 + N_x N_y N_z \cdot \text{mod}_3(\tilde{p}-1) + \lfloor (\tilde{p}-1) \div 3 \rfloor$$

$$q = 1 + N_x N_y N_z \cdot \text{mod}_3(\tilde{q}-1) + \lfloor (\tilde{q}-1) \div 3 \rfloor$$

$$\vec{\mathbf{e}} = \begin{bmatrix} E_x^{1,1,1} \\ \vdots \\ E_x^{N_x,N_y,N_z} \\ E_y^{1,1,1} \\ \vdots \\ E_y^{N_x,N_y,N_z} \\ E_z^{1,1,1} \\ \vdots \\ E_z^{N_x,N_y,N_z} \end{bmatrix} \rightarrow \tilde{\mathbf{e}} = \begin{bmatrix} E_x^{1,1,1} \\ E_y^{1,1,1} \\ E_z^{1,1,1} \\ E_x^{2,1,1} \\ E_y^{2,1,1} \\ E_z^{2,1,1} \\ \vdots \\ E_x^{N_x,1,1} \\ E_y^{N_x,1,1} \\ E_z^{N_x,1,1} \\ \vdots \\ E_x^{N_x,N_y,N_z} \\ E_y^{N_x,N_y,N_z} \\ E_z^{N_x,N_y,N_z} \end{bmatrix}$$

We still raster first along x, then y, and then z, but we group the x, y, and z components together instead of separate.

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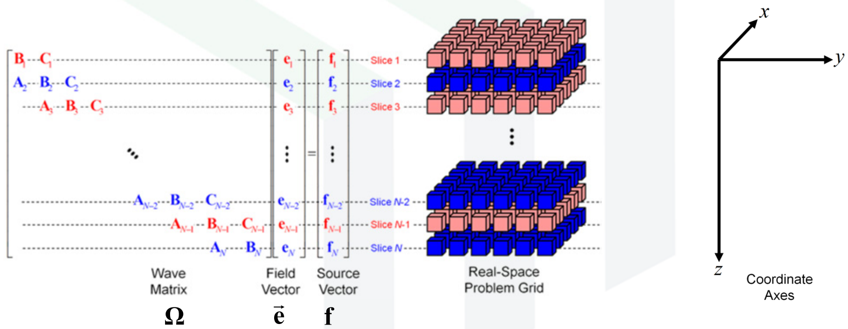
Visual Interpretation of Reordered Equation

The matrix $\tilde{\mathbf{A}}$ now has a very important "block tridiagonal" symmetry. Each slice through the grid corresponds to a row in the block matrix equation composed of three square matrices $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ and a column vector $\mathbf{f}$ that is usually all zeros.



Slice Data →

$\mathbf{A}_i$ quantifies coupling to the i-1 slice.
$\mathbf{B}_i$ quantifies coupling of fields within the i^{th} slice
$\mathbf{C}_i$ quantifies coupling to the i+1 slice.
$\mathbf{f}_i$ is a source condition in the i^{th} slice

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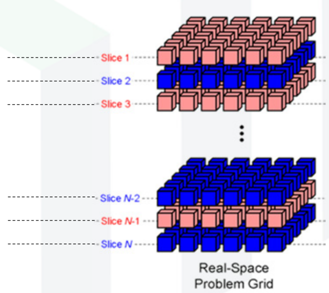
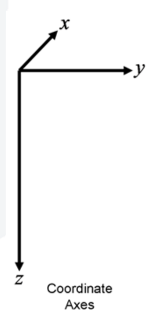
Slice Equations

We can think of the block tridiagonal matrix equation on the previous slide as the block matrix form of the following set of matrix equations. These "slice equations" relate fields in immediately adjacent slices.

$$\mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{f}_1$$
$$\mathbf{A}_2\mathbf{e}_1 + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{f}_2$$
$$\mathbf{A}_3\mathbf{e}_2 + \mathbf{B}_3\mathbf{e}_3 + \mathbf{C}_3\mathbf{e}_4 = \mathbf{f}_3$$
$$\vdots$$
$$\mathbf{A}_{N-2}\mathbf{e}_{N-3} + \mathbf{B}_{N-2}\mathbf{e}_{N-2} + \mathbf{C}_{N-2}\mathbf{e}_{N-1} = \mathbf{f}_{N-2}$$
$$\mathbf{A}_{N-1}\mathbf{e}_{N-2} + \mathbf{B}_{N-1}\mathbf{e}_{N-1} + \mathbf{C}_{N-1}\mathbf{e}_{N} = \mathbf{f}_{N-1}$$
$$\mathbf{A}_{N}\mathbf{e}_{N-1} + \mathbf{B}_{N}\mathbf{e}_{N} = \mathbf{f}_{N}$$





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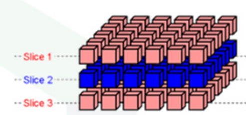
Slice Absorption Method

Steps to Calculate Slice Data for a Single Slice



Step 1: Build a grid containing three slices where the center slice is the slice for which to calculate the slice data. Simple Dirichlet boundary conditions can be used for the *z*-axis boundaries because only Slice 2 is of interest here.

Step 2: Construct the standard 3D-FDFD matrix for three adjacent slices. The slice of interest should be the middle slice.

$$\mathbf{\Omega}_{123} = \mathbf{C}^h \left[\boldsymbol{\mu}_{123}\right]^{-1} \mathbf{C}^e - \left[\boldsymbol{\varepsilon}_{123}\right]$$
$$\mathbf{f}_{123} = \mathbf{0}$$

Step 3: Reorder the data

$\tilde{\mathbf{\Omega}}_{123} \rightarrow$ reordered columns and rows

$\tilde{\mathbf{f}}_{123} \rightarrow$ reordered rows

$$\tilde{\mathbf{\Omega}}_{123} = \text{reorder}\left(\mathbf{\Omega}_{123}\right)$$
$$\tilde{\mathbf{f}}_{123} = \text{reorder}\left(\mathbf{f}_{123}\right)$$

Step 4: Extract the slice data from the middle row of the block matrix equation.

$$\begin{bmatrix} \mathbf{B}_1 & \mathbf{C}_1 & \mathbf{0} \\ \mathbf{A}_2 & \mathbf{B}_2 & \mathbf{C}_2 \\ \mathbf{0} & \mathbf{A}_3 & \mathbf{B}_3 \end{bmatrix} \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \mathbf{f}_3 \end{bmatrix}$$

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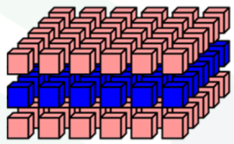
Absorbing a Slice (1 of 5)



<u>Three Slice Equations</u>

We can write the slice equations for three adjacent slices. The center slice is the i^{th} slice.

$$\begin{aligned} \mathbf{A}_{i-1}\mathbf{e}_{i-2} + \mathbf{B}_{i-1}\mathbf{e}_{i-1} + \mathbf{C}_{i-1}\mathbf{e}_{i} &= \mathbf{f}_{i-1} \\ \mathbf{A}_{i}\mathbf{e}_{i-1} + \mathbf{B}_{i}\mathbf{e}_{i} + \mathbf{C}_{i}\mathbf{e}_{i+1} &= \mathbf{f}_{i} \\ \mathbf{A}_{i+1}\mathbf{e}_{i} + \mathbf{B}_{i+1}\mathbf{e}_{i+1} + \mathbf{C}_{i+1}\mathbf{e}_{i+2} &= \mathbf{f}_{i+1} \end{aligned}$$

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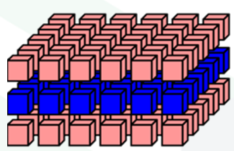
Absorbing a Slice (2 of 5)



We solve the middle equation for $\mathbf{e}_i$.

