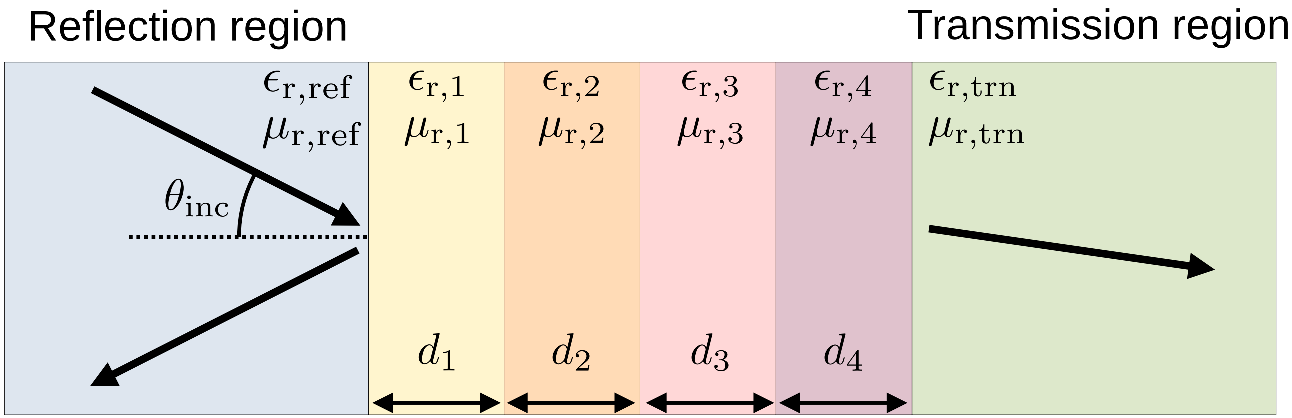
Lecture 12

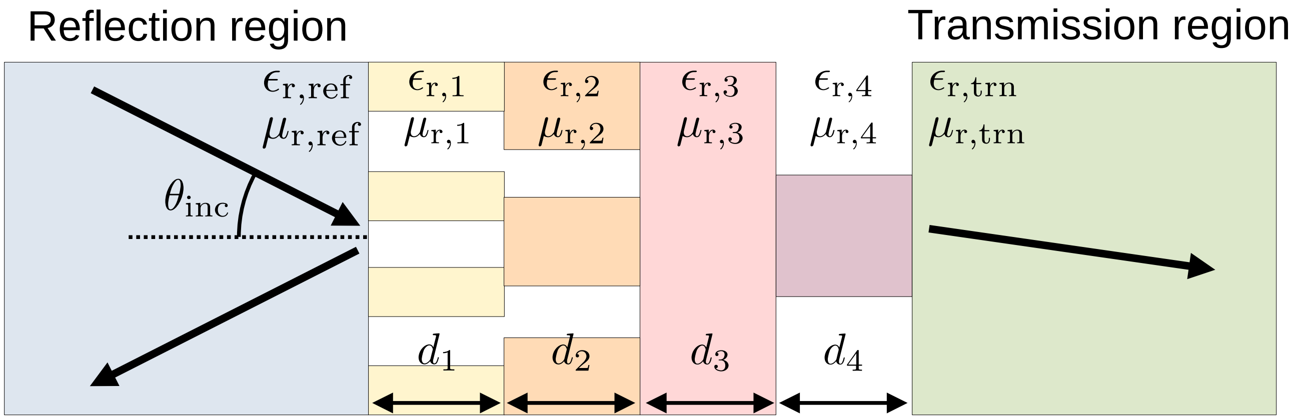
Rigorous Coupled-Wave Analysis (RCWA)

Rigorous Coupled-Wave Analysis

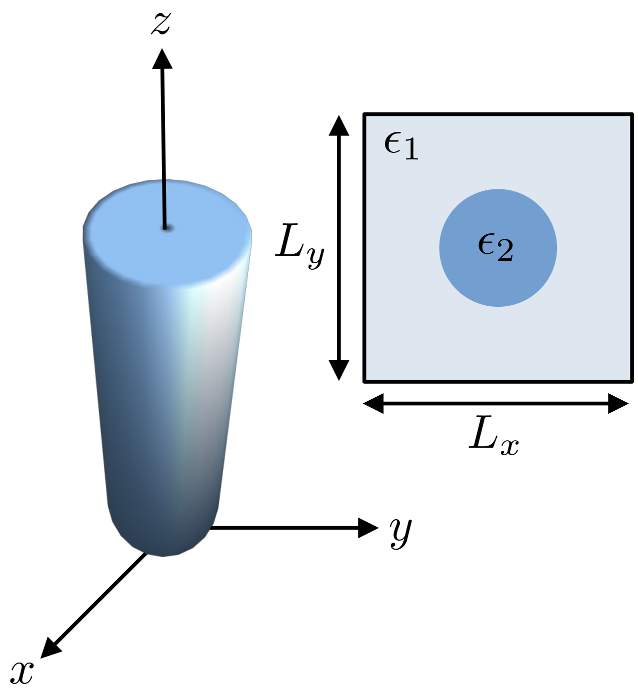
Transfer matrix method: all layers are uniform



RCWA: layers may be non-uniform along x and y



Maxwell Equations in Fourier Space



The periodic unit cell may be non-uniform along x and y but must be uniform along z.

Maxwell equations

$$\nabla \times \mathbf{H} = j\omega\epsilon\mathbf{E}$$
$$\nabla \times \mathbf{E} = -j\omega\mu\mathbf{H}$$

The products $\epsilon\mathbf{E}$ and $\mu\mathbf{H}$ become convolutions when going into Fourier space since both the fields and the material parameters are functions of x and y

Since the unit cell is periodic along x and y, we can express all quantities as Fourier series

$$\epsilon_r(x,y) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} a_{m,n} e^{j(m\mathbf{T}_1 + n\mathbf{T}_2)\cdot\mathbf{r}}$$

where the Fourier coefficients are given by

$$a_{m,n} = \frac{1}{L_x L_y}\int_{-L_x/2}^{L_x/2} \epsilon_r(x,y) e^{-j(m\mathbf{T}_1 + n\mathbf{T}_2)\cdot\mathbf{r}} dxdy$$

Maxwell Equations in Fourier Space

$$\epsilon_r(x,y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} a_{m,n} e^{j(m\mathbf{T}_1 + n\mathbf{T}_2)\cdot\mathbf{r}}$$

$$a_{m,n} = \frac{1}{L_x L_y} \int_{-L_x/2}^{L_x/2} \epsilon_r(x,y) e^{-j(m\mathbf{T}_1 + n\mathbf{T}_2)\cdot\mathbf{r}} dxdy$$

$$\mu_r(x,y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,n} e^{j(m\mathbf{T}_1 + n\mathbf{T}_2)\cdot\mathbf{r}}$$

$$b_{m,n} = \frac{1}{L_x L_y} \int_{-L_x/2}^{L_x/2} \mu_r(x,y) e^{-j(m\mathbf{T}_1 + n\mathbf{T}_2)\cdot\mathbf{r}} dxdy$$

Similarly, the fields are expressed in terms of spatial harmonics

$$\mathbf{E}(x,y,z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \mathbf{S}(m,n;z) e^{-j\mathbf{k}_{\parallel}(m,n)\cdot\mathbf{r}}$$

$$\mathbf{H}(x,y,z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \mathbf{U}(m,n;z) e^{-j\mathbf{k}_{\parallel}(m,n)\cdot\mathbf{r}}$$

where the tangential k-vectors are

$$\mathbf{k}_{\parallel}(m,n) = \mathbf{k}_{\parallel,\text{inc}} - m\mathbf{T}_1 - n\mathbf{T}_2$$

Normalizing Maxwell Equations

Maxwell equations

$$\nabla \times \mathbf{H} = j\omega\epsilon\mathbf{E}$$

$$\nabla \times \mathbf{E} = -j\omega\mu\mathbf{H}$$

We express and simplify Maxwell equations in each layer of the system

Normalization of the **H** field

$$\tilde{\mathbf{H}} = -j\eta_0\mathbf{H}$$

$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0\epsilon_{\mathrm{r}}E_x$$

$$\frac{\partial \tilde{H}_x}{\partial z} - \frac{\partial \tilde{H}_z}{\partial x} = k_0\epsilon_{\mathrm{r}}E_y$$

$$\frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_x}{\partial y} = k_0\epsilon_{\mathrm{r}}E_z$$

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = k_0\mu_{\mathrm{r}}\tilde{H}_x$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0\mu_{\mathrm{r}}\tilde{H}_y$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = k_0\mu_{\mathrm{r}}\tilde{H}_z$$

$$\epsilon_r(x, y) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} a_{m,n}e^{j(m\mathbf{T}_1+n\mathbf{T}_2)\cdot\mathbf{r}}$$

$$\mu_r(x, y) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} b_{m,n}e^{j(m\mathbf{T}_1+n\mathbf{T}_2)\cdot\mathbf{r}}$$

$$\mathbf{E}(x, y, z) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \mathbf{S}(m, n; z)e^{-j\mathbf{k}_{\parallel}(m,n)\cdot\mathbf{r}}$$

$$\mathbf{H}(x, y, z) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \mathbf{U}(m, n; z)e^{-j\mathbf{k}_{\parallel}(m,n)\cdot\mathbf{r}}$$

Example of Transforming Maxwell Equations

$$\mathbf{E}(x,y,z) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \mathbf{S}(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}}$$

$$\epsilon_r(x,y) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} a_{m,n}e^{j(m\mathbf{T}_1+n\mathbf{T}_2)\cdot\mathbf{r}}$$

$$\mathbf{H}(x,y,z) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \mathbf{U}(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}}$$

$$\frac{\partial\tilde{H}_z}{\partial y} - \frac{\partial\tilde{H}_y}{\partial z} = k_0\epsilon_\mathrm{r}E_x$$

$$-jk_y(m,n)\sum_m\sum_n U_z(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}} - \sum_m\sum_n \frac{\partial U_y}{\partial z}(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}} = k_0\underbrace{\left[\sum_m\sum_n a_{m,n}e^{j(m\mathbf{T}_1+n\mathbf{T}_2)\cdot\mathbf{r}}\right]\left[\sum_m\sum_n S_x(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}}\right]}$$

Cauchy product $\left(\sum_{n=0}^{\infty}a_n\right)\left(\sum_{n=0}^{\infty}b_n\right) = \sum_{n=0}^{\infty}\sum_{m=0}^{n}a_{n-m}b_m$

$$-jk_y(m,n)\sum_m\sum_n U_z(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}} - \sum_m\sum_n \frac{\partial U_y}{\partial z}(m,n;z)e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}} = k_0\sum_m\sum_n\left[\sum_p\sum_q a_{m-p,n-q}e^{j[(m-p)\mathbf{T}_1+(n-q)\mathbf{T}_2]\cdot\mathbf{r}}S_x(p,q;z)e^{-j\mathbf{k}_\parallel(p,q)\cdot\mathbf{r}}\right]$$

$$\sum_m\sum_n\left\{\left[-jk_y(m,n)U_z(m,n;z) - \frac{\partial U_y}{\partial z}(m,n;z)\right]e^{-j\mathbf{k}_\parallel(m,n)\cdot\mathbf{r}} = k_0\left[\sum_p\sum_q a_{m-p,n-q}S_x(p,q;z)e^{j[(m-p)\mathbf{T}_1+(n-q)\mathbf{T}_2]\cdot\mathbf{r}-j\mathbf{k}_\parallel(p,q)\cdot\mathbf{r}}\right]\right\}$$

Example of Transforming Maxwell Equations

$$\sum_m \sum_n \left\{ \left[-jk_y(m,n)U_z(m,n;z) - \frac{\partial U_y}{\partial z}(m,n;z) \right] e^{-j\mathbf{k}_{\parallel}(m,n)\cdot\mathbf{r}} = k_0 \left[\sum_p \sum_q a_{m-p,n-q} S_x(p,q;z) e^{j[(m-p)\mathbf{T}_1 + (n-q)\mathbf{T}_2]\cdot\mathbf{r} - j\mathbf{k}_{\parallel}(p,q)\cdot\mathbf{r}} \right] \right\}$$

$$e^{j[(m-p)\mathbf{T}_1+(n-q)\mathbf{T}_2]\cdot\mathbf{r}-j\mathbf{k}_{\parallel}(p,q)\cdot\mathbf{r}} = e^{j[(m-p)\mathbf{T}_1+(n-q)\mathbf{T}_2]\cdot\mathbf{r}-j(\mathbf{k}_{\parallel,\mathrm{inc}}-p\mathbf{T}_1-q\mathbf{T}_2)\cdot\mathbf{r}} = e^{-k(\mathbf{k}_{\parallel,\mathrm{inc}}-m\mathbf{T}_1-n\mathbf{T}_2)} = e^{-j\mathbf{k}_{\parallel}(m,n)\cdot\mathbf{r}}$$

Using the fact that $\mathbf{k}_{\parallel}(m,n) = \mathbf{k}_{\parallel,\mathrm{inc}} - m\mathbf{T}_1 - n\mathbf{T}_2$

↓

$$\sum_m \sum_n \left\{ -jk_y(m,n)U_z(m,n;z) - \frac{\partial U_y}{\partial z}(m,n;z) = k_0 \sum_p \sum_q a_{m-p,n-q} S_x(p,q;z) \right\}$$

↓

Since the equation must be valid for any *m* and *n*

$$-jk_y(m,n)U_z(m,n;z) - \frac{\partial U_y}{\partial z}(m,n;z) = k_0 \sum_p \sum_q a_{m-p,n-q} S_x(p,q;z)$$

Normalizing Maxwell Equations

Maxwell equations

$$\nabla \times \mathbf{H} = j\omega\epsilon\mathbf{E}$$
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We express and simplify Maxwell equations in each layer of the system

Normalization of the **H** field

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$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0\epsilon_\mathrm{r}E_x$$

$$\frac{\partial \tilde{H}_x}{\partial z} - \frac{\partial \tilde{H}_z}{\partial x} = k_0\epsilon_\mathrm{r}E_y$$

$$\frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_x}{\partial y} = k_0\epsilon_\mathrm{r}E_z$$