$$\begin{aligned} \mathbf{A}_{i-1}\mathbf{e}_{i-2} + \mathbf{B}_{i-1}\mathbf{e}_{i-1} + \mathbf{C}_{i-1}\mathbf{e}_{i} &= \mathbf{f}_{i-1} \\ \mathbf{A}_{i}\mathbf{e}_{i-1} + \mathbf{B}_{i}\mathbf{e}_{i} + \mathbf{C}_{i}\mathbf{e}_{i+1} &= \mathbf{f}_{i} \quad \longrightarrow \quad \mathbf{e}_i = \mathbf{B}_i^{-1}\left(\mathbf{f}_i - \mathbf{A}_i\mathbf{e}_{i-1} - \mathbf{C}_i\mathbf{e}_{i+1}\right) \\ \mathbf{A}_{i+1}\mathbf{e}_{i} + \mathbf{B}_{i+1}\mathbf{e}_{i+1} + \mathbf{C}_{i+1}\mathbf{e}_{i+2} &= \mathbf{f}_{i+1} \end{aligned}$$

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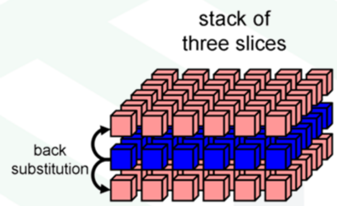
Absorbing a Slice (3 of 5)



<u>Substitute New Expression into First and Third Equation</u>

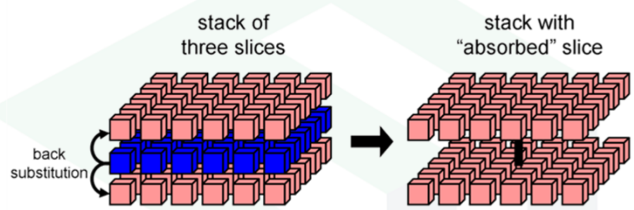
We eliminate $\mathbf{e}_i$ from these equations by substituting our new expression into the first and third equations.

$$\mathbf{A}_{i-1}\mathbf{e}_{i-2} + \mathbf{B}_{i-1}\mathbf{e}_{i-1} + \mathbf{C}_{i-1}\mathbf{e}_{i} = \mathbf{f}_{i-1}$$

$$\mathbf{e}_i = \mathbf{B}_i^{-1}\left(\mathbf{f}_i - \mathbf{A}_i\mathbf{e}_{i-1} - \mathbf{C}_i\mathbf{e}_{i+1}\right)$$

$$\mathbf{A}_{i+1}\mathbf{e}_{i} + \mathbf{B}_{i+1}\mathbf{e}_{i+1} + \mathbf{C}_{i+1}\mathbf{e}_{i+2} = \mathbf{f}_{i+1}$$

Absorbing a Slice (4 of 5)



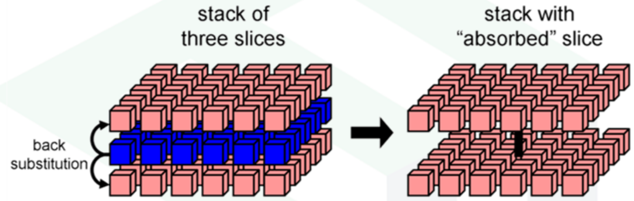
<u>Revised Slice Equations for Slice i-1 and i+1</u>

These are the equations after the substitution.

$$\mathbf{A}_{i-1}\mathbf{e}_{i-2} + \mathbf{B}_{i-1}\mathbf{e}_{i-1} + \mathbf{C}_{i-1}\mathbf{B}_i^{-1}\left(\mathbf{f}_i - \mathbf{A}_i\mathbf{e}_{i-1} - \mathbf{C}_i\mathbf{e}_{i+1}\right) = \mathbf{f}_{i-1}$$

$$\mathbf{A}_{i+1}\mathbf{B}_i^{-1}\left(\mathbf{f}_i - \mathbf{A}_i\mathbf{e}_{i-1} - \mathbf{C}_i\mathbf{e}_{i+1}\right) + \mathbf{B}_{i+1}\mathbf{e}_{i+1} + \mathbf{C}_{i+1}\mathbf{e}_{i+2} = \mathbf{f}_{i+1}$$

Absorbing a Slice (5 of 5)



<u>Revised Slice Equations for Slice *i*-1 and *i*+1</u>

We expand the equations and collect the coefficients on common electric field terms. This puts the remaining two slice equations back into their original form, but with revised slice data.

$$\mathbf{A}_{i-1}\mathbf{e}_{i-2} + \left(\mathbf{B}_{i-1} - \mathbf{C}_{i-1}\mathbf{B}_i^{-1}\mathbf{A}_i\right)\mathbf{e}_{i-1} + \left(-\mathbf{C}_{i-1}\mathbf{B}_i^{-1}\mathbf{C}_i\right)\mathbf{e}_{i+1} = \mathbf{f}_{i-1} - \mathbf{C}_{i-1}\mathbf{B}_i^{-1}\mathbf{f}_i$$

$$\left(-\mathbf{A}_{i+1}\mathbf{B}_i^{-1}\mathbf{A}_i\right)\mathbf{e}_{i-1} + \left(\mathbf{B}_{i+1} - \mathbf{A}_{i+1}\mathbf{B}_i^{-1}\mathbf{C}_i\right)\mathbf{e}_{i+1} + \mathbf{C}_{i+1}\mathbf{e}_{i+2} = \mathbf{f}_{i+1} - \mathbf{A}_{i+1}\mathbf{B}_i^{-1}\mathbf{f}_i$$

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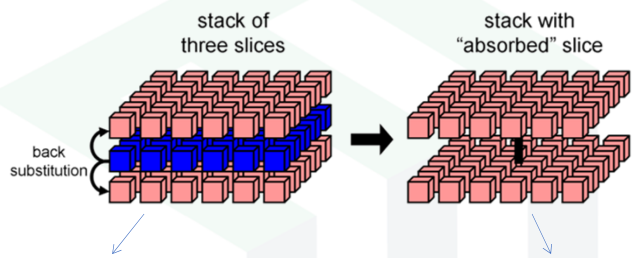
Absorbing a Slice (Summary)



Three slice equations

$$\mathbf{A}_{i-1}\mathbf{e}_{i-2} + \mathbf{B}_{i-1}\mathbf{e}_{i-1} + \mathbf{C}_{i-1}\mathbf{e}_i = \mathbf{f}_{i-1}$$
$$\mathbf{A}_i\mathbf{e}_{i-1} + \mathbf{B}_i\mathbf{e}_i + \mathbf{C}_i\mathbf{e}_{i+1} = \mathbf{f}_i$$
$$\mathbf{A}_{i+1}\mathbf{e}_i + \mathbf{B}_{i+1}\mathbf{e}_{i+1} + \mathbf{C}_{i+1}\mathbf{e}_{i+2} = \mathbf{f}_{i+1}$$

Algebraically eliminate $\mathbf{e}_i$

$$\mathbf{A}'_{i-1}\mathbf{e}_{i-2} + \mathbf{B}'_{i-1}\mathbf{e}_{i-1} + \mathbf{C}'_{i-1}\mathbf{e}_{i+1} = \mathbf{f}'_{i-1}$$
$$\mathbf{A}'_{i+1}\mathbf{e}_{i-1} + \mathbf{B}'_{i+1}\mathbf{e}_{i+1} + \mathbf{C}'_{i+1}\mathbf{e}_{i+2} = \mathbf{f}'_{i+1}$$

$$\mathbf{A}'_{i-1} = \mathbf{A}_{i-1} \qquad \mathbf{A}'_{i+1} = -\mathbf{A}_{i+1}\mathbf{B}_i^{-1}\mathbf{A}_i$$
$$\mathbf{B}'_{i-1} = \mathbf{B}_{i-1} - \mathbf{C}_{i-1}\mathbf{B}_i^{-1}\mathbf{A}_i \qquad \mathbf{B}'_{i+1} = \mathbf{B}_{i+1} - \mathbf{A}_{i+1}\mathbf{B}_i^{-1}\mathbf{C}_i$$
$$\mathbf{C}'_{i-1} = -\mathbf{C}_{i-1}\mathbf{B}_i^{-1}\mathbf{C}_i \qquad \mathbf{C}'_{i+1} = \mathbf{C}_{i+1}$$
$$\mathbf{f}'_{i-1} = \mathbf{f}_{i-1} - \mathbf{C}_{i-1}\mathbf{B}_i^{-1}\mathbf{f}_i \qquad \mathbf{f}'_{i+1} = \mathbf{f}_{i+1} - \mathbf{A}_{i+1}\mathbf{B}_i^{-1}\mathbf{f}_i$$

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Forward Absorption from Top

Two slice equations

$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{f}_1$$
$$\mathbf{A}_2\mathbf{e}_1 + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{f}_2$$

Algebraically eliminate $\mathbf{E}_1$

$$\mathbf{A}_2'\mathbf{e}_0 + \mathbf{B}_2'\mathbf{e}_2 + \mathbf{C}_2'\mathbf{e}_3 = \mathbf{f}_2'$$

$$\mathbf{A}_2' = -\mathbf{A}_2\mathbf{b}_1^{-1}\mathbf{A}_1$$
$$\mathbf{B}_2' = \mathbf{B}_2 - \mathbf{A}_2\mathbf{B}_1^{-1}\mathbf{c}_1$$
$$\mathbf{C}_2' = \mathbf{C}_2$$
$$\mathbf{f}_2' = \mathbf{f}_2 - \mathbf{A}_2\mathbf{B}_1^{-1}\mathbf{f}_1$$

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Backward Absorption from Bottom

Two slice equations

$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{f}_1$$
$$\mathbf{A}_2\mathbf{e}_1 + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{f}_2$$

Algebraically eliminate $\mathbf{E}_1$

$$\mathbf{A}_1'\mathbf{e}_0 + \mathbf{B}_1'\mathbf{e}_1 + \mathbf{C}_1'\mathbf{e}_3 = \mathbf{f}_1'$$

$$\mathbf{A}_1' = \mathbf{A}_1$$
$$\mathbf{B}_1' = \mathbf{B}_1 - \mathbf{C}_1\mathbf{B}_2^{-1}\mathbf{A}_2$$
$$\mathbf{C}_1' = -\mathbf{C}_1\mathbf{B}_2^{-1}\mathbf{C}_2$$
$$\mathbf{f}_1' = \mathbf{f}_1 - \mathbf{C}_1\mathbf{B}_2^{-1}\mathbf{f}_2$$

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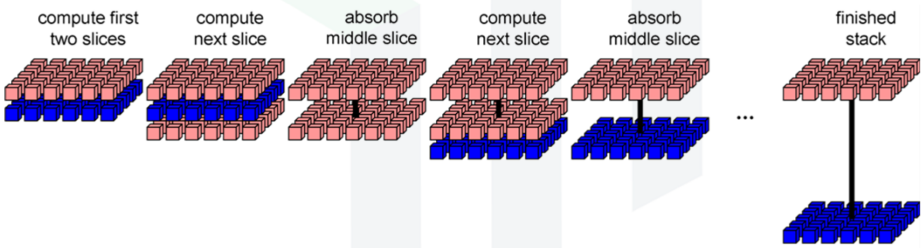
Slice Absorption Procedure

Using the slice absorption procedure described on the previous slide, we can methodically progress through a large stack of slices, one slice at a time, and reduce the entire stack to just two adjacent slices by “absorbing” all interior slices.



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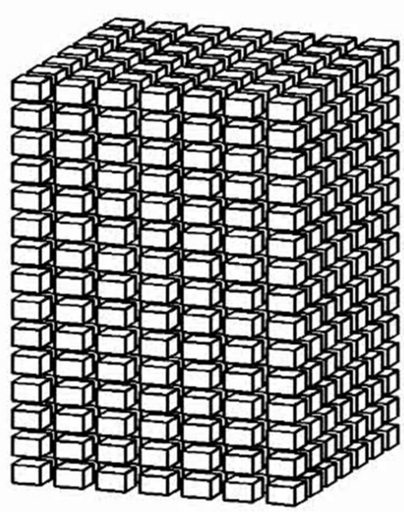
Animation of Slice Absorption Method



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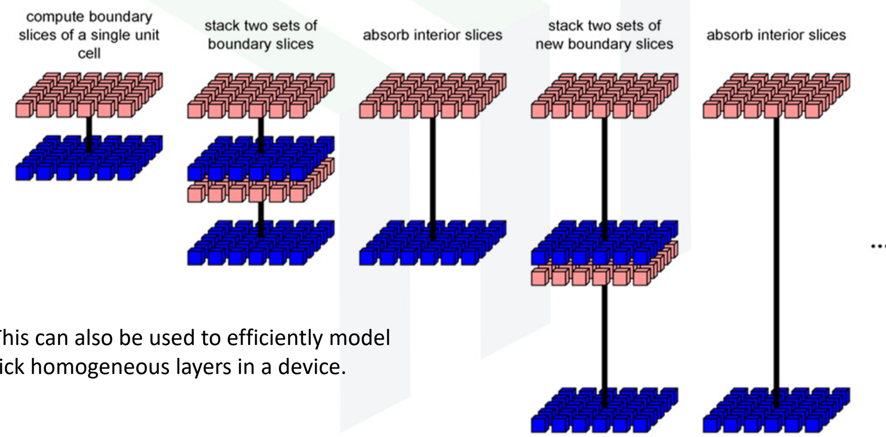
Cascading and Doubling

Given two outer slices describing the unit cell of a periodic structure, we can perform an efficient cascading and doubling procedure to quickly describe large stacks.



Note: This can also be used to efficiently model very thick homogeneous layers in a device.

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Plane Wave Source

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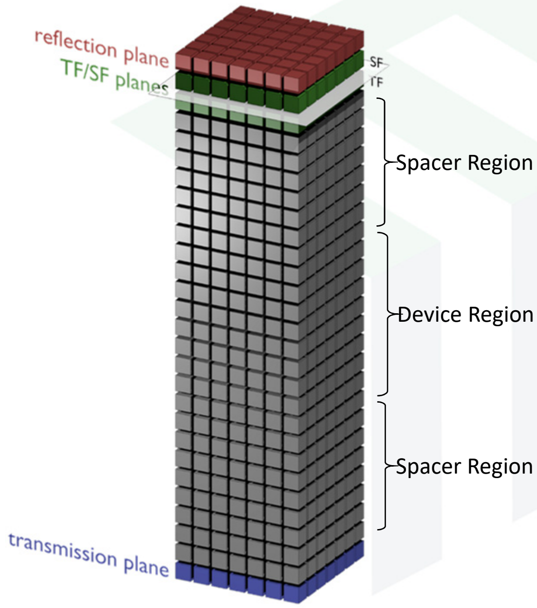
Total-Field/Scattered-Field Framework



Grid Strategy
The grid strategy for SAM is just like FDFD.

For doubly-periodic devices, an absorbing boundary is only needed at the z-axis boundaries.

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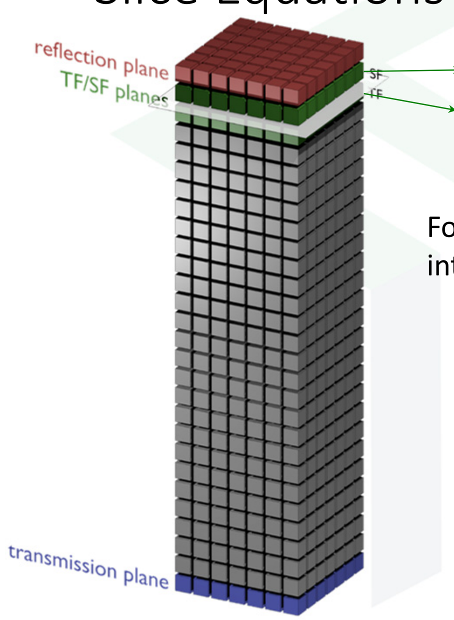
Slice Equations at TF/SF Interface



$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{0}$$ scattered-field

$$\mathbf{A}_2\mathbf{e}_1 + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{0}$$ total-field

For simplicity, we'll call the TF/SF interface slices 1 and 2.