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = k_0\mu_\mathrm{r}\tilde{H}_x$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0\mu_\mathrm{r}\tilde{H}_y$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = k_0\mu_\mathrm{r}\tilde{H}_z$$

$$-jk_y(m,n)U_z(m,n;z) - \frac{\partial U_y}{\partial z}(m,n;')= k_0\sum_p\sum_q a_{m-p,n-q}S_x(p,q;z)$$

$$\frac{\partial U_x}{\partial z}(m,n;z) + jk_x(m,n)U_z(m,n;z) = k_0\sum_p\sum_q a_{m-p,n-q}S_y(p,q;z)$$

$$jk_y(m,n)U_x(m,n;z) - jk_xU_y(m,n;z) = k_0\sum_p\sum_q a_{m-p,n-q}S_z(p,q;z)$$

$$-jk_y(m,n)S_z(m,n;z) - \frac{\partial S_y}{\partial z}(m,n;z) = k_0\sum_p\sum_q b_{m-p,n-q}U_x(p,q;z)$$

$$\frac{\partial S_x}{\partial z}(m,n;z) + jk_x(m,n)S_z(m,n;z) = k_0\sum_p\sum_q b_{m-p,n-q}U_y(p,q;z)$$

$$jk_y(m,n)S_x(m,n;z) - jk_xS_y(m,n;z) = k_0\sum_p\sum_q b_{m-p,n-q}U_z(p,q;z)$$

Normalizing Fourier Space Maxwell Equations

Additional normalizations

$$z' = k_0 z$$

$$\tilde{k}_i = k_i / k_0$$

$$-j\tilde{k}_y(m,n)U_z(m,n;z') - \frac{\partial U_y}{\partial z'}(m,n;z') = \sum_p \sum_q a_{m-p,n-q} S_x(p,q;z')$$

$$\frac{\partial U_x}{\partial z'}(m,n;z') + j\tilde{k}_x(m,n)U_z(m,n;z') = \sum_p \sum_q a_{m-p,n-q} S_y(p,q;z')$$

$$j\tilde{k}_y(m,n)U_x(m,n;z') - j\tilde{k}_x U_y(m,n;z') = \sum_p \sum_q a_{m-p,n-q} S_z(p,q;z')$$

$$-j\tilde{k}_y(m,n)S_z(m,n;z') - \frac{\partial S_y}{\partial z'}(m,n;z') = \sum_p \sum_q b_{m-p,n-q} U_x(p,q;z')$$

$$\frac{\partial S_x}{\partial z'}(m,n;z') + j\tilde{k}_x(m,n)S_z(m,n;z') = \sum_p \sum_q b_{m-p,n-q} U_y(p,q;z')$$

$$j\tilde{k}_y(m,n)S_x(m,n;z') - j\tilde{k}_x S_y(m,n;z') = \sum_p \sum_q b_{m-p,n-q} U_z(p,q;z')$$

Understanding the Matrix Formulation

$$-j\tilde{k}_y(m,n)U_z(m,n;z') - \frac{\partial U_y}{\partial z'}(m,n;z') = \sum_p \sum_q a_{m-p,n-q} S_x(p,q;z')$$

Numerically, we limit ourselves to ±M and ±N harmonics

$$m = -M, \ \dots \ , 0, \ \dots \ , M$$

$$n = -N, \ \dots \ , 0, \ \dots \ , N$$

Convolution matrix

$$-j\overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_z - \frac{d}{dz'}\mathbf{u}_y = \overline{\overline{\epsilon}}_{\mathrm{r}} \cdot \mathbf{s}_x$$

$$\mathbf{s}_x = \begin{bmatrix} S_{x,-M,-N} \\ \vdots \\ S_{x,0,0} \\ \vdots \\ S_{x,M,N} \end{bmatrix}$$

Diagonal matrix containing the k_y component of each spatial harmonic

$$\overline{\overline{\mathrm{K}}}_y = \begin{bmatrix} \tilde{k}_{y,-M,-N} & & & & 0 \\ & \ddots & & & \\ & & \tilde{k}_{y,0,0} & & \\ & & & \ddots & \\ 0 & & & & \tilde{k}_{y,M,N} \end{bmatrix}$$

$$\mathbf{u}_z = \begin{bmatrix} U_{z,-M,-N} \\ \vdots \\ U_{z,0,0} \\ \vdots \\ U_{z,M,N} \end{bmatrix} \qquad \mathbf{u}_y = \begin{bmatrix} U_{y,-M,-N} \\ \vdots \\ U_{y,0,0} \\ \vdots \\ U_{y,M,N} \end{bmatrix}$$

Remember that $\mathbf{k}_{\|}(m,n) = \mathbf{k}_{\|,\mathrm{inc}} - m\mathbf{T}_1 - n\mathbf{T}_2$

Complete Matrix Formulation

Additional normalizations

$$z' = k_0 z$$

$$\tilde{k}_i = k_i / k_0$$

$$-j\tilde{k}_y(m,n)U_z(m,n;z') - \frac{\partial U_y}{\partial z'}(m,n;z') = \sum_q \sum_r a_{m-q,n-r} S_x(q,r;z')$$

$$\frac{\partial U_x}{\partial z'}(m,n;z') + j\tilde{k}_x(m,n)U_z(m,n;z') = \sum_q \sum_r a_{m-q,n-r} S_y(q,r;z')$$

$$j\tilde{k}_y(m,n)U_x(m,n;z') - j\tilde{k}_x U_y(m,n;z') = \sum_q \sum_r a_{m-q,n-r} S_z(q,r;z')$$

$$-j\tilde{k}_y(m,n)S_z(m,n;z') - \frac{\partial S_y}{\partial z'}(m,n;z') = \sum_q \sum_r b_{m-q,n-r} U_x(q,r;z')$$

$$\frac{\partial S_x}{\partial z'}(m,n;z') + j\tilde{k}_x(m,n)S_z(m,n;z') = \sum_q \sum_r b_{m-q,n-r} U_y(q,r;z')$$

$$j\tilde{k}_y(m,n)S_x(m,n;z') - j\tilde{k}_x S_y(m,n;z') = \sum_q \sum_r b_{m-q,n-r} U_z(q,r;z')$$

→

Matrix formulation

$$-j\overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_z - \frac{d}{dz'}\mathbf{u}_y = \overline{\overline{\epsilon}}_\mathrm{r} \cdot \mathbf{s}_x$$

$$\frac{d}{dz'}\mathbf{u}_x + j\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_z = \overline{\overline{\epsilon}}_\mathrm{r} \cdot \mathbf{s}_y$$

$$\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_y - \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_x = j\overline{\overline{\epsilon}}_\mathrm{r} \cdot \mathbf{s}_z$$

$$-j\overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_z - \frac{d}{dz'}\mathbf{s}_y = \overline{\overline{\mu}}_\mathrm{r} \cdot \mathbf{u}_x$$

$$\frac{d}{dz'}\mathbf{s}_x + j\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_z = \overline{\overline{\mu}}_\mathrm{r} \cdot \mathbf{u}_y$$

$$\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_y - \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_x = j\overline{\overline{\mu}}_\mathrm{r} \cdot \mathbf{u}_z$$

Eliminating Longitudinal Components

Matrix formulation

$$\left.\begin{aligned} \frac{d}{dz'}\mathbf{u}_x + j\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_z &= \overline{\overline{\epsilon}}_\mathrm{r} \cdot \mathbf{s}_y \\ -j\overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_z - \frac{d}{dz'}\mathbf{u}_y &= \overline{\overline{\epsilon}}_\mathrm{r} \cdot \mathbf{s}_x \end{aligned}\right\} \longrightarrow \left\{\begin{aligned} \frac{d}{dz'}\mathbf{u}_x &= \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_x + \left(\overline{\overline{\epsilon}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x\right) \cdot \mathbf{s}_y \\ \frac{d}{dz'}\mathbf{u}_y &= \left(\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\epsilon}}_\mathrm{r}\right) \cdot \mathbf{s}_x - \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_y \end{aligned}\right.$$

$$\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_y - \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_x = j\overline{\overline{\epsilon}}_\mathrm{r} \cdot \mathbf{s}_z \longrightarrow \mathbf{s}_z = -j\overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \left(\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_y - \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_x\right)$$

$$\left.\begin{aligned} \frac{d}{dz'}\mathbf{s}_x + j\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_z &= \overline{\overline{\mu}}_\mathrm{r} \cdot \mathbf{u}_y \\ -j\overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_z - \frac{d}{dz'}\mathbf{s}_y &= \overline{\overline{\mu}}_\mathrm{r} \cdot \mathbf{u}_x \end{aligned}\right\} \longrightarrow \left\{\begin{aligned} \frac{d}{dz'}\mathbf{s}_x &= \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_x + \left(\overline{\overline{\mu}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x\right) \cdot \mathbf{u}_y \\ \frac{d}{dz'}\mathbf{s}_y &= \left(\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mu}}_\mathrm{r}\right) \cdot \mathbf{u}_x - \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_y \end{aligned}\right.$$

$$\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_y - \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_x = j\overline{\overline{\mu}}_\mathrm{r} \cdot \mathbf{u}_z \longrightarrow \mathbf{u}_z = -j\overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \left(\overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_y - \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_x\right)$$

Expression of P and Q Matrices

$$\begin{cases} \dfrac{d}{dz'}\mathbf{u}_x = \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{s}_x + \left(\overline{\overline{\epsilon}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x\right) \cdot \mathbf{s}_y \\ \dfrac{d}{dz'}\mathbf{u}_y = \left(\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\epsilon}}_\mathrm{r}\right) \cdot \mathbf{s}_x - \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \cdot \mathbf{s}_y \end{cases} \longrightarrow \frac{d}{dz'}\begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y\end{bmatrix} = \underbrace{\begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\epsilon}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\epsilon}}_\mathrm{r} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}}_{\overline{\overline{\mathrm{Q}}}} \cdot \begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix}$$

$$\begin{cases} \dfrac{d}{dz'}\mathbf{s}_x = \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y \cdot \mathbf{u}_x + \left(\overline{\overline{\mu}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x\right) \cdot \mathbf{u}_y \\ \dfrac{d}{dz'}\mathbf{s}_y = \left(\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mu}}_\mathrm{r}\right) \cdot \mathbf{u}_x - \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \cdot \mathbf{u}_y \end{cases} \longrightarrow \frac{d}{dz'}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} = \underbrace{\begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\mu}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mu}}_\mathrm{r} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}}_{\overline{\overline{\mathrm{P}}}} \cdot \begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y\end{bmatrix}$$

Comparison with TMM formulation

$$\overline{\overline{\mathrm{P}}} = \frac{1}{\epsilon_\mathrm{r}}\begin{bmatrix} \tilde{k}_x\tilde{k}_y & \epsilon_\mathrm{r}\mu_\mathrm{r} - \tilde{k}_x^2 \\ \tilde{k}_y^2 - \epsilon_\mathrm{r}\mu_\mathrm{r} & -\tilde{k}_x\tilde{k}_y \end{bmatrix} \qquad \overline{\overline{\mathrm{Q}}} = \frac{1}{\mu_\mathrm{r}}\begin{bmatrix} \tilde{k}_x\tilde{k}_y & \epsilon_\mathrm{r}\mu_\mathrm{r} - \tilde{k}_x^2 \\ \tilde{k}_y^2 - \epsilon_\mathrm{r}\mu_\mathrm{r} & -\tilde{k}_x\tilde{k}_y \end{bmatrix}$$

Electric Field System of Equations

$$\frac{d}{dz'}\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix} = \overline{\overline{\mathrm{P}}}\cdot\begin{bmatrix}\mathbf{u}_x\\ \mathbf{u}_y\end{bmatrix}$$

$$\frac{d}{dz'}\begin{bmatrix}\mathbf{u}_x\\ \mathbf{u}_y\end{bmatrix} = \overline{\overline{\mathrm{Q}}}\cdot\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix}$$

→

$$\frac{d^2}{d\tilde{z}^2}\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix} - \overline{\overline{\Omega}}^2\cdot\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix} = 0$$

where $\overline{\overline{\Omega}}^2 = \overline{\overline{\mathrm{P}}}\cdot\overline{\overline{\mathrm{Q}}}$

General solution

$$\begin{bmatrix}\mathbf{s}_x(z')\\ \mathbf{s}_y(z')\end{bmatrix} = e^{-\overline{\overline{\Omega}}z'}\cdot\mathbf{s}_0^{+} + e^{+\overline{\overline{\Omega}}z'}\cdot\mathbf{s}_0^{-}$$

↓

$$\begin{bmatrix}\mathbf{s}_x(z')\\ \mathbf{s}_y(z')\end{bmatrix} = \overline{\overline{\mathrm{W}}}\cdot e^{-\overline{\overline{\lambda}}z'}\cdot\mathbf{c}^{+} + \overline{\overline{\mathrm{W}}}\cdot e^{+\overline{\overline{\lambda}}z'}\cdot\mathbf{c}^{-}$$

From the TMM, we have

$$e^{\pm\overline{\overline{\Omega}}z'} = \overline{\overline{\mathrm{W}}}\cdot e^{\pm\overline{\overline{\lambda}}z'}\cdot\overline{\overline{\mathrm{W}}}^{-1}$$

$\overline{\overline{\mathrm{W}}}$: matrix of the eigen-vectors of $\overline{\overline{\Omega}}$

$\overline{\overline{\lambda}}$: matrix of the eigen-values of $\overline{\overline{\Omega}}$

Similarly for the magnetic field

$$\begin{bmatrix}\mathbf{u}_x(z')\\ \mathbf{u}_y(z')\end{bmatrix} = -\overline{\overline{\mathrm{V}}}\cdot e^{-\overline{\overline{\lambda}}z'}\cdot\mathbf{c}^{+} + \overline{\overline{\mathrm{V}}}\cdot e^{+\overline{\overline{\lambda}}z'}\cdot\mathbf{c}^{-}$$

where $\overline{\overline{\mathrm{V}}} = \overline{\overline{\mathrm{Q}}}\cdot\overline{\overline{\mathrm{W}}}\cdot\overline{\overline{\lambda}}^{-1}$

Complete Solution

Combined electric and magnetic solutions

$$\mathbf{\Psi}(z') = \begin{bmatrix} \mathbf{s}_x(z') \\ \mathbf{s}_y(z') \\ \mathbf{u}_x(z') \\ \mathbf{u}_y(z') \end{bmatrix} = \begin{bmatrix} \overline{\overline{\mathrm{W}}} & \overline{\overline{\mathrm{W}}} \\ -\overline{\overline{\mathrm{V}}} & \overline{\overline{\mathrm{V}}} \end{bmatrix} \cdot \begin{bmatrix} e^{-\overline{\overline{\lambda}}z'} & 0 \\ 0 & e^{+\overline{\overline{\lambda}}z'} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{c}^{+} \\ \mathbf{c}^{-} \end{bmatrix}$$

Forward/backward mode amplitudes within a layer

1) Compute P and Q from the layer parameters and the incidence angle

$$\overline{\overline{\mathrm{P}}} = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\mu}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mu}}_\mathrm{r} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

$$\overline{\overline{\mathrm{Q}}} = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\epsilon}}_\mathrm{r} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\epsilon}}_\mathrm{r} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_\mathrm{r}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

2) Compute Ω

$$\overline{\overline{\Omega}}^2 = \overline{\overline{\mathrm{P}}} \cdot \overline{\overline{\mathrm{Q}}}$$

3) Find the eigen-vectors and eigen-values of Ω^2

$\overline{\overline{\mathrm{W}}}$: matrix of the eigen-vectors of $\overline{\overline{\Omega}}$