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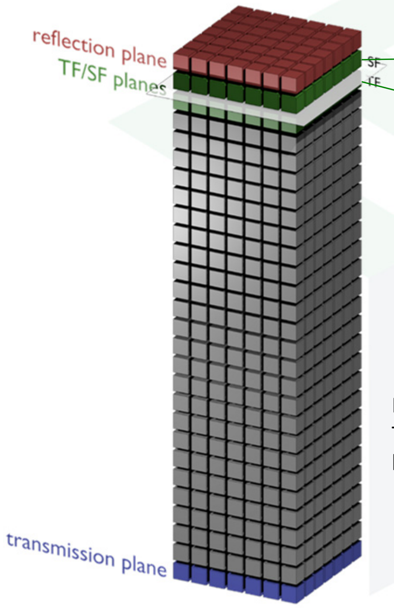
TF/SF Corrections (1 of 2)



$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\boxed{\mathbf{e}_2} = \mathbf{0} \qquad \text{Eq. (1)}$$

$$\mathbf{A}_2\boxed{\mathbf{e}_1} + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{0} \qquad \text{Eq. (2)}$$

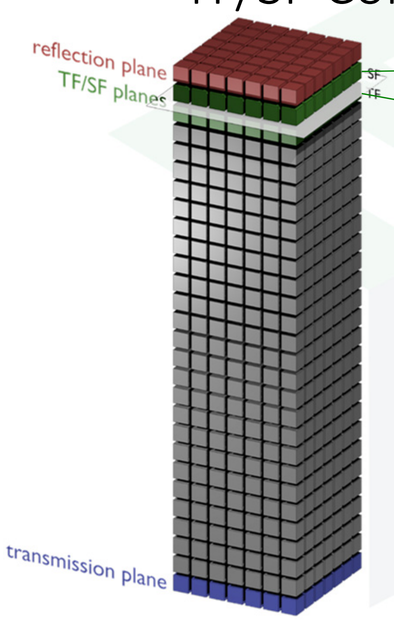
Eq. (1) exists in the SF region, but $\mathbf{e}_2$ is a TF quantity. The source in slice 2 must be subtracted from it to make it look like a SF quantity.

$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\left(\mathbf{e}_2 - \mathbf{f}_{2,\mathrm{src}}\right) = \mathbf{0}$$

Eq. (2) exists in the TF region, but $\mathbf{e}_1$ is a SF quantity. The source in slice 1 must be added to it to make it look like a TF quantity.

$$\mathbf{A}_2\left(\mathbf{e}_1 + \mathbf{f}_{1,\mathrm{src}}\right) + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{0}$$

TF/SF Corrections (2 of 2)



$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{C}_1\mathbf{f}_{2,\mathrm{src}}$$

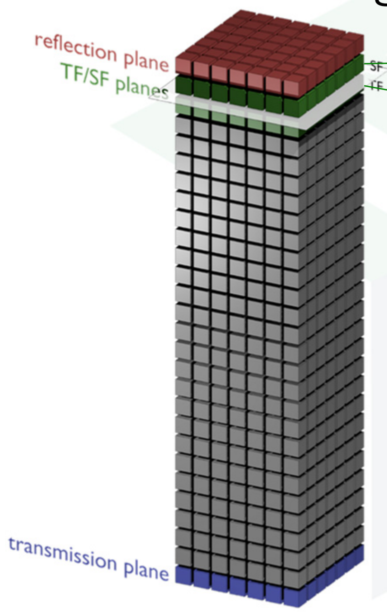
$$\mathbf{A}_2\mathbf{e}_1 + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = -\mathbf{A}_2\mathbf{f}_{1,\mathrm{src}}$$

From the above equations, we make the following observations:

- The slice data can be calculated without considering the source or TF/SF framework.
- We must calculate the source function into two adjacent planes.
- The TF/SF source is easily incorporated through the right hand side of the above equations.

$$\mathbf{f}_1 = \mathbf{C}_1\mathbf{f}_{2,\mathrm{src}} \qquad \mathbf{f}_2 = -\mathbf{A}_2\mathbf{f}_{1,\mathrm{src}}$$

Calculating the Source Terms



$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{f}_1 \qquad \mathbf{f}_1 = \mathbf{C}_1\mathbf{f}_{2,\text{src}}$$

$$\mathbf{A}_2\mathbf{e}_1 + \mathbf{B}_2\mathbf{e}_2 + \mathbf{C}_2\mathbf{e}_3 = \mathbf{f}_2 \qquad \mathbf{f}_2 = -\mathbf{A}_2\mathbf{f}_{1,\text{src}}$$

$$\mathbf{f}_{1,\text{src}} = \text{reorder}\left(\begin{bmatrix} p_x e^{-j\left(k_{x,\text{inc}}\mathbf{x}+k_{y,\text{inc}}\mathbf{y}\right)} \\ p_y e^{-j\left(k_{x,\text{inc}}\mathbf{x}+k_{y,\text{inc}}\mathbf{y}\right)} \\ p_z e^{-j\left(k_{x,\text{inc}}\mathbf{x}+k_{y,\text{inc}}\mathbf{y}\right)} \end{bmatrix} \right)$$

$$\mathbf{f}_{2,\text{src}} = e^{-jk_{z,\text{inc}}\Delta z}\mathbf{f}_{1,\text{src}}$$

Unit Amplitude Source

$$|\vec{p}| = 1$$

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Transparent Boundary Condition

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Notes on the TBC

- Requires homogeneous materials where TBC is implemented (can be generalized)
- Energy can only be propagating in a single direction (ensured by TF/SF)
- TBC handles evanescent fields naturally so no spacer layer is needed.
  - Smaller matrices
  - More efficient simulations
- FFT operators are slow to construct, but there may be a better way

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Matrix Tilt Operator

Given the field in a slice $\mathbf{e}_i$, we need a matrix operator $\mathbf{T}$ that will remove the phase tilt across the grid giving just the periodic envelope term from Bloch's theorem.

$$\mathbf{a}_i = \mathbf{T}\mathbf{e}_i$$

This is calculated as

$$\mathbf{T} = \text{reorder}\left(\begin{bmatrix} \mathbf{T}' & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{T}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{T}' \end{bmatrix} \right) \qquad \mathbf{T}' = \text{diag}\left[e^{j\left(k_{x,\text{inc}}\mathbf{x} + k_{y,\text{inc}}\mathbf{y}\right)} \right]$$

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Matrix 2D-FFT Operator

Given the amplitude component $\mathbf{a}_i$ of the field in a slice, we need another matrix operator $\mathbf{F}$ that will calculate a 2D FFT in order to calculate the amplitudes of the spatial harmonics in that slice.

$$\mathbf{s}_i = \mathbf{F}\mathbf{a}_i$$

The 2D-FFT is defined as

$$H(m,n) = \sum_p \sum_q h(p,q) e^{-j2\pi\left(\frac{mp}{M}+\frac{nq}{N}\right)}$$

$$m,p = 0,1,\ldots,N_x \qquad n,p = 0,1,\ldots,N_y$$

From this, we can construct $\mathbf{F}'$.

$$\hat{\mathbf{h}} = \mathbf{F}'\mathbf{h}$$

The full-vector 2D-FFT matrix operator is then

$$\mathbf{F} = \text{reorder}\left(\begin{bmatrix} \mathbf{F}' & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{F}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{F}' \end{bmatrix}\right)$$

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Matrix Phase Operator

Given the spatial harmonics, we need an operator that will add the correct phase to each spatial harmonic to propagate them across one slice.