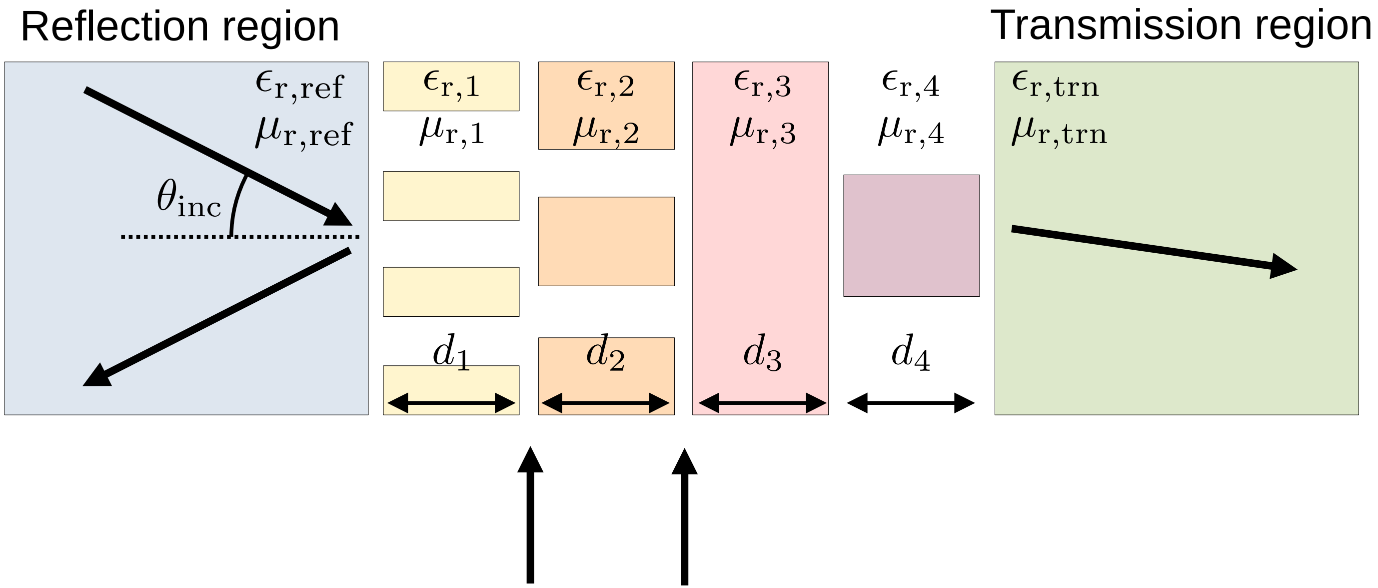
$\overline{\overline{\lambda}}$: matrix of the eigen-values of $\overline{\overline{\Omega}}$

4) Compute V

$$\overline{\overline{\mathrm{V}}} = \overline{\overline{\mathrm{Q}}} \cdot \overline{\overline{\mathrm{W}}} \cdot \overline{\overline{\lambda}}^{-1}$$

Remember that $\mathbf{k}_{\|}(m,n) = \mathbf{k}_{\|,\mathrm{inc}} - m\mathbf{T}_1 - n\mathbf{T}_2$

Problem Simplification Using Gap Media



As for the TMM formulation, we insert zero-thickness gaps in between the layers to symmetrize them.

Parameters of the Gap Medium

We define the gap media as being vacuum. Since these gaps are homogeneous layers, we do not need to compute convolution matrices.

$$\overline{\overline{Q}} = \begin{bmatrix} \overline{\overline{K}}_x \cdot \overline{\overline{K}}_y & \overline{\overline{I}} - \overline{\overline{K}}_x \cdot \overline{\overline{K}}_x \\ \overline{\overline{K}}_y \cdot \overline{\overline{K}}_y - \overline{\overline{I}} & -\overline{\overline{K}}_y \cdot \overline{\overline{K}}_x \end{bmatrix}$$

$$\overline{\overline{\lambda}} = \begin{bmatrix} j\overline{\overline{K}}_z & \overline{\overline{0}} \\ \overline{\overline{0}} & j\overline{\overline{K}}_z \end{bmatrix}$$

$$\overline{\overline{K}}_z = \left(\sqrt{\overline{\overline{I}} - \overline{\overline{K}}_y^2 - \overline{\overline{K}}_y^2} \right)^*$$

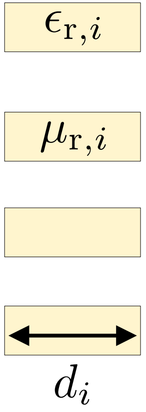
The conjugate is to satisfy the convention

$$e^{-jkz}$$

$$\overline{\overline{W}}_0 = \begin{bmatrix} \overline{\overline{I}} & \overline{\overline{0}} \\ \overline{\overline{0}} & \overline{\overline{I}} \end{bmatrix}$$

$$\overline{\overline{V}}_0 = \overline{\overline{Q}} \cdot \overline{\overline{\lambda}}^{-1}$$

Scattering Matrix of Each Layer



Scattering matrices using gap media

$$\overline{\overline{\mathrm{S}}}_{11}^{(i)} = \left(\overline{\overline{\mathrm{A}}}_i - \overline{\overline{\mathrm{X}}}_i \cdot \overline{\overline{\mathrm{B}}}_i \cdot \overline{\overline{\mathrm{A}}}_i^{-1} \cdot \overline{\overline{\mathrm{X}}}_i \cdot \overline{\overline{\mathrm{B}}}_i\right)^{-1} \cdot \left(\overline{\overline{\mathrm{X}}}_i \cdot \overline{\overline{\mathrm{B}}}_i \cdot \overline{\overline{\mathrm{A}}}_i^{-1} \cdot \overline{\overline{\mathrm{X}}}_i \cdot \overline{\overline{\mathrm{A}}}_i - \overline{\overline{\mathrm{B}}}_i\right)$$

$$\overline{\overline{\mathrm{S}}}_{12}^{(i)} = \left(\overline{\overline{\mathrm{A}}}_i - \overline{\overline{\mathrm{X}}}_i \cdot \overline{\overline{\mathrm{B}}}_i \cdot \overline{\overline{\mathrm{A}}}_i^{-1} \cdot \overline{\overline{\mathrm{X}}}_i \cdot \overline{\overline{\mathrm{B}}}_i\right)^{-1} \cdot \overline{\overline{\mathrm{X}}}_i \cdot \left(\overline{\overline{\mathrm{A}}}_i - \overline{\overline{\mathrm{B}}}_i \cdot \overline{\overline{\mathrm{A}}}_i^{-1} \cdot \overline{\overline{\mathrm{B}}}_i\right)$$

$$\overline{\overline{\mathrm{S}}}_{21}^{(i)} = \overline{\overline{\mathrm{S}}}_{12}^{(i)}$$

$$\overline{\overline{\mathrm{S}}}_{22}^{(i)} = \overline{\overline{\mathrm{S}}}_{11}^{(i)}$$

gap parameters

where

$$\begin{cases} \overline{\overline{\mathrm{A}}}_i = \overline{\overline{\mathrm{W}}}_i^{-1} + \overline{\overline{\mathrm{V}}}_i^{-1} \cdot \overline{\overline{\mathrm{V}}}_0 \\ \overline{\overline{\mathrm{B}}}_i = \overline{\overline{\mathrm{W}}}_i^{-1} - \overline{\overline{\mathrm{V}}}_i^{-1} \cdot \overline{\overline{\mathrm{V}}}_0 \\ \overline{\overline{\mathrm{X}}}_i = e^{-\overline{\overline{\lambda}}_i k_0 d_i} \end{cases}$$

1) Compute P and Q from the layer parameters and the incidence angle

$$\overline{\overline{\mathrm{P}}}_i = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\mu}}_{\mathrm{r},i} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mu}}_{\mathrm{r},i} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

$$\overline{\overline{\mathrm{Q}}}_i = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\epsilon}}_{\mathrm{r},i} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\epsilon}}_{\mathrm{r},i} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

2) Compute Ω

$$\overline{\overline{\Omega}}_i^2 = \overline{\overline{\mathrm{P}}}_i \cdot \overline{\overline{\mathrm{Q}}}_i$$

3) Find the eigen-vectors and eigen-values of Ω^2

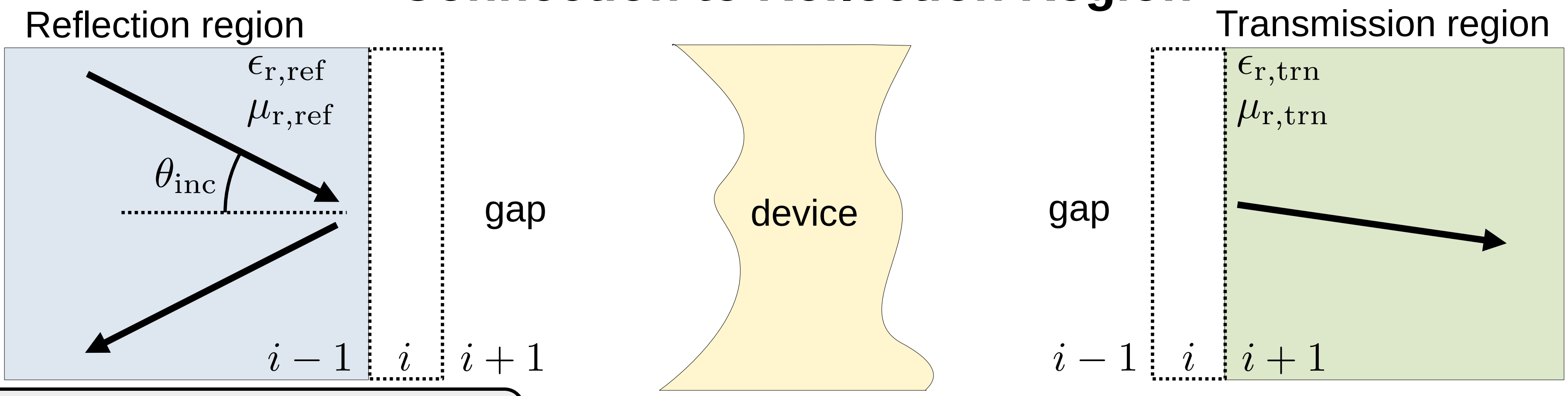
$\overline{\overline{\mathrm{W}}}_i$: matrix of the eigen-vectors

$\overline{\overline{\lambda}}_i$: matrix of the eigen-values

4) Compute V

$$\overline{\overline{\mathrm{V}}}_i = \overline{\overline{\mathrm{Q}}}_i \cdot \overline{\overline{\mathrm{W}}}_i \cdot \overline{\overline{\lambda}}_i^{-1}$$

Connection to Reflection Region



$$\overline{\overline{\mathrm{S}}}_{11}^{(\mathrm{ref})} = -\overline{\overline{\mathrm{A}}}_{\mathrm{ref}}^{-1} \cdot \overline{\overline{\mathrm{B}}}_{\mathrm{ref}}$$

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

$$\overline{\overline{\mathrm{S}}}_{21}^{(\mathrm{ref})} = \frac{1}{2}\left(\overline{\overline{\mathrm{A}}}_{\mathrm{ref}} - \overline{\overline{\mathrm{B}}}_{\mathrm{ref}} \cdot \overline{\overline{\mathrm{A}}}_{\mathrm{ref}}^{-1} \cdot \overline{\overline{\mathrm{B}}}_{\mathrm{ref}}\right)$$

$$\overline{\overline{\mathrm{S}}}_{22}^{(\mathrm{ref})} = \overline{\overline{\mathrm{B}}}_{\mathrm{ref}} \cdot \overline{\overline{\mathrm{A}}}_{\mathrm{ref}}^{-1}$$

$$\overline{\overline{\mathrm{A}}}_{\mathrm{ref}} = \overline{\overline{\mathrm{I}}} + \overline{\overline{\mathrm{V}}}_{0}^{-1} \cdot \overline{\overline{\mathrm{V}}}_{\mathrm{ref}}$$

$$\overline{\overline{\mathrm{B}}}_{\mathrm{ref}} = \overline{\overline{\mathrm{I}}} - \overline{\overline{\mathrm{V}}}_{0}^{-1} \cdot \overline{\overline{\mathrm{V}}}_{\mathrm{ref}}$$

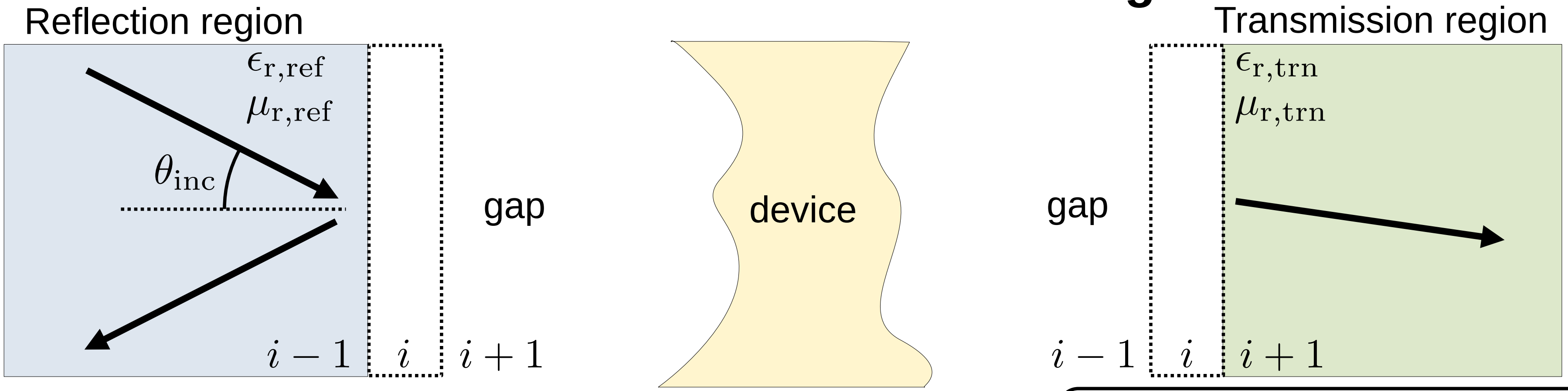
The incidence region is homogeneous, so we do not need to compute convolution matrices

$$\overline{\overline{\mathrm{K}}}_{z,\mathrm{ref}} = \left(\sqrt{\overline{\overline{\mathrm{I}}}\epsilon_{\mathrm{r,ref}}^{*}\mu_{\mathrm{r,ref}}^{*} - \overline{\overline{\mathrm{K}}}_{x}^{2} - \overline{\overline{\mathrm{K}}}_{y}^{2}}\right)^{*} \qquad \overline{\overline{\lambda}}_{\mathrm{ref}} = \begin{bmatrix} j\overline{\overline{\mathrm{K}}}_{z,\mathrm{ref}} & \overline{\overline{0}} \\ \overline{\overline{0}} & j\overline{\overline{\mathrm{K}}}_{z,\mathrm{ref}} \end{bmatrix}$$

$$\overline{\overline{\mathrm{Q}}}_{\mathrm{ref}} = \frac{1}{\epsilon_{\mathrm{r,ref}}} \begin{bmatrix} \overline{\overline{\mathrm{K}}}_{x} \cdot \overline{\overline{\mathrm{K}}}_{y} & \overline{\overline{\mathrm{I}}}\epsilon_{\mathrm{r,ref}}\mu_{\mathrm{r,ref}} - \overline{\overline{\mathrm{K}}}_{x} \cdot \overline{\overline{\mathrm{K}}}_{x} \\ \overline{\overline{\mathrm{K}}}_{y} \cdot \overline{\overline{\mathrm{K}}}_{y} - \overline{\overline{\mathrm{I}}}\epsilon_{\mathrm{r,ref}}\mu_{\mathrm{r,ref}} & -\overline{\overline{\mathrm{K}}}_{y} \cdot \overline{\overline{\mathrm{K}}}_{x} \end{bmatrix}$$

$$\overline{\overline{\mathrm{W}}}_{\mathrm{inc}} = \begin{bmatrix} \overline{\overline{\mathrm{I}}} & \overline{\overline{0}} \\ \overline{\overline{0}} & \overline{\overline{\mathrm{I}}} \end{bmatrix} \qquad \overline{\overline{\mathrm{V}}}_{\mathrm{ref}} = \overline{\overline{\mathrm{Q}}}_{\mathrm{ref}} \cdot \overline{\overline{\lambda}}_{\mathrm{ref}}^{-1}$$