$$\mathbf{s}_{i+1} = \mathbf{Z}_i \mathbf{s}_i$$

This is calculated as

$$\mathbf{Z} = \text{reorder}\left(\begin{bmatrix} \mathbf{Z}' & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{Z}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{Z}' \end{bmatrix}\right) \qquad \mathbf{Z}' = \begin{bmatrix} e^{-jk_z(1,1)\Delta z} & & 0 \\ & \ddots & \\ 0 & & e^{-jk_z(M,N)\Delta z} \end{bmatrix}$$

$$k_z(m,n) = \sqrt{k_0^2 \mu_r \varepsilon_r - k_x^2(m) - k_y^2(n)}$$

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Overall Matrix Propagators

We need to calculate a single matrix operator that will calculate the field in an adjacent slice.

$$\mathbf{e}_{i+1} = \mathbf{P}_i \mathbf{e}_i$$

1. Remove phase tilt. $\mathbf{T} \cdot \mathbf{e}_i$
2. FFT the field to transform to Fourier-space. $\mathbf{F} \cdot \mathbf{T} \cdot \mathbf{e}_i$
3. Add phase to the spatial harmonics. $\mathbf{Z}_i \cdot \mathbf{F} \cdot \mathbf{T} \cdot \mathbf{e}_i$
4. Inverse-FFT the field to transform to real-space. $\mathbf{F}^{-1} \cdot \mathbf{Z}_i \cdot \mathbf{F} \cdot \mathbf{T} \cdot \mathbf{e}_i$
5. Reincorporate the phase tilt. $\mathbf{T}^{-1} \cdot \mathbf{F}^{-1} \cdot \mathbf{Z}_i \cdot \mathbf{F} \cdot \mathbf{T} \cdot \mathbf{e}_i$

The overall propagator is therefore

$$\mathbf{P}_i = \mathbf{T}^{-1}\mathbf{F}^{-1}\mathbf{Z}_i\mathbf{F}\mathbf{T} = \left(\mathbf{F}\mathbf{T}\right)^{-1} \mathbf{Z}_i \left(\mathbf{F}\mathbf{T}\right)$$

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TBC at Top of Grid

The slice equation for the top slice (slice #1) can be written as

$$\mathbf{A}_1 \boxed{\mathbf{e}_0} + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{f}_1$$

The term $\mathbf{e}_0$ does not exist because it resides outside of the grid. Assuming the field at the top of the grid is only moving outward (bottom to top), we can calculate $\mathbf{e}_0$ from $\mathbf{e}_1$ using the matrix propagator calculated in the reflection region.

$$\mathbf{e}_0 = \mathbf{P}_{\text{ref}}\mathbf{e}_1$$

Substituting this into the original slice equation yields

$$\mathbf{B}_1'\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_2 = \mathbf{f}_1 \qquad \mathbf{B}_1' = \mathbf{B}_1 + \mathbf{A}_1\mathbf{P}_{\text{ref}}$$

After this calculation, we no longer need $\mathbf{A}_1$.

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TBC at Bottom of Grid

The slice equation for the bottom slice (slice N) can be written as

$$\mathbf{A}_N \mathbf{e}_{N-1} + \mathbf{B}_N \mathbf{e}_N + \mathbf{C}_N \boxed{\mathbf{e}_{N+1}} = \mathbf{f}_N$$

The term $\mathbf{e}_{N+1}$ does not exist because it resides outside of the grid. Assuming the field at the bottom of the grid is only moving outward (top to bottom), we can calculate $\mathbf{e}_{N+1}$ from $\mathbf{e}_N$ using the matrix propagator calculated in the transmission region.

$$\mathbf{e}_{N+1} = \mathbf{P}_{\text{trn}} \mathbf{e}_N$$

Substituting this into the original slice equation yields

$$\mathbf{A}_N \mathbf{e}_{N-1} + \mathbf{B}'_N \mathbf{e}_N = \mathbf{f}_N \qquad \mathbf{B}'_N = \mathbf{B}_N + \mathbf{C}_N \mathbf{P}_{\text{trn}}$$

After this calculation, we no longer need $\mathbf{C}_N$.

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Field Solution

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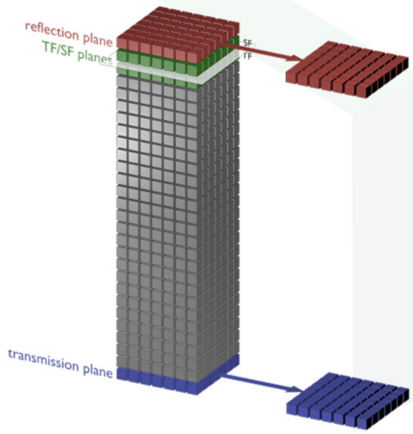
Final Matrix Problem

The slice absorption method algorithm is implemented until only two slices remain. These are usually the reflection and transmission record planes. A final matrix equation is constructed from the remaining two slice equations.



$$\mathbf{A}_1'\mathbf{e}_0 + \mathbf{B}_1'\mathbf{e}_1 + \mathbf{C}_1'\mathbf{e}_2 = \mathbf{f}_1'$$

$$\begin{bmatrix} \mathbf{B}_1' & \mathbf{C}_1' \\ \mathbf{A}_N' & \mathbf{B}_N' \end{bmatrix} \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_N \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1' \\ \mathbf{f}_N' \end{bmatrix}$$

$$\mathbf{A}_N'\mathbf{e}_1 + \mathbf{B}_N'\mathbf{e}_N + \mathbf{C}_N'\mathbf{e}_{N+1} = \mathbf{f}_N'$$

Recall that $\mathbf{A}_1$ and $\mathbf{C}_N$ are no longer needed because these described coupling to slices from outside of the grid.

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Field Solution

The fields in the record planes are calculated as

$$\begin{bmatrix} \mathbf{e}_{\text{ref}} \\ \mathbf{e}_{\text{trn}} \end{bmatrix} = \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_N \end{bmatrix} = \begin{bmatrix} \mathbf{B}_1 & \mathbf{C}_1 \\ \mathbf{A}_N & \mathbf{B}_N \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_N \end{bmatrix}$$

We can recover the vector components of the field in each slice as follows.

$$\begin{bmatrix} \mathbf{e}_{x,\text{ref}} \\ \mathbf{e}_{y,\text{ref}} \\ \mathbf{e}_{z,\text{ref}} \end{bmatrix} = \text{reorder}^{-1}\left(\mathbf{e}_{\text{ref}}\right) \qquad \begin{bmatrix} \mathbf{e}_{x,\text{trn}} \\ \mathbf{e}_{y,\text{trn}} \\ \mathbf{e}_{z,\text{trn}} \end{bmatrix} = \text{reorder}^{-1}\left(\mathbf{e}_{\text{trn}}\right)$$

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Calculating Diffraction Efficiencies

The amplitudes of the spatial harmonics are calculated as

$$\mathbf{s}_{\text{ref}} = (\mathbf{FT})\mathbf{e}_{\text{ref}} \qquad \mathbf{s}_{\text{trn}} = (\mathbf{FT})\mathbf{e}_{\text{trn}}$$

Assuming the incident wave is given unit amplitude, the diffraction efficiencies are calculated as usual.

$$R_{\text{DE}}(m,n) = \left|\vec{S}_{\text{ref}}(m,n)\right|^2 \frac{\text{Re}\left[-k_{z,\text{ref}}(m,n)/\mu_{\text{r,inc}}\right]}{\text{Re}\left[k_{z,\text{inc}}/\mu_{\text{r,inc}}\right]}$$

$$T_{\text{DE}}(m,n) = \left|\vec{S}_{\text{trn}}(m,n)\right|^2 \frac{\text{Re}\left[k_{z,\text{trn}}(m,n)/\mu_{\text{r,trn}}\right]}{\text{Re}\left[k_{z,\text{inc}}/\mu_{\text{r,inc}}\right]}$$

These equations assume the source was given unit amplitude.

$$\left|\vec{S}_{\text{inc}}\right| = 1$$

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Fourier-Space SAM

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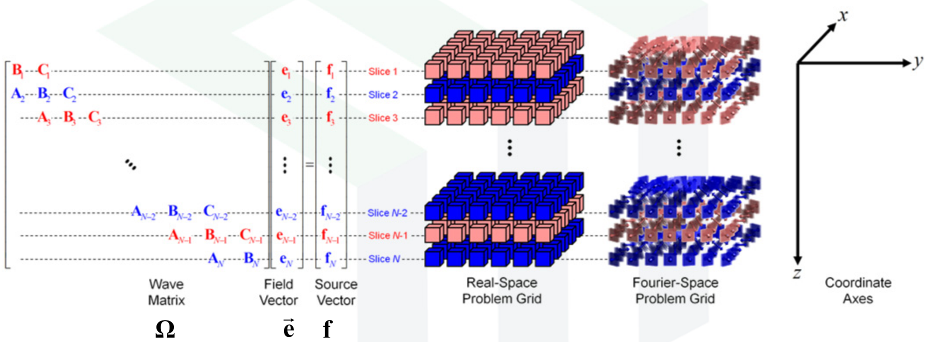
Comparison to Real-Space SAM



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Formulation of Fourier-Space SAM

$$\mathbf{D}_{y'}^{e}\mathbf{e}_z - \mathbf{D}_{z'}^{e}\mathbf{e}_y = \boldsymbol{\mu}_{xx}\tilde{\mathbf{h}}_x \quad\Rightarrow\quad \mathbf{K}_{y'}^{e}\mathbf{s}_z - \mathbf{D}_{z'}^{e}\mathbf{s}_y = [\![\mu_{xx}]\!]\mathbf{u}_x$$

$$\mathbf{D}_{z'}^{e}\mathbf{e}_x - \mathbf{D}_{x'}^{e}\mathbf{e}_z = \boldsymbol{\mu}_{yy}\tilde{\mathbf{h}}_y \quad\Rightarrow\quad \mathbf{D}_{z'}^{e}\mathbf{s}_x - \mathbf{K}_{x'}^{e}\mathbf{s}_z = [\![\mu_{yy}]\!]\mathbf{u}_y$$

$$\mathbf{D}_{x'}^{e}\mathbf{e}_y - \mathbf{D}_{y'}^{e}\mathbf{e}_x = \boldsymbol{\mu}_{zz}\tilde{\mathbf{h}}_z \quad\Rightarrow\quad \mathbf{K}_{x'}^{e}\mathbf{s}_y - \mathbf{K}_{y'}^{e}\mathbf{s}_x = [\![\mu_{zz}]\!]\mathbf{u}_z$$

$$\mathbf{D}_{y'}^{h}\tilde{\mathbf{h}}_z - \mathbf{D}_{z'}^{h}\tilde{\mathbf{h}}_y = \boldsymbol{\varepsilon}_{xx}\mathbf{e}_x \quad\Rightarrow\quad \mathbf{K}_{y'}^{h}\mathbf{u}_z - \mathbf{D}_{z'}^{h}\mathbf{u}_y = [\![\varepsilon_{xx}]\!]\mathbf{s}_x$$

$$\mathbf{D}_{z'}^{h}\tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^{h}\tilde{\mathbf{h}}_z = \boldsymbol{\varepsilon}_{yy}\mathbf{e}_y \quad\Rightarrow\quad \mathbf{D}_{z'}^{h}\mathbf{u}_x - \mathbf{K}_{x'}^{h}\mathbf{u}_z = [\![\varepsilon_{yy}]\!]\mathbf{s}_y$$

$$\mathbf{D}_{x'}^{h}\tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^{h}\tilde{\mathbf{h}}_x = \boldsymbol{\varepsilon}_{zz}\mathbf{e}_z \quad\Rightarrow\quad \mathbf{K}_{x'}^{h}\mathbf{u}_y - \mathbf{K}_{y'}^{h}\mathbf{u}_x = [\![\varepsilon_{zz}]\!]\mathbf{s}_z$$

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Example Simulations

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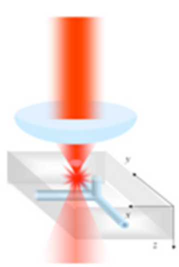
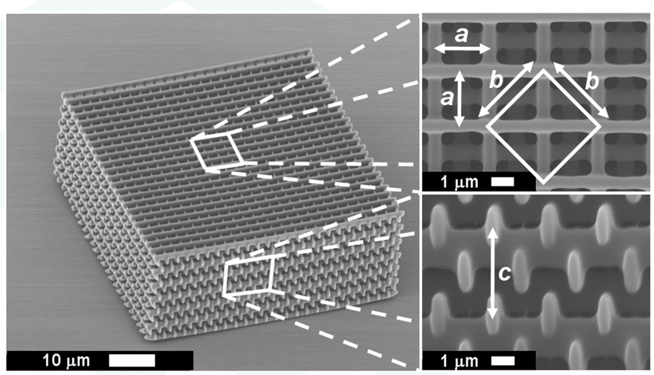
Photonic Crystals Fabricated by Multi-Photon Direct Laser Writing





This is a scanning electron microscope image of a photonic crystal designed to operate in the infrared.

R. C. Rumpf, A. Tal, S. M. Kuebler, "Rigorous electromagnetic analysis of volumetrically complex media using the slice absorption method," J. Opt. Soc. Am. A **24**(10), 3123-3134, 2007.

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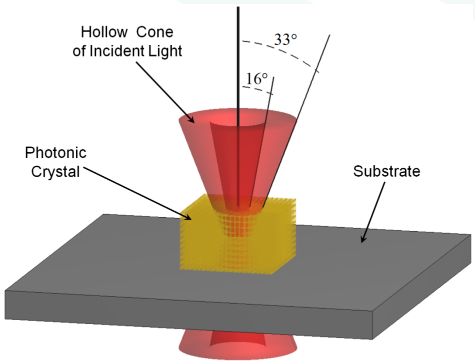
Fourier Transform Infrared Spectrometer

Samples are illuminated by a hollow Gaussian beam produced by a Cassegrain optic.



Reflected infrared energy at near normal reflection angle is collected and measured.

R. C. Rumpf, A. Tal, S. M. Kuebler, "Rigorous electromagnetic analysis of volumetrically complex media using the slice absorption method," J. Opt. Soc. Am. A **24**(10), 3123-3134, 2007.

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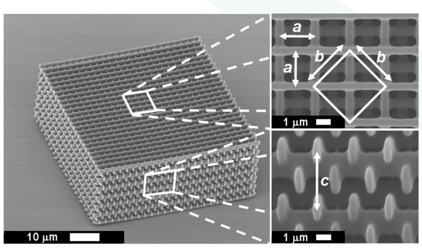
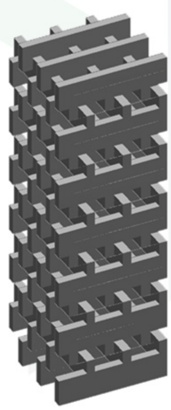
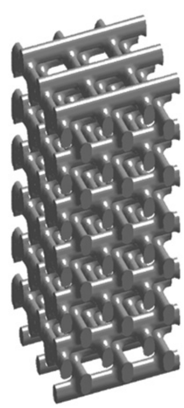
Predicting Accurate Geometry

To predict the geometry of the photonic crystal more accurately, the DLW process was simulated in MATLAB.