Connection to Transmission Region



The transmission region is homogeneous, so we do not need to compute convolution matrices

$$\overline{\overline{\mathrm{K}}}_{z,\mathrm{trn}} = \left(\sqrt{\overline{\overline{\mathrm{I}}}\epsilon^*_{\mathrm{r,trn}}\mu^*_{\mathrm{r,trn}} - \overline{\overline{\mathrm{K}}}_x^2 - \overline{\overline{\mathrm{K}}}_y^2}\right)^*$$

$$\overline{\overline{\lambda}}_{\mathrm{trn}} = \begin{bmatrix} j\overline{\overline{\mathrm{K}}}_{z,\mathrm{trn}} & \overline{\overline{0}} \\ \overline{\overline{0}} & j\overline{\overline{\mathrm{K}}}_{z,\mathrm{trn}} \end{bmatrix}$$

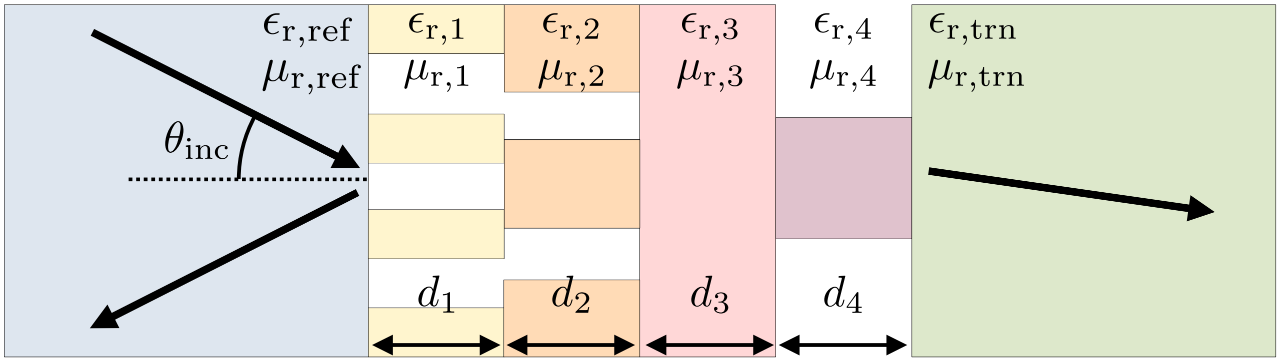
$$\overline{\overline{\mathrm{Q}}}_{\mathrm{trn}} = \frac{1}{\epsilon_{\mathrm{r,trn}}} \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\mathrm{I}}}\epsilon_{\mathrm{r,trn}}\mu_{\mathrm{r,trn}} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mathrm{I}}}\epsilon_{\mathrm{r,trn}}\mu_{\mathrm{r,trn}} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

$$\overline{\overline{\mathrm{W}}}_{\mathrm{trn}} = \begin{bmatrix} \overline{\overline{\mathrm{I}}} & \overline{\overline{0}} \\ \overline{\overline{0}} & \overline{\overline{\mathrm{I}}} \end{bmatrix} \qquad \overline{\overline{\mathrm{V}}}_{\mathrm{trn}} = \overline{\overline{\mathrm{Q}}}_{\mathrm{trn}} \cdot \overline{\overline{\lambda}}_{\mathrm{trn}}^{-1}$$

$$\begin{aligned} \overline{\overline{\mathrm{S}}}_{11}^{(\mathrm{trn})} &= \overline{\overline{\mathrm{B}}}_{\mathrm{trn}} \cdot \overline{\overline{\mathrm{A}}}_{\mathrm{trn}}^{-1} \\ \overline{\overline{\mathrm{S}}}_{12}^{(\mathrm{trn})} &= \frac{1}{2}\left(\overline{\overline{\mathrm{A}}}_{\mathrm{trn}} - \overline{\overline{\mathrm{B}}}_{\mathrm{trn}} \cdot \overline{\overline{\mathrm{A}}}_{\mathrm{trn}}^{-1} \cdot \overline{\overline{\mathrm{B}}}_{\mathrm{trn}}\right) \\ \overline{\overline{\mathrm{S}}}_{21}^{(\mathrm{trn})} &= 2\overline{\overline{\mathrm{A}}}_{\mathrm{trn}}^{-1} \\ \overline{\overline{\mathrm{S}}}_{22}^{(\mathrm{trn})} &= -\overline{\overline{\mathrm{A}}}_{\mathrm{trn}}^{-1} \cdot \overline{\overline{\mathrm{B}}}_{\mathrm{trn}} \end{aligned}$$

$$\begin{aligned} \overline{\overline{\mathrm{A}}}_{\mathrm{trn}} &= \overline{\overline{\mathrm{I}}} + \overline{\overline{\mathrm{V}}}_0^{-1} \cdot \overline{\overline{\mathrm{V}}}_{\mathrm{trn}} \\ \overline{\overline{\mathrm{B}}}_{\mathrm{trn}} &= \overline{\overline{\mathrm{I}}} - \overline{\overline{\mathrm{V}}}_0^{-1} \cdot \overline{\overline{\mathrm{V}}}_{\mathrm{trn}} \end{aligned}$$

Global Scattering Matrix



$$\overline{\overline{S}}^{(global)} = \overline{\overline{S}}^{(ref)} \otimes \left[\overline{\overline{S}}^{(1)} \otimes \overline{\overline{S}}^{(2)} \otimes \cdots \otimes \overline{\overline{S}}^{(N-1)} \otimes \overline{\overline{S}}^{(N)}\right] \otimes \overline{\overline{S}}^{(trn)}$$

Redheffer product

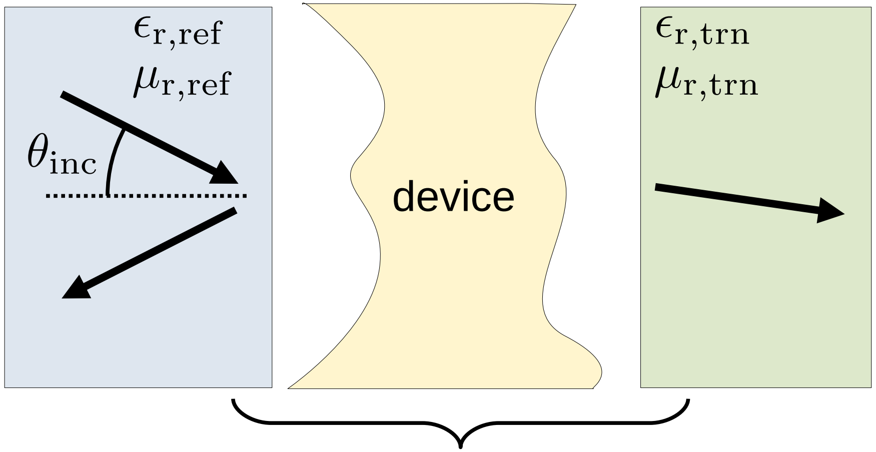
$$\overline{\overline{S}}_{11}^{(AB)} = \overline{\overline{S}}_{11}^{(A)} + \overline{\overline{S}}_{12}^{(A)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{11}^{(B)} \cdot \overline{\overline{S}}_{22}^{(A)}\right)^{-1} \cdot \overline{\overline{S}}_{11}^{(B)} \cdot \overline{\overline{S}}_{21}^{(A)}$$

$$\overline{\overline{S}}_{12}^{(AB)} = \overline{\overline{S}}_{12}^{(A)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{11}^{(B)} \cdot \overline{\overline{S}}_{22}^{(A)}\right)^{-1} \cdot \overline{\overline{S}}_{12}^{(B)}$$

$$\overline{\overline{S}}_{21}^{(AB)} = \overline{\overline{S}}_{21}^{(B)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{22}^{(A)} \cdot \overline{\overline{S}}_{11}^{(B)}\right)^{-1} \cdot \overline{\overline{S}}_{21}^{(A)}$$

$$\overline{\overline{S}}_{22}^{(AB)} = \overline{\overline{S}}_{22}^{(B)} + \overline{\overline{S}}_{21}^{(B)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{22}^{(A)} \cdot \overline{\overline{S}}_{11}^{(B)}\right)^{-1} \cdot \overline{\overline{S}}_{22}^{(A)} \cdot \overline{\overline{S}}_{12}^{(B)}$$

How to Define the Fields ?



$$\begin{bmatrix} \mathbf{c}'^{-}_{\mathrm{inc}} \\ \mathbf{c}'^{+}_{\mathrm{trn}} \end{bmatrix} = \begin{bmatrix} \overline{\overline{\mathrm{S}}}_{11}^{(\mathrm{global})} & \overline{\overline{\mathrm{S}}}_{12}^{(\mathrm{global})} \\ \overline{\overline{\mathrm{S}}}_{21}^{(\mathrm{global})} & \overline{\overline{\mathrm{S}}}_{22}^{(\mathrm{global})} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{c}'^{+}_{\mathrm{inc}} \\ \mathbf{c}'^{-}_{\mathrm{trn}} \end{bmatrix}$$

We assume the light is incident only from the left → $\mathbf{c}'^{-}_{\mathrm{trn}} = 0$

Reflection $\mathbf{c}'^{-}_{\mathrm{ref}} = \overline{\overline{\mathrm{S}}}_{11}^{(\mathrm{global})} \cdot \mathbf{c}'^{+}_{\mathrm{inc}}$

Transmission $\mathbf{c}'^{+}_{\mathrm{trn}} = \overline{\overline{\mathrm{S}}}_{21}^{(\mathrm{global})} \cdot \mathbf{c}'^{+}_{\mathrm{inc}}$

$$\begin{bmatrix} \mathbf{s}_x(z') \\ \mathbf{s}_y(z') \end{bmatrix} = \overline{\overline{\mathrm{W}}} \cdot e^{-\overline{\overline{\lambda}} z'} \cdot \mathbf{c}^{+} + \overline{\overline{\mathrm{W}}} \cdot e^{\overline{\overline{\lambda}} z'} \cdot \mathbf{c}^{-}$$

Remember that: $\overline{\overline{\mathrm{W}}} = \overline{\overline{\mathrm{I}}}$ and we can set $z' = 0$

$$\mathbf{c} = \begin{bmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{bmatrix}$$

$$\mathbf{E}_{\mathrm{ref}} = \overline{\overline{\mathrm{S}}}_{11}^{(\mathrm{global})} \cdot \mathbf{E}_{\mathrm{inc}}$$

$$\mathbf{E}_{\mathrm{trn}} = \overline{\overline{\mathrm{S}}}_{21}^{(\mathrm{global})} \cdot \mathbf{E}_{\mathrm{inc}}$$

where

$$\mathbf{E}_{\mathrm{inc}} = \begin{bmatrix} p_x \boldsymbol{\delta}_0 \\ p_y \boldsymbol{\delta}_0 \end{bmatrix}$$

x and y field polarizations

Vector of zeros with a one in the middle corresponding to 0^{th} order

How to Define the Scattered Power ?

$$\mathbf{E}_{\text{ref}} = \overline{\overline{\text{S}}}_{11}^{(\text{global})} \cdot \mathbf{E}_{\text{inc}}$$

$$\mathbf{E}_{\text{trn}} = \overline{\overline{\text{S}}}_{21}^{(\text{global})} \cdot \mathbf{E}_{\text{inc}}$$

where $\mathbf{E}_{\text{ref}} = \begin{bmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{bmatrix}$ and $\mathbf{E}_{\text{trn}} = \begin{bmatrix} \mathbf{t}_x \\ \mathbf{t}_y \end{bmatrix}$

$$E_z = -\frac{k_x E_x + k_y E_y}{k_z} \longrightarrow \begin{cases} \mathbf{r}_z = -\overline{\overline{\text{K}}}_{z,\text{ref}}^{-1} \cdot \left(\overline{\overline{\text{K}}}_x \cdot \mathbf{r}_x + \overline{\overline{\text{K}}}_y \cdot \mathbf{r}_y \right) \\ \mathbf{t}_z = -\overline{\overline{\text{K}}}_{z,\text{trn}}^{-1} \cdot \left(\overline{\overline{\text{K}}}_x \cdot \mathbf{t}_x + \overline{\overline{\text{K}}}_y \cdot \mathbf{t}_y \right) \end{cases}$$

Field reflection and transmission coefficients of each spatial harmonic

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

Power reflection and transmission coefficients of each spatial harmonic

$$\mathbf{R} = \frac{\text{Re}\left[\overline{\overline{\text{K}}}_{z,\text{ref}}\right] \cdot |\mathbf{r}|^2}{\text{Re}\left[k_{z,\text{inc}}\right]} \qquad \mathbf{T} = \frac{\text{Re}\left[\overline{\overline{\text{K}}}_{z,\text{trn}}/\mu_{\text{r,trn}}\right] \cdot |\mathbf{t}|^2}{\text{Re}\left[k_{z,\text{inc}}/\mu_{\text{r,inc}}\right]}$$

Total scattered power $R_{\text{tot}} = \sum \mathbf{R}$ $\qquad T_{\text{tot}} = \sum \mathbf{T}$

What Have We Learned So Far….

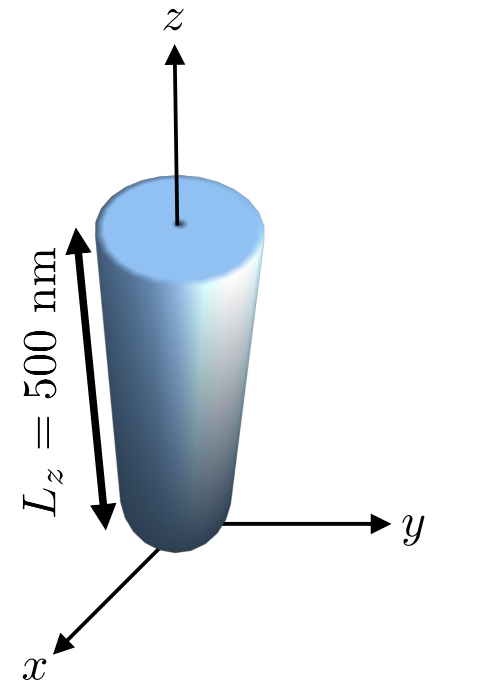
- The RCWA technique is built on the same principle as the TMM technique. The main difference is that the RCWA technique considers that the layers may be periodically varying.
- Periodic variations of the permittivity and permeability are expressed in terms of Fourier series.
- The fields are also expressed in terms of Fourier series since they follow the periodicity of the structure.
- This allows us to rewrite Maxwell equations in Fourier space and build and system of matrix equations for all spatial harmonics (diffraction orders + evanescent waves).
- In Fourier space, the multiplications between the permittivity/permeability and the fields become convolutions. These convolutions are conveniently transformed into matrix multiplications.
- As for the TMM technique, we use zero-thickness gap media in between each layer to symmetrize them and simplify the problem. This time, the gap media are simply vacuum.
- In contrast to the TMM technique, we now have to compute the eigen-vectors/values for each of the spatially varying layer.

RCWA Python Implementation

In what follows, I am using

```
import numpy as np
from scipy.linalg import expm
```

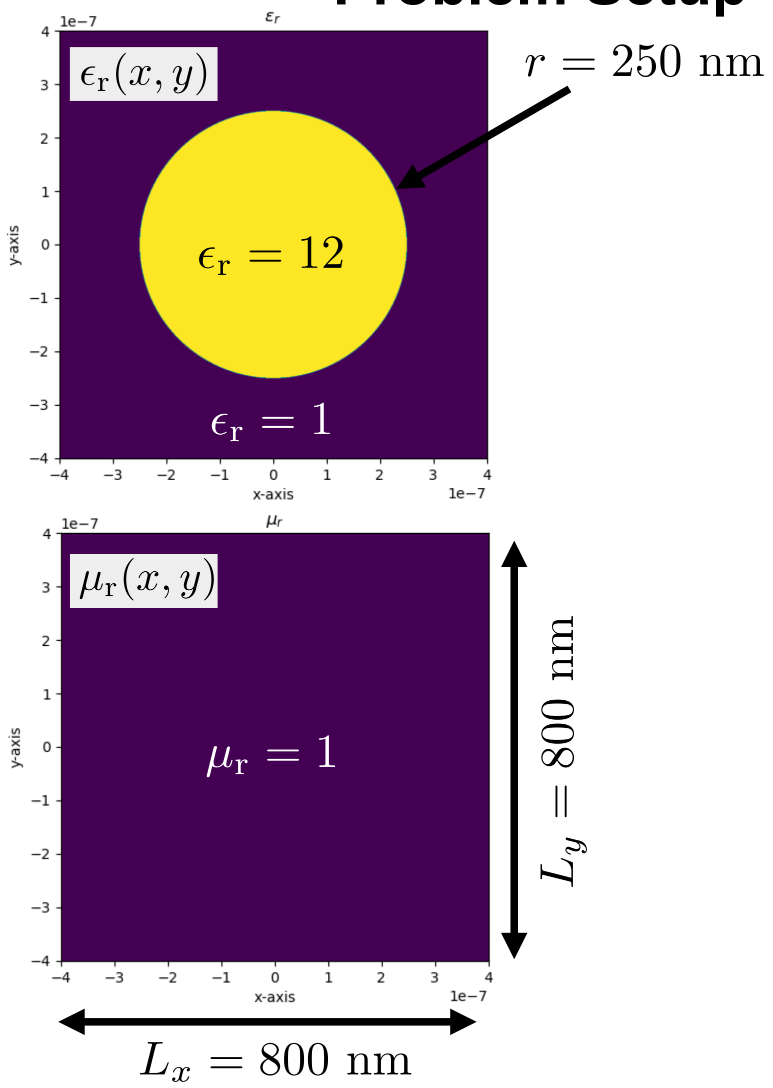
Problem Setup



Spatial harmonics

$$m = -M, \ \ldots \ , 0, \ \ldots \ , M$$

$$n = -N, \ \ldots \ , 0, \ \ldots \ , N$$




```
er1 = 1         # epsilon in reflection medium
mr1 = 1         # mu in reflection medium
er2 = 1         # epsilon in transmission medium
mr2 = 1         # mu in transmission medium

pol_inc = 'TM' # source polarization: TM, TE

wavelength = 1000e-9  # wavelength in m

theta = 0      # incidence angle in rad
phi   = 0      # incidence angle in rad

Lx = 800e-9    # dimension of the unit cell along x in m
Ly = 800e-9    # dimension of the unit cell along y in m
Lz = [500e-9]

M = 3          # Number of spatial harmonics along x
N = 3          # Number of spatial hamronics along y

# DEFINE LAYER(S)
r = 250*1e-9

Nx = 1024      # number of cells along x
Ny = Nx        # number of cells along y

mr = np.ones((Nx,Ny))

dx = Lx/Nx
xa = np.arange(Nx)*dx
xa = xa - np.mean(xa)

dy = Ly/Ny
ya = np.arange(Ny)*dy
ya = ya - np.mean(ya)

Y,X = np.meshgrid(ya,xa)
A = (X**2 + Y**2) <= r**2

er = 12*A + (1-A)
```

Computing Convolution Matrix

Takes Fourier transform of the material matrix →

$$\sum_p \sum_q a_{m-p,n-q} S_x(p,q;z')$$

$$\bar{\bar{\epsilon}}_{\mathrm{r}} \cdot \mathbf{s}_x$$

$$\mathbf{s}_x = \begin{bmatrix} S_{x,-M,-N} \\ \vdots \\ S_{x,0,0} \\ \vdots \\ S_{x,M,N} \end{bmatrix}$$

Spatial harmonics

$$m = -M, \ \ldots \ , 0, \ \ldots \ , M$$

$$n = -N, \ \ldots \ , 0, \ \ldots \ , N$$

contains

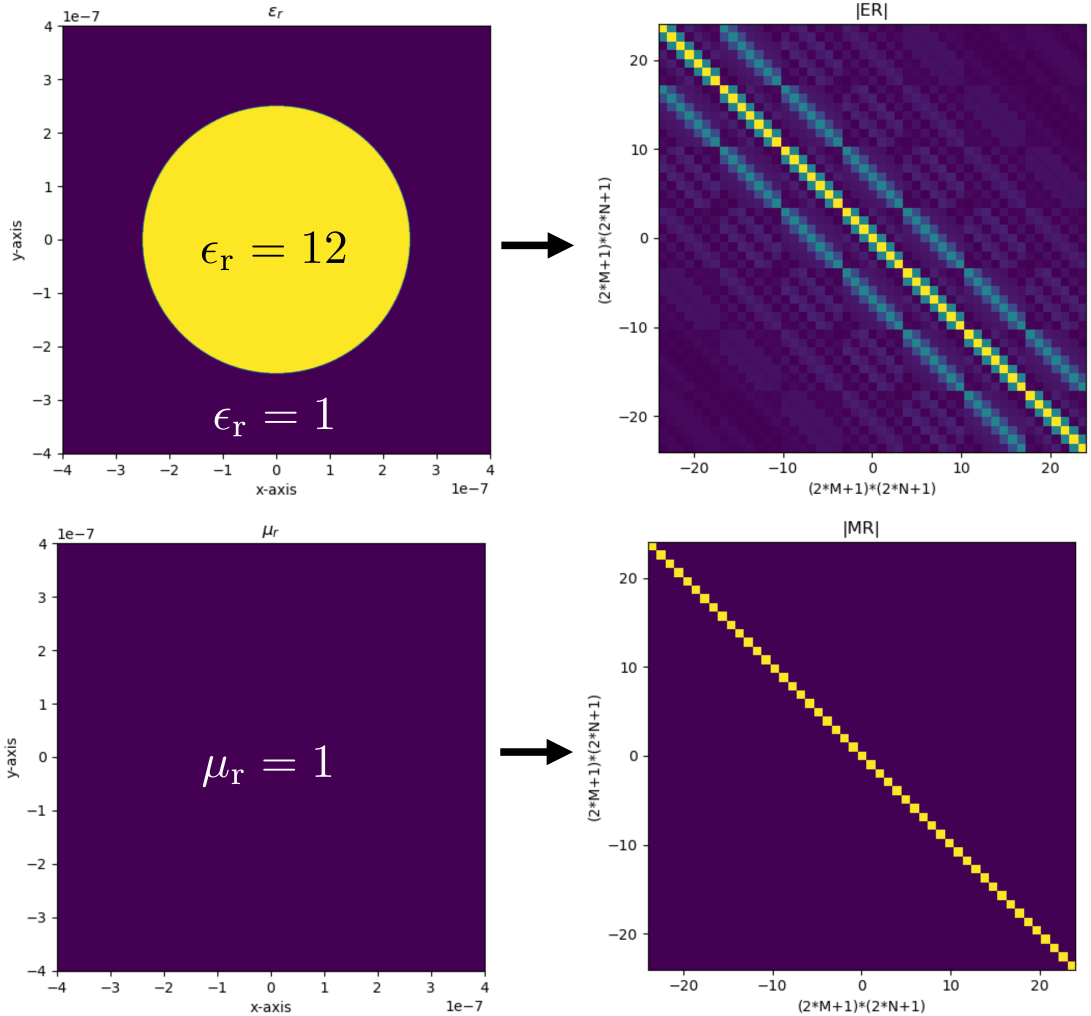
$$(2M+1)(2N+1)$$

spatial harmonics

```
def convmat(A,M,N):

    Nx,Ny = np.shape(A)
    p = np.arange(-M,M+1)
    q = np.arange(-N,N+1)
    P,Q = 2*M+1, 2*N+1

    A = np.fft.fftshift(np.fft.fft2(A))/(Nx*Ny)

    p0 = np.floor(Nx/2)
    q0 = np.floor(Ny/2)

    row = (Q-1)*P + (P-1)
    col = (Q-1)*P + (P-1)

    C = np.zeros((row+1,col+1),dtype=np.complex128)

    for qrow in range(Q):
        for prow in range(P):

            row = qrow*P + prow

            for qcol in range(Q):
                for pcol in range(P):

                    col = qcol*P + pcol

                    pfft = p[prow] - p[pcol]
                    qfft = q[qrow] - q[qcol]

                    C[row,col] = A[int(p0+pfft),int(q0+qfft)]

    return C
```

Computing Convolution Matrices

Direct space / **Convolution matrices**



Off-diagonal terms create coupling between spatial harmonics

```
ERc = [convmat(er,M,N)]
MRc = [convmat(mr,M,N)]
```

Builds a list as it may contain several layers

Since M=N=3, we have

$$(2M+1)(2N+1) = 49$$

spatial harmonics

Spatial harmonics

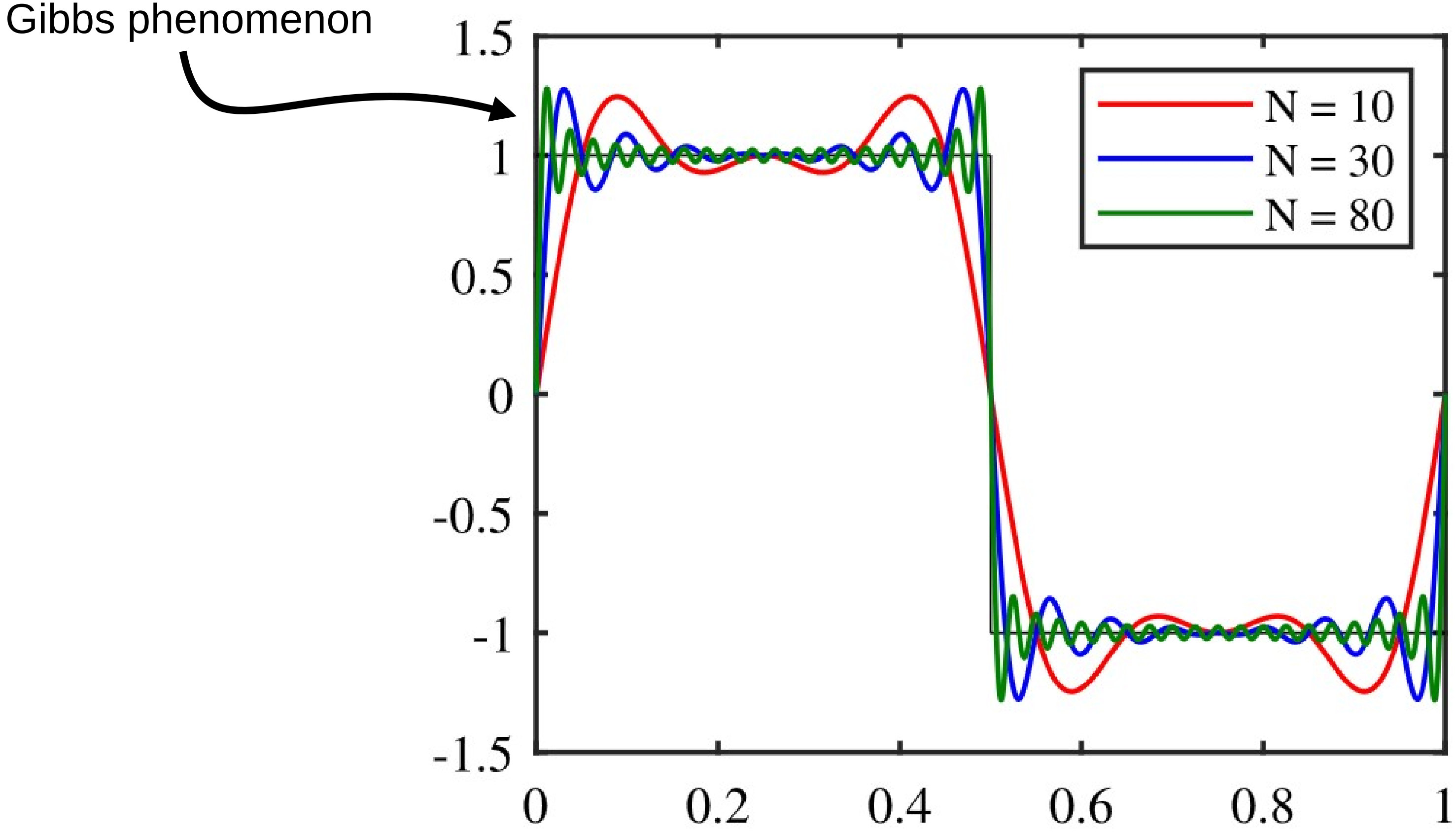
$$m = -M, \dots, 0, \dots, M$$

$$n = -N, \dots, 0, \dots, N$$

Drawback of Fourier Methods

Fourier series approximation of a square function

Gibbs phenomenon



We are never really simulating the actual structure but a Fourier reconstruction of it.

https://doi.org/10.1016/j.cma.2019.112781

Defining Incidence Source Field

Defining TE and TM incident field polarization

$$\hat{\mathbf{p}}_{\mathrm{TE}} = \begin{cases} \hat{\mathbf{y}} & \mathbf{k}_\mathrm{i} \parallel \hat{\mathbf{n}} \quad \text{(normal incidence)} \\ \hat{\mathbf{n}} \times \hat{\mathbf{k}}_\mathrm{i} & \mathbf{k}_\mathrm{i} \nparallel \hat{\mathbf{n}} \end{cases}$$

$$\hat{\mathbf{p}}_{\mathrm{TM}} = \hat{\mathbf{k}}_\mathrm{i} \times \hat{\mathbf{p}}_{\mathrm{TE}}$$

$$\mathbf{E} = A_{\mathrm{TE}}\hat{\mathbf{p}}_{\mathrm{TE}} + A_{\mathrm{TM}}\hat{\mathbf{p}}_{\mathrm{TM}}$$

$$\mathbf{E}_{\mathrm{inc}} = \begin{bmatrix} p_x \boldsymbol{\delta}_0 \\ p_y \boldsymbol{\delta}_0 \end{bmatrix}$$

```
# incident normalized wave vector
kinc = np.array([np.sin(theta)*np.cos(phi),\
np.sin(theta)*np.sin(phi),np.cos(theta)])

# vector normal to medium
nvec = np.array([0,0,1])

# definition of polarization vector
if theta == 0:
    ate = np.array([0,1,0])
else:
    ate = np.cross(kinc,nvec)/np.linalg.norm(np.cross(kinc,nvec))

atm  = np.cross(ate,kinc)/np.linalg.norm(np.cross(ate,kinc))

if theta == 0:
    atm0, ate0 = atm, ate
    atm = np.cos(phi)*atm0 - np.sin(phi)*ate0
    ate = np.sin(phi)*atm0 + np.cos(phi)*ate0

if pol_inc == 'TM':
    Pol = atm
elif pol_inc == 'TE':
    Pol = ate

# Create Dirac vector
MN = (2*M+1)*(2*N+1)
Delta = np.zeros((MN,1))
middle = int(np.floor(MN/2))
Delta[middle] = 1

# Compute Source Field
Esrc = np.concatenate((Pol[0]*Delta, Pol[1]*Delta))
```

Defining K-Vector Matrices

Spatial harmonics

$$m = -M, \ \ldots \ , 0, \ \ldots \ , M$$

$$n = -N, \ \ldots \ , 0, \ \ldots \ , N$$

Tangential k-vector

$$\mathbf{k}_{\|}(m,n) = \mathbf{k}_{\|,\text{inc}} - m\mathbf{T}_1 - n\mathbf{T}_2$$

$$\overline{\overline{\text{K}}}_{z,\text{ref}} = \left(\sqrt{\overline{\overline{\text{I}}}\epsilon^*_{\text{r,ref}}\mu^*_{\text{r,ref}} - \overline{\overline{\text{K}}}_y^2 - \overline{\overline{\text{K}}}_y^2}\right)^*$$

$$\overline{\overline{\text{K}}}_{z,\text{trn}} = \left(\sqrt{\overline{\overline{\text{I}}}\epsilon^*_{\text{r,trn}}\mu^*_{\text{r,trn}} - \overline{\overline{\text{K}}}_y^2 - \overline{\overline{\text{K}}}_y^2}\right)^*$$

$$\overline{\overline{\text{K}}}_{z} = \left(\sqrt{\overline{\overline{\text{I}}} - \overline{\overline{\text{K}}}_y^2 - \overline{\overline{\text{K}}}_y^2}\right)^*$$

```
# Number of spatial harmonics
m = np.arange(-M,M+1)
n = np.arange(-N,N+1)

# Generate k-vectors
mr1er1 = mr1*er1
mr2er2 = mr2*er2

kinc  = np.emath.sqrt(mr1er1)*kinc

kx    = kinc[0]-m*wavelength/Lx
ky    = kinc[1]-n*wavelength/Ly

ky,kx = np.meshgrid(ky,kx)

kzRef = np.conj(np.emath.sqrt(\
np.conj(mr1er1)-kx**2-ky**2))
kzTrn = np.conj(np.emath.sqrt(\
np.conj(mr2er2)-kx**2-ky**2))
kzGap = np.conj(np.emath.sqrt(1-kx**2-ky**2))

Kx    = np.diag(kx.flatten('F'))
Ky    = np.diag(ky.flatten('F'))
KzRef = np.diag(kzRef.flatten('F'))
KzTrn = np.diag(kzTrn.flatten('F'))
KzGap = np.diag(kzGap.flatten('F'))

KxKy, KyKx = Kx.dot(Ky), Ky.dot(Kx)
KyKy, KxKx = Ky.dot(Ky), Kx.dot(Kx)
```

Defining Gap Media Parameters

$$\overline{\overline{\mathrm{Q}}} = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\mathrm{I}}} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mathrm{I}}} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

$$\overline{\overline{\lambda}} = \begin{bmatrix} j\overline{\overline{\mathrm{K}}}_z & \overline{\overline{0}} \\ \overline{\overline{0}} & j\overline{\overline{\mathrm{K}}}_z \end{bmatrix}$$

$$\overline{\overline{\mathrm{V}}}_0 = \overline{\overline{\mathrm{Q}}} \cdot \overline{\overline{\lambda}}^{-1}$$

```
One, ID = np.identity(MN), np.identity(MN*2)
Zer = np.zeros((MN,MN))
Q0  = np.concatenate((np.concatenate((KxKy, One-KxKx),axis=1),\
                     np.concatenate((KyKy-One, -KyKx),axis=1)))

L0 = np.concatenate((np.concatenate((1j*KzGap, Zer),axis=1),\
                     np.concatenate((Zer, 1j*KzGap),axis=1)))

V0 = Q0.dot(np.linalg.inv(L0))
iV0 = np.linalg.inv(V0)

# Initialize scattering matrices
SR_0 = np.zeros(((MN)*2,(MN)*2))
ST_0 = ID

S11d, S22d, S12d, S21d = SR_0, SR_0, ST_0, ST_0
```

Implementation of the Redheffer Product

Used to combine scattering matrices $\overline{\overline{S}}^{(A)} \otimes \overline{\overline{S}}^{(B)} = \overline{\overline{S}}^{(AB)}$

$$\overline{\overline{S}}_{11}^{(AB)} = \overline{\overline{S}}_{11}^{(A)} + \overline{\overline{S}}_{12}^{(A)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{11}^{(B)} \cdot \overline{\overline{S}}_{22}^{(A)} \right)^{-1} \cdot \overline{\overline{S}}_{11}^{(B)} \cdot \overline{\overline{S}}_{21}^{(A)}$$

$$\overline{\overline{S}}_{12}^{(AB)} = \overline{\overline{S}}_{12}^{(A)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{11}^{(B)} \cdot \overline{\overline{S}}_{22}^{(A)} \right)^{-1} \cdot \overline{\overline{S}}_{12}^{(B)}$$

$$\overline{\overline{S}}_{21}^{(AB)} = \overline{\overline{S}}_{21}^{(B)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{22}^{(A)} \cdot \overline{\overline{S}}_{11}^{(B)} \right)^{-1} \cdot \overline{\overline{S}}_{21}^{(A)}$$

$$\overline{\overline{S}}_{22}^{(AB)} = \overline{\overline{S}}_{22}^{(B)} + \overline{\overline{S}}_{21}^{(B)} \cdot \left(\overline{\overline{I}} - \overline{\overline{S}}_{22}^{(A)} \cdot \overline{\overline{S}}_{11}^{(B)} \right)^{-1} \cdot \overline{\overline{S}}_{22}^{(A)} \cdot \overline{\overline{S}}_{12}^{(B)}$$

```
def redheffer(SA11,SA12,SA21,SA22,SB11,SB12,SB21,SB22):

    I = np.identity(len(SA11))

    D = SA12.dot(np.linalg.inv(I - SB11.dot(SA22)))
    F = SB21.dot(np.linalg.inv(I - SA22.dot(SB11)))

    SAB11 = SA11 + D.dot(SB11.dot(SA21))
    SAB12 = D.dot(SB12)
    SAB21 = F.dot(SA21)
    SAB22 = SB22 + F.dot(SA22.dot(SB12))

    return SAB11,SAB12,SAB21,SAB22
```

Defining Layer Loop

$$\overline{\overline{\mathrm{P}}}_i = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\mu}}_{\mathrm{r},i} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\mu}}_{\mathrm{r},i} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\epsilon}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

$$\overline{\overline{\mathrm{Q}}}_i = \begin{bmatrix} \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y & \overline{\overline{\epsilon}}_{\mathrm{r},i} - \overline{\overline{\mathrm{K}}}_x \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \\ \overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_y - \overline{\overline{\epsilon}}_{\mathrm{r},i} & -\overline{\overline{\mathrm{K}}}_y \cdot \overline{\overline{\mu}}_{\mathrm{r},i}^{-1} \cdot \overline{\overline{\mathrm{K}}}_x \end{bmatrix}$$

$$\overline{\overline{\Omega}}_i^2 = \overline{\overline{\mathrm{P}}}_i \cdot \overline{\overline{\mathrm{Q}}}_i$$

Eigen-mode decomposition

$$\overline{\overline{\mathrm{V}}}_i = \overline{\overline{\mathrm{Q}}}_i \cdot \overline{\overline{\mathrm{W}}}_i \cdot \overline{\overline{\lambda}}_i^{-1}$$

$$\overline{\overline{\mathrm{A}}}_i = \overline{\overline{\mathrm{W}}}_i^{-1} + \overline{\overline{\mathrm{V}}}_i^{-1} \cdot \overline{\overline{\mathrm{V}}}_0$$

$$\overline{\overline{\mathrm{B}}}_i = \overline{\overline{\mathrm{W}}}_i^{-1} - \overline{\overline{\mathrm{V}}}_i^{-1} \cdot \overline{\overline{\mathrm{V}}}_0$$

$$\overline{\overline{\mathrm{X}}}_i = e^{-\overline{\overline{\lambda}}_i k_0 d_i}$$

```
for n in range(len(ERc)):

    ER, MR = ERc[n], MRc[n]
    iER, iMR = np.linalg.inv(ER), np.linalg.inv(MR)
    KxiER, KyiER, KxiMR, KyiMR = Kx.dot(iER), Ky.dot(iER), Kx.dot(iMR), Ky.dot(iMR)

    Pm = np.concatenate((np.concatenate((KxiER.dot(Ky), MR-KxiER.dot(Kx)),axis=1),\
                         np.concatenate((KyiER.dot(Ky)-MR, -KyiER.dot(Kx)),axis=1)))

    Qm = np.concatenate((np.concatenate((KxiMR.dot(Ky), ER-KxiMR.dot(Kx)),axis=1),\
                         np.concatenate((KyiMR.dot(Ky)-ER, -KyiMR.dot(Kx)),axis=1)))

    omega = Pm.dot(Qm)

    eV, W = np.linalg.eig(omega)
    eV = np.diag(np.emath.sqrt(eV))
    V = Qm.dot(W).dot(np.linalg.inv(eV))
    iW, iV = np.linalg.inv(W), np.linalg.inv(V).dot(V0)

    A = iW + iV
    B = iW - iV

    X = expm(-eV*Lz[n]*2*np.pi/wavelength)

    iA = np.linalg.inv(A)
    Num = A - X.dot(B).dot(iA).dot(X).dot(B)

    S11 = np.linalg.solve(Num, X.dot(B).dot(iA).dot(X).dot(A) - B)
    S12 = np.linalg.solve(Num, X.dot(A - B.dot(iA).dot(B)))
    S21 = S12
    S22 = S11

    # Compute device scattering matrices
    S11d,S12d,S21d,S22d = redheffer(S11d,S12d,S21d,S22d,S11,S12,S21,S22)
```

Connection to Reflection and Transmission Regions

Reflection region

```
mr1er1O = mr1er1*One
Qref = 1/mr1*np.concatenate\
  ((np.concatenate((KxKy, mr1er1O-KxKx),axis=1),\
   np.concatenate((KyKy-mr1er1O, -KyKx),axis=1)))

Lref = np.concatenate\
  ((np.concatenate((1j*KzRef, Zer),axis=1),\
       np.concatenate((Zer, 1j*KzRef),axis=1)))

Vref = Qref.dot(np.linalg.inv(Lref))
iV0Vref = iV0.dot(Vref)

A = ID + iV0Vref
B = ID - iV0Vref

iA = np.linalg.inv(A)
iAB = iA.dot(B)

S11ref = -iAB
S12ref = 2*iA
S21ref = 0.5*(A - B.dot(iAB))
S22ref = B.dot(iA)

S11,S12,S21,S22 = redheffer(S11ref,S12ref,S21ref,\
  S22ref,S11d,S12d,S21d,S22d)
```

Transmission region

```
mr2er2O = mr2er2*One
Qtrn = 1/mr2*np.concatenate(\
  (np.concatenate((KxKy, mr2er2O-KxKx),axis=1),\
   np.concatenate((KyKy-mr2er2O, -KyKx),axis=1)))

Ltrn = np.concatenate(\
   (np.concatenate((1j*KzTrn, Zer),axis=1),\
   np.concatenate((Zer, 1j*KzTrn),axis=1)))

Vtrn = Qtrn.dot(np.linalg.inv(Ltrn))
iV0Vtrn = iV0.dot(Vtrn)

A = ID + iV0Vtrn
B = ID - iV0Vtrn

iA  = np.linalg.inv(A)
iAB = iA.dot(B)

S11trn = B.dot(iA)
S12trn = 0.5*(A - B.dot(iAB))
S21trn = 2*iA
S22trn = -iAB

S11,S12,S21,S22 = redheffer(S11,S12,S21,\
  S22,S11trn,S12trn,S21trn,S22trn)
```

Computing Scattered Power

$$\mathbf{E}_{\text{ref}} = \overline{\overline{\text{S}}}_{11}^{(\text{global})} \cdot \mathbf{E}_{\text{inc}}$$

$$\mathbf{E}_{\text{trn}} = \overline{\overline{\text{S}}}_{21}^{(\text{global})} \cdot \mathbf{E}_{\text{inc}}$$

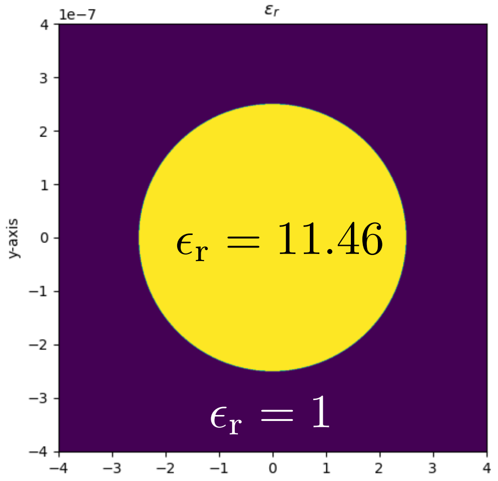
```
T = S21.dot(Esrc)
R = S11.dot(Esrc)

Rx = R[0:MN]
Ry = R[MN:]
Rz = -np.linalg.inv(KzRef).dot(Kx.dot(Rx) + Ky.dot(Ry))

Tx = T[0:MN]
Ty = T[MN:]
Tz = -np.linalg.inv(KzTrn).dot(Kx.dot(Tx) + Ky.dot(Ty))

# transmission power coefficient
Tcoef = np.real(mr1/mr2*KzTrn/kinc[2])

# getting the zeroth order scattering parameters
r0 = np.array([Rx[middle,0], Ry[middle,0], Rz[middle,0]])
t0 = np.array([Tx[middle,0], Ty[middle,0], Tz[middle,0]])

# transmission field amplitude
FA = np.emath.sqrt(Tcoef[middle,middle])

r0tm, t0tm = atm.dot(r0), FA*atm.dot(t0)
r0te, t0te = ate.dot(r0), FA*ate.dot(t0)

# COMPUTE DIFFRACTION EFFICIENCES
# For reflected field
reff = np.abs(Rx)**2 + np.abs(Ry)**2 + np.abs(Rz)**2
R = np.real(KzRef/kinc[2]).dot(reff)
Rtot = np.sum(R)

# For transmitted field
teff = np.abs(Tx)**2 + np.abs(Ty)**2 + np.abs(Tz)**2
T = Tcoef.dot(teff)
Ttot = np.sum(T)
```

Example of how to compute the scattered power going in the 0th order

$$\mathbf{R} = \frac{\text{Re}\left[\overline{\overline{\text{K}}}_{z,\text{ref}}\right] \cdot |\mathbf{r}|^2}{\text{Re}\left[k_{z,\text{inc}}\right]} \qquad R_{\text{tot}} = \sum \mathbf{R}$$

$$\mathbf{T} = \frac{\text{Re}\left[\overline{\overline{\text{K}}}_{z,\text{trn}}/\mu_{\text{r,trn}}\right] \cdot |\mathbf{t}|^2}{\text{Re}\left[k_{z,\text{inc}}/\mu_{\text{r,ref}}\right]} \qquad T_{\text{tot}} = \sum \mathbf{T}$$

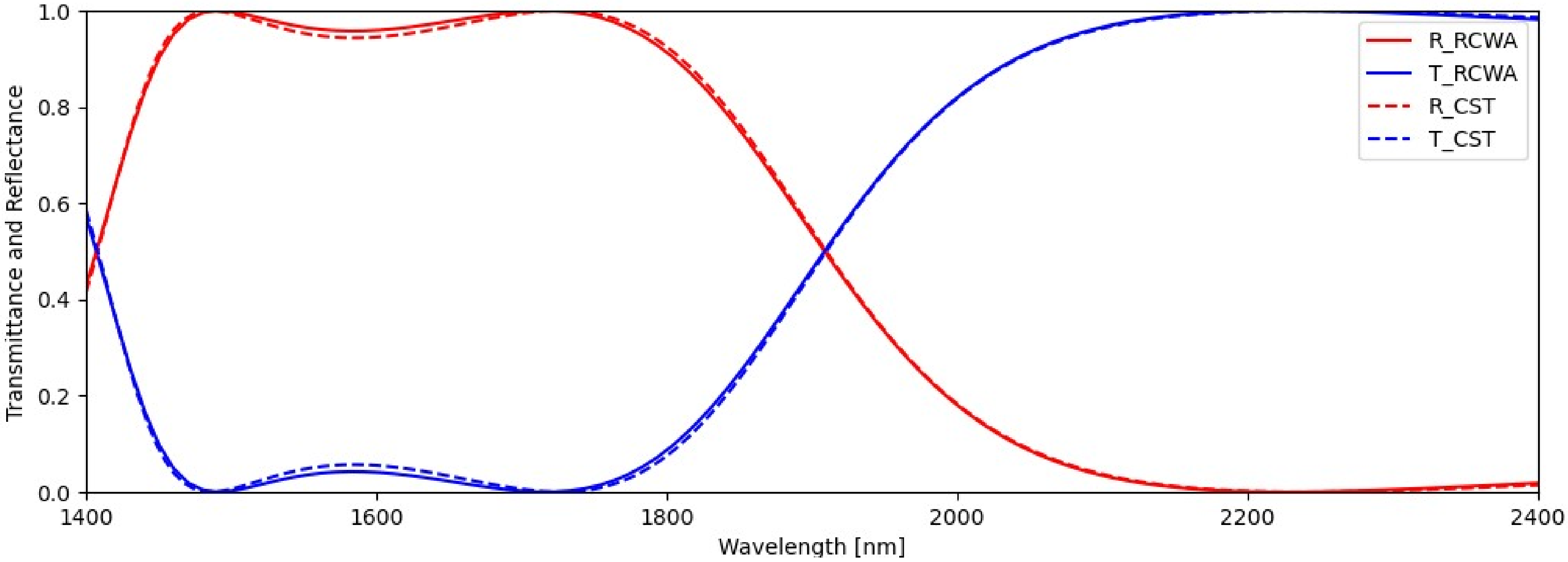
Frequency Response



Simulation parameters

$$L_x = L_y = 800 \text{ nm}$$
$$L_z = 500 \text{ nm}$$
$$r = 250 \text{ nm}$$
$$N = M = 7$$

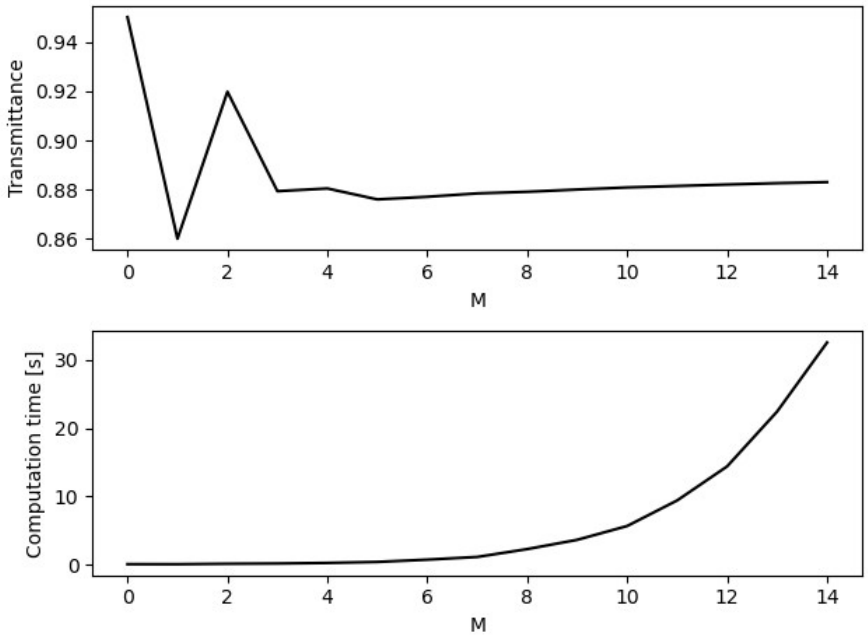
CST Studio is a commercial simulation software



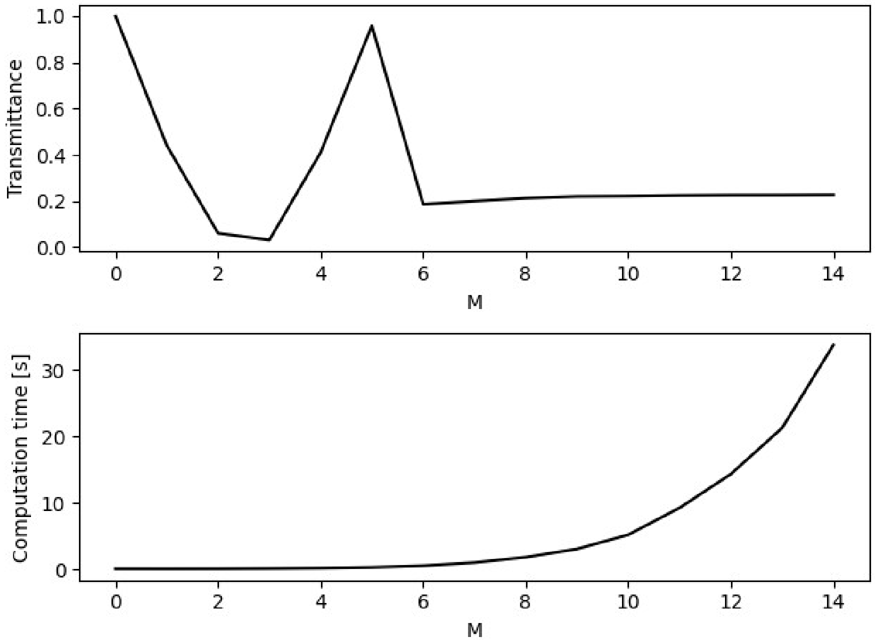
Convergence and Computation Time

Computation done for a single frequency point

$\epsilon_{\mathrm{r,puck}} = 12$



$\epsilon_{\mathrm{r,puck}} = 50$



Here we consider that M = N, so the total number of spatial harmonics is $(2M+1)^2$

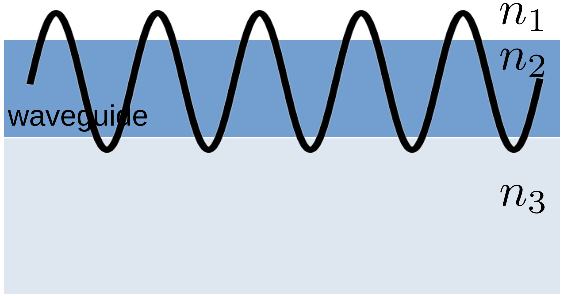
What Have We Learned So Far….

- For each layer, we only define the cross-sections of $\epsilon_r(x,y)$ and $\mu_r(x,y)$ since the layers are considered uniform in the z-direction.
- We specify a finite set of spatial harmonics in the x- and y-directions. The more spatial harmonics, the more accurate the simulation but the longer the computation time.
- RCWA typically gives good results for low index materials. For high index materials (like metals) the technique requires more spatial harmonics, which increases computation time.

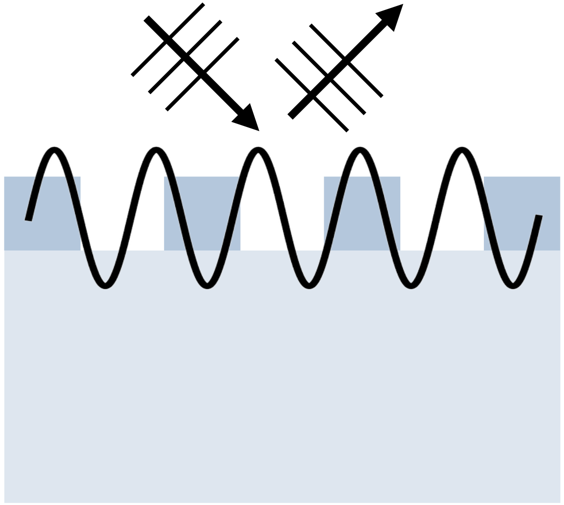
Guided-Mode Resonances

Guided-Mode Resonances (GMR)

In a waveguide, the light does not escape and does not couple from the outside

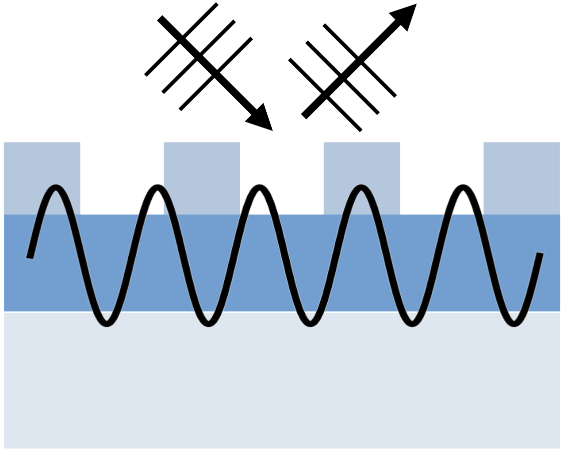


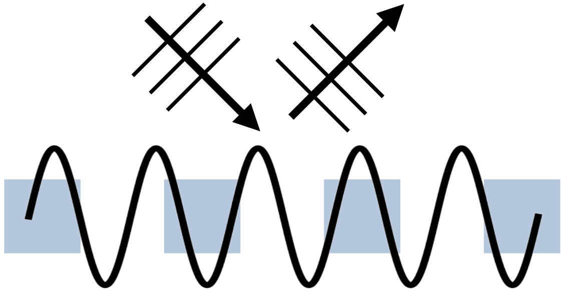
$n_2 > n_1$ and $n_2 > n_3$



The grating itself may support GMR

Adding a grating on top of the waveguide enables in and out coupling

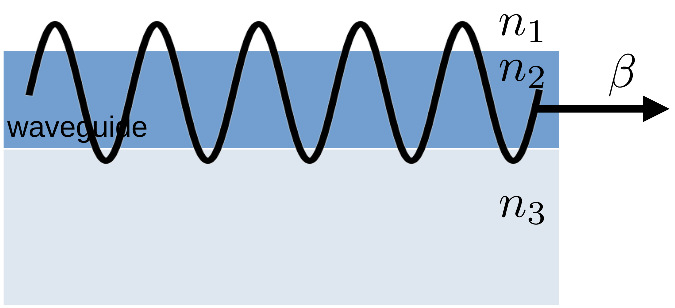




Even a simple array of particles may support GMR

Guided-mode resonances are a generalization of <u>Wood anomalies</u> to dielectric structures

Waveguide Propagation Constant

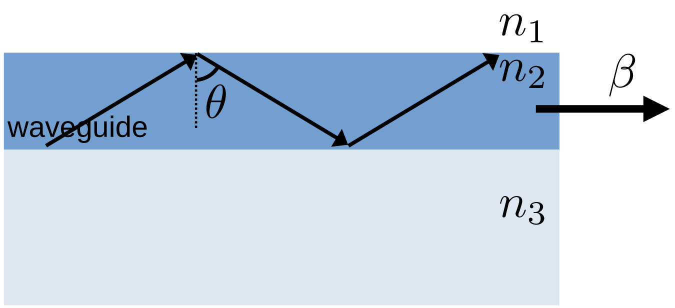


$n_2 > n_1$ and $n_2 > n_3$

The modes that propagate inside the waveguide have a propagation constant β and "see" an effective refractive index n_{eff}

$$\beta = k_0 n_{\text{eff}}$$

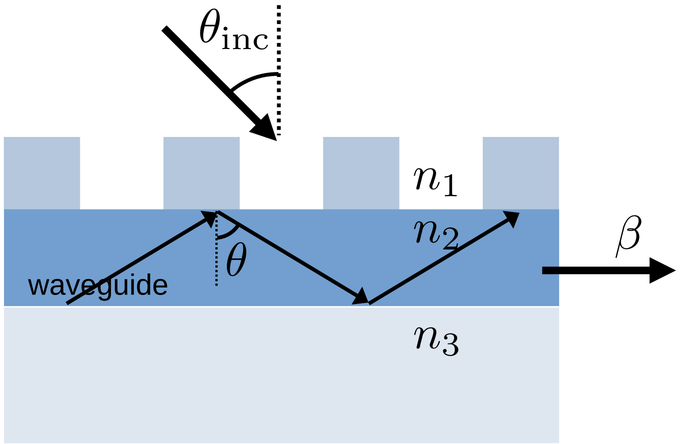
where $n_1, n_3 < n_{\text{eff}} < n_2$



Using a ray tracing approach, we see that the propagation constant may be expressed in terms of the propagation angle θ

$$\beta = k_0 n_{\text{eff}} = k_0 n_2 \sin\theta$$

Coupling to a Waveguide Mode with a Grating



$$\beta = k_0 n_{\rm eff} = k_0 n_2 \sin\theta$$

Grating equation

$$\underbrace{n_2 \sin\theta_m}_{n_{\rm eff}} = n_1 \sin\theta_{\rm inc} - m\frac{\lambda_0}{L}$$

Knowing that

$$n_1, n_3 < n_{\rm eff} < n_2$$

$$\max(n_1, n_3) < \left| n_1 \sin\theta_{\rm inc} - m\frac{\lambda_0}{L} \right| < n_2$$

Coupling to a Waveguide Mode with a Grating

Condition for GMR existence

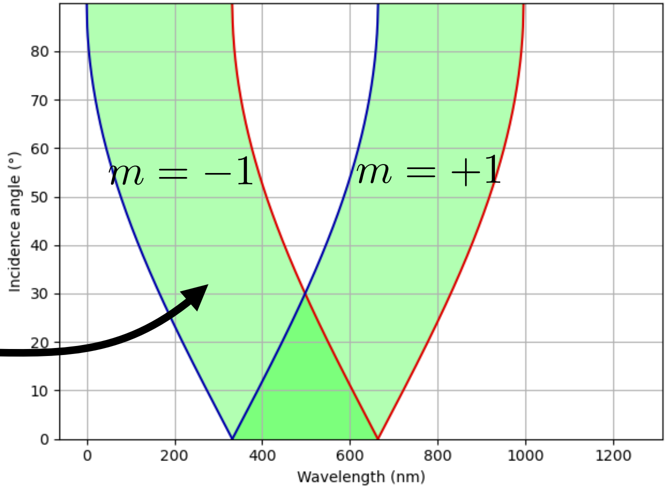
$$\max(n_1, n_3) < \left| n_1 \sin\theta_{\text{inc}} - m\frac{\lambda_0}{L} \right| < n_2$$

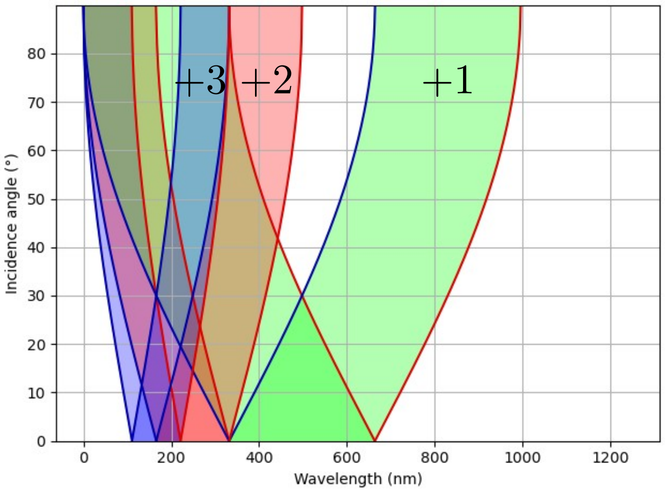
$$\rightarrow \begin{cases} \theta_{\text{inc}}^{\text{min}} = \arcsin\left\{ \dfrac{1}{n_1}\left[m\dfrac{\lambda_0}{L} \pm \max(n_1, n_3) \right] \right\} \\[2ex] \theta_{\text{inc}}^{\text{max}} = \arcsin\left\{ \dfrac{1}{n_1}\left[m\dfrac{\lambda_0}{L} \pm n_2 \right] \right\} \end{cases}$$

$$L = 332 \text{ nm}$$
$$n_1 = 1 = n_3$$
$$n_2 = 2$$

With m = -3, …, +3

GMR may exist

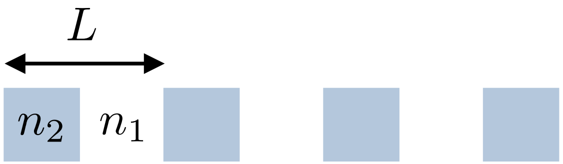




Code for Predicting GMR

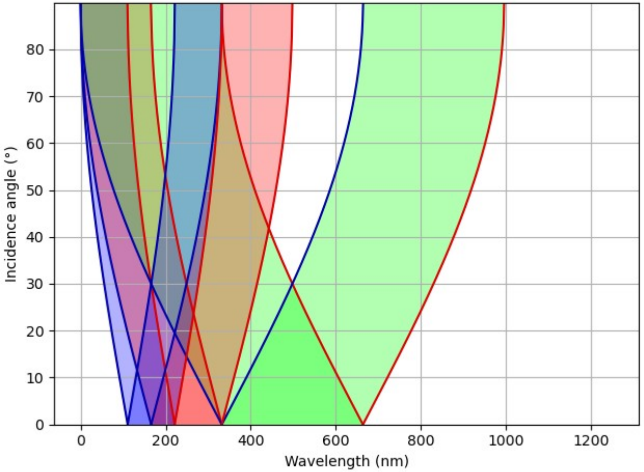
```
import numpy as np
import matplotlib.pyplot as pl
# ================================================
P = 300      # array period in [nm]
e1 = 1       # er of superstrate
eg = 7.5     # grating effective refractive index
e3 = 1       # er of substrate
N = 1        # number of diffraction orders to display (up to 3)
lam = np.linspace(0,2400,1000)   # wavelength in [nm]
# ================================================
n1, ng, n3 = np.sqrt(e1), np.sqrt(eg), np.sqrt(e3)
C = ['#00FF00','#FF0000','#0000FF']
pl.figure()
for m in range(-N,N+1):

    if m == 0:
        continue
    if m < 0:
        tet_min = np.arcsin( 1/n1*(m*lam/P + max(n1,n3)),dtype=np.complex128)
        tet_max = np.arcsin( 1/n1*(m*lam/P + ng),dtype=np.complex128)
    elif m > 0:
        tet_min = np.arcsin( 1/n1*(m*lam/P - max(n1,n3)),dtype=np.complex128)
        tet_max = np.arcsin( 1/n1*(m*lam/P - ng),dtype=np.complex128)

    y1 = np.real(tet_min)*180/np.pi
    y2 = np.real(tet_max)*180/np.pi

    pl.plot(lam,y1,'#0000AA',lw=1.5)
    pl.plot(lam,y2,'#DD0000',lw=1.5)
    pl.fill_between(lam, y1, y2,color=C[abs(m)-1],alpha=0.3)

pl.xlabel('Wavelength (nm)')
pl.ylabel('Incidence angle (°)')
pl.ylim([0,89.9])
pl.xlim([lam[0],lam[-1]])
pl.grid()
pl.tight_layout()
pl.show()
```

Varying Parameters

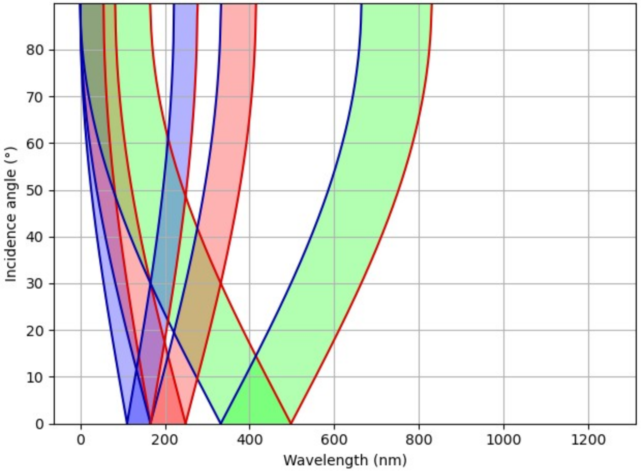


$$\begin{cases} \theta_{\text{inc}}^{\text{min}} = \arcsin\left\{\frac{1}{n_1}\left[m\frac{\lambda_0}{L} \pm \max(n_1, n_3)\right]\right\} \\ \theta_{\text{inc}}^{\text{max}} = \arcsin\left\{\frac{1}{n_1}\left[m\frac{\lambda_0}{L} \pm n_2\right]\right\} \end{cases}$$

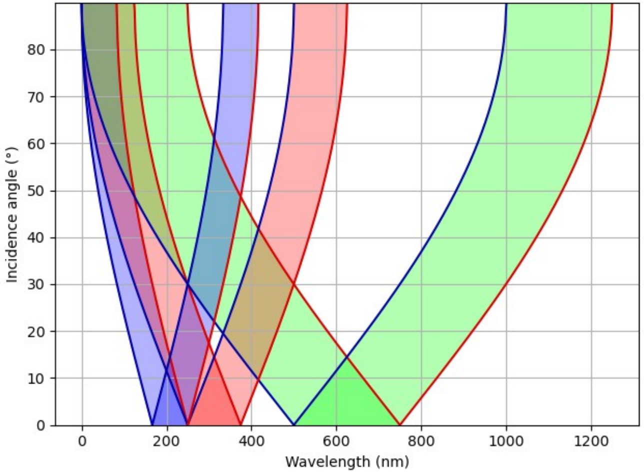
$L = 332$ nm
$n_1 = 1 = n_3$
$n_2 = 2$



$L = 332$ nm
$n_1 = 1 = n_3$
$n_2 = 1.5$



$L = 500$ nm
$n_1 = 1 = n_3$
$n_2 = 1.5$

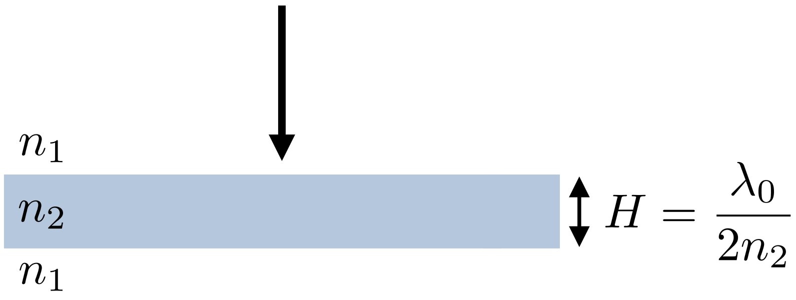


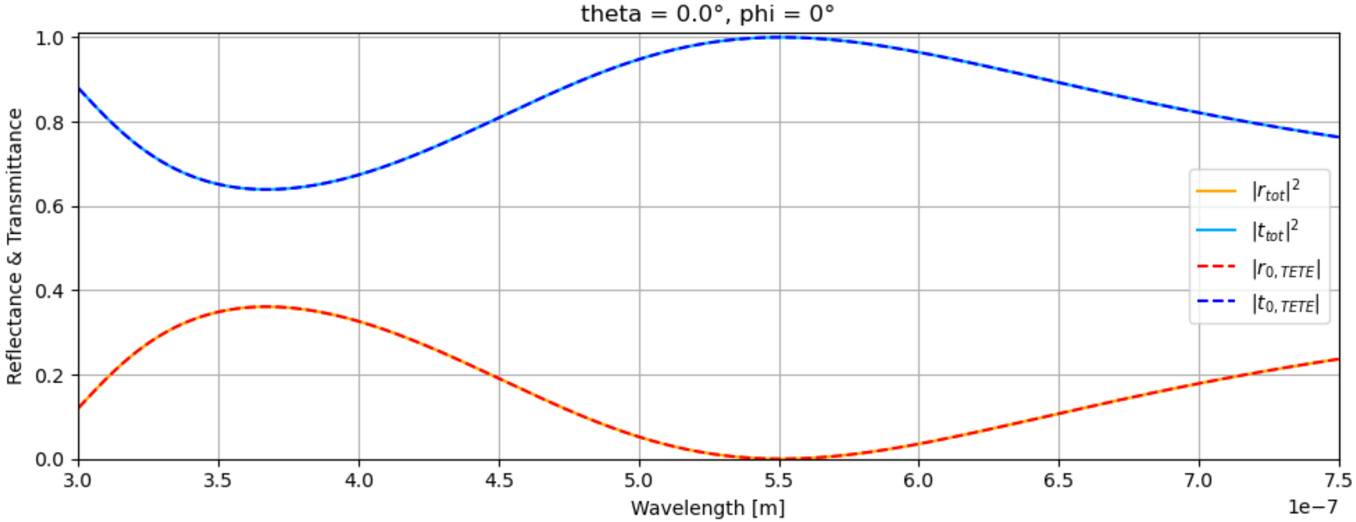
GMR Design Example

Design of an “invisible” slab at normal incidence

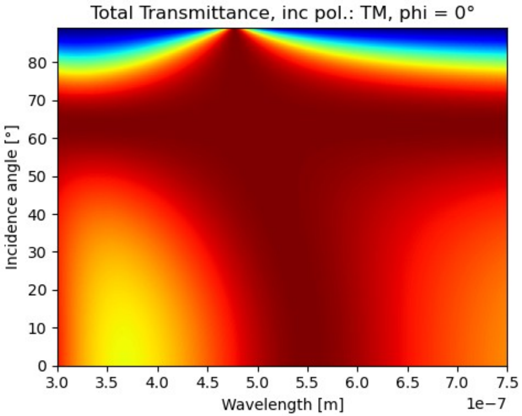
Parameters

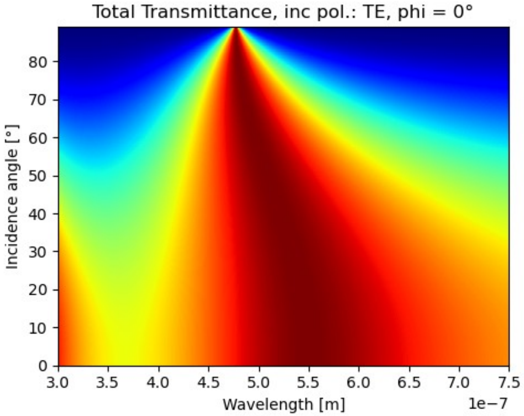
$$\begin{cases} \lambda_0 = 550 \text{ nm} \\ H = 137.5 \text{ nm} \\ n