Idealized Geometry



Realistic Geometry

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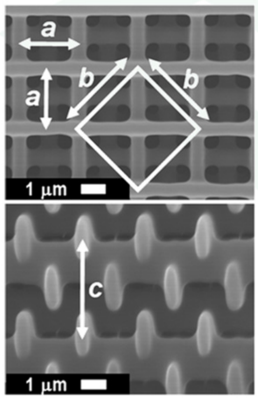
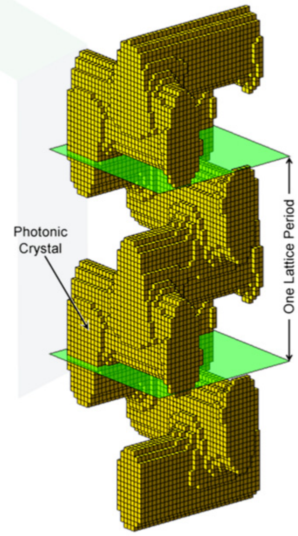
Numerical Representation of Device





R. C. Rumpf, A. Tal, S. M. Kuebler, "Rigorous electromagnetic analysis of volumetrically complex media using the slice absorption method," J. Opt. Soc. Am. A **24**(10), 3123-3134, 2007.

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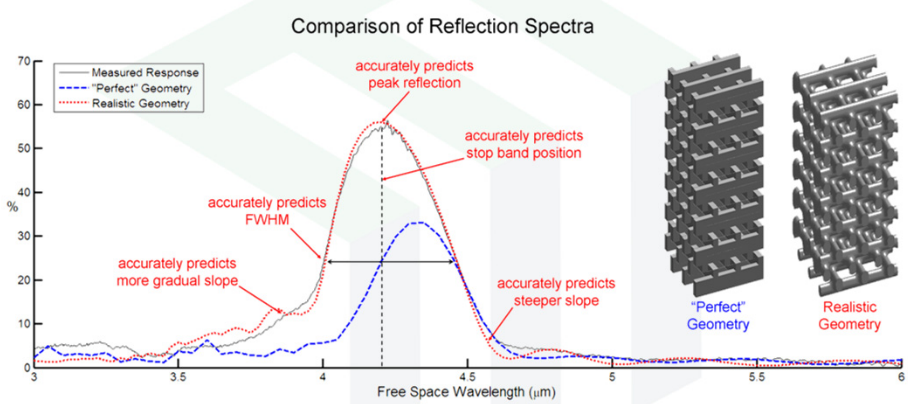
Results from SAM



There is am important lesson here in terms of the importance of incorporating realistic geometry into your models.

R. C. Rumpf, A. Tal, S. M. Kuebler, "Rigorous electromagnetic analysis of volumetrically complex media using the slice absorption method," J. Opt. Soc. Am. A **24**(10), 3123-3134, 2007.

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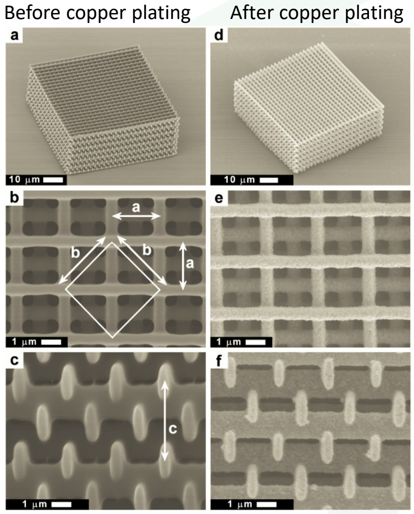
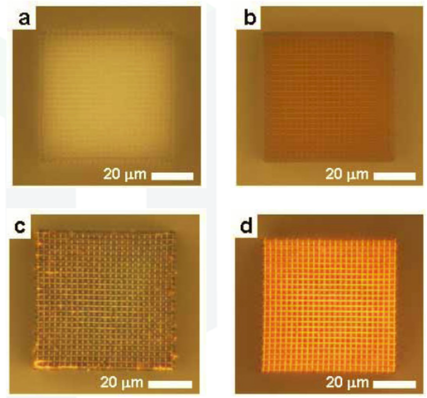
Metallo-Dielectric Photonic Crystals

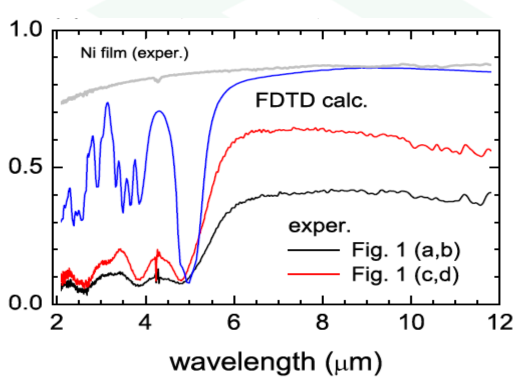


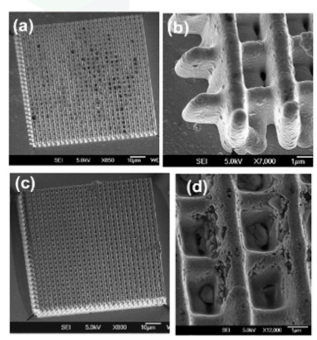


A. Tal, Y.-S. Chen, H. E. Williams, R. C. Rumpf, S. M. Kuebler, "Fabrication and characterization of three-dimensional copper metallodielectric photonic crystals," Optics Express **15**(26), 18283-18293, 2007.

"State-of-the-Art" Simulation of Reflectance

Results obtained by Lumerical and Misawa's research group.

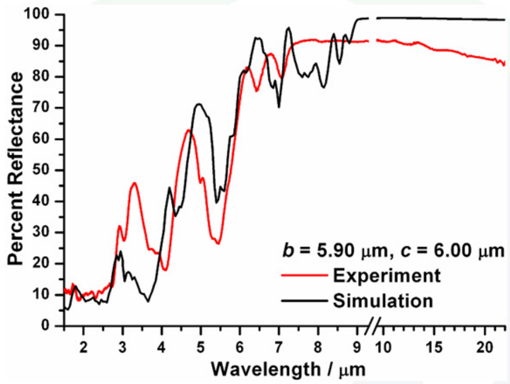


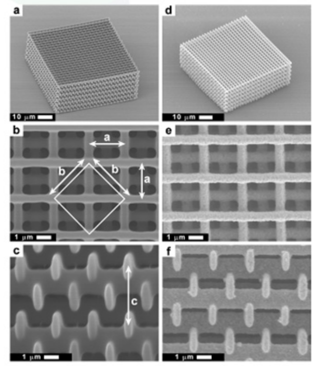


V. Mizeikis, S. Juodkazis, R. Tarozaite, J. Juodkazyte, K. Juodkazis, H. Misawa, "Fabrication and properties of metalo-dielectric photonic crystal structures for infrared spectral region," Opt. Express 15, 8454-8464 (2007)

A Better Simulation of Reflectance

Results obtained by UCF/Rumpf team…





A. Tal, Y. -S. Chen, H. E. Williams, R. C. Rumpf, and S. M. Kuebler, "Fabrication and characterization of three-dimensional copper metallodielectric photonic crystals," Opt. Express **15**, 18283-18293 (2007)

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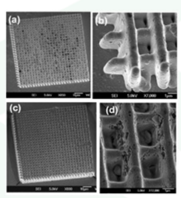
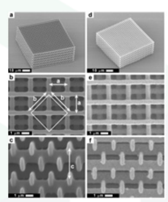
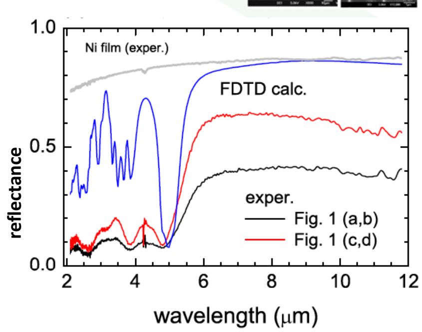
Side-by-Side Comparison

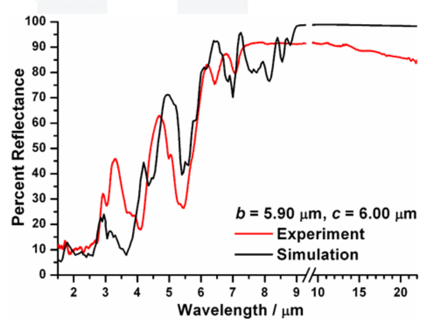
Results obtained with Lumerical's **FDTD** software



Results obtained by UCF/Rumpf







V. Mizeikis, S. Juodkazis, R. Tarozaite, J. Juodkazyte, K. Juodkazis, H. Misawa, "Fabrication and properties of metalo-dielectric photonic crystal structures for infrared spectral region," Opt. Express 15, 8454-8464 (2007)

A. Tal, Y. -S. Chen, H. E. Williams, R. C. Rumpf, and S. M. Kuebler, "Fabrication and characterization of three-dimensional copper metallodielectric photonic crystals," Opt. Express **15**, 18283-18293 (2007)

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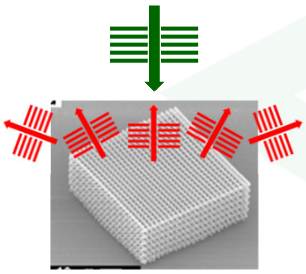
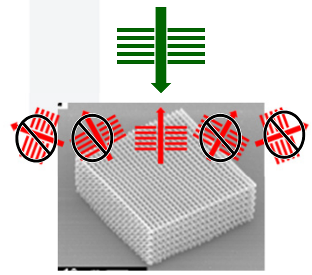
What Was Their Big Mistake?



Below 10 μm (or so), this photonic crystal is a diffracting structure.

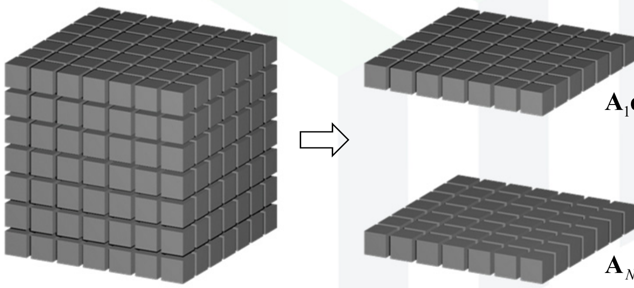


The optical configuration inside the FTIR cuts off the higher order modes. Essentially, it is only the zero-order diffracted mode that gets detected.

Dispersion Analysis Using the SAM

Starting Point

Using the standard SAM algorithm, it is possible to reduce a unit cell to two slice equations, one at each boundary of the unit cell.



$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_N = \mathbf{0}$$

$$\mathbf{A}_N\mathbf{e}_1 + \mathbf{B}_N\mathbf{e}_N + \mathbf{C}_N\mathbf{e}_{N+1} = \mathbf{0}$$

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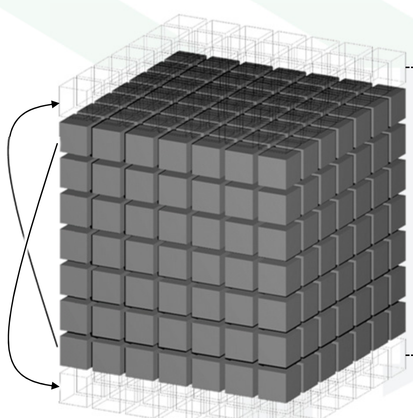
Derivation of the Eigen-Value Problem (1 of 3)

Assuming the unit cell is infinitely periodic in the z direction, boundary conditions allow $\mathbf{e}_0$ and $\mathbf{e}_{N+1}$ to be written in terms of slices contained in the unit cell.



$$\mathbf{e}_0 = e^{j\beta_z\Lambda_z}\mathbf{e}_N$$

$$\mathbf{e}_{N+1} = e^{-j\beta_z\Lambda_z}\mathbf{e}_1$$

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Derivation of the Eigen-Value Problem (2 of 3)

Substituting the new expressions into the slice equations gives

$$\mathbf{A}_1\mathbf{e}_0 + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_N = \mathbf{0} \qquad \mathbf{A}_N\mathbf{e}_1 + \mathbf{B}_N\mathbf{e}_N + \mathbf{C}_N\mathbf{e}_{N+1} = \mathbf{0}$$

$$\mathbf{e}_0 = e^{j\beta_z\Lambda_z}\mathbf{e}_N \qquad \mathbf{e}_{N+1} = e^{-j\beta_z\Lambda_z}\mathbf{e}_1$$

$$\Downarrow \qquad \Downarrow$$

$$\mathbf{A}_1 e^{j\beta_z\Lambda_z}\mathbf{e}_N + \mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_N = \mathbf{0} \qquad \mathbf{A}_N\mathbf{e}_1 + \mathbf{B}_N\mathbf{e}_N + \mathbf{C}_N e^{-j\beta_z\Lambda_z}\mathbf{e}_1 = \mathbf{0}$$

After some algebraic manipulation to get $e^{j\beta_z\Lambda_z}$ on the right-hand side of the equations, we get

$$\mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_N = -e^{j\beta_z\Lambda_z}\mathbf{A}_1\mathbf{e}_N \qquad -\mathbf{C}_N\mathbf{e}_1 = e^{j\beta_z\Lambda_z}\mathbf{A}_N\mathbf{e}_1 + e^{j\beta_z\Lambda_z}\mathbf{B}_N\mathbf{e}_N$$

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Derivation of the Eigen-Value Problem (3 of 3)

Our last two equations can be written in block matrix form as

$$\begin{aligned}\mathbf{B}_1\mathbf{e}_1 + \mathbf{C}_1\mathbf{e}_N &= -e^{j\beta_z\Lambda_z}\mathbf{A}_1\mathbf{e}_N \\ -\mathbf{C}_N\mathbf{e}_1 &= e^{j\beta_z\Lambda_z}\mathbf{A}_N\mathbf{e}_1 + e^{j\beta_z\Lambda_z}\mathbf{B}_N\mathbf{e}_N\end{aligned} \quad \rightarrow \quad \begin{bmatrix}\mathbf{B}_1 & \mathbf{C}_1 \\ -\mathbf{C}_N & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{e}_1 \\ \mathbf{e}_N\end{bmatrix} = e^{j\beta_z\Lambda_z}\begin{bmatrix}\mathbf{0} & -\mathbf{A}_1 \\ \mathbf{A}_N & \mathbf{B}_N\end{bmatrix}\begin{bmatrix}\mathbf{e}_1 \\ \mathbf{e}_N\end{bmatrix}$$

This has the form of a generalized eigen-value problem

$$\mathbf{A}\mathbf{x} = v\mathbf{B}\mathbf{x}$$

$$\mathbf{A} = \begin{bmatrix}\mathbf{B}_1 & \mathbf{C}_1 \\ -\mathbf{C}_N & \mathbf{0}\end{bmatrix} \quad \mathbf{B} = \begin{bmatrix}\mathbf{0} & -\mathbf{A}_1 \\ \mathbf{A}_N & \mathbf{B}_N\end{bmatrix} \quad \mathbf{x} = \begin{bmatrix}\mathbf{e}_1 \\ \mathbf{e}_N\end{bmatrix} \quad v = e^{j\beta_z\Lambda_z}$$

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Parameter Retrieval

The effective parameters of the unit cell can be determined one of two ways:

1. **Field Averaging** – The eigen-vectors give the field values at the boundary slices. From these, the fields in all interior slices can be calculated. After all the fields are known, the field averaging technique can be implemented.

2. **T-Matrix Parameter Retrieval** – The effective properties of the unit cell can be retrieved from the eigen-value following the T-matrix parameter retrieval method.

$$e^{j\beta_z\Lambda_z} \quad \rightarrow \quad \tilde{n}_{\text{eff}} = \frac{\ln v - 2\pi m}{k_0\Lambda_z} \qquad m \equiv \text{branch \#} \qquad \begin{aligned} n_{\text{o}} &= \text{Re}\left[n_{\text{eff}}\right] \\ \kappa &= \text{Im}\left[n_{\text{eff}}\right] \end{aligned}$$

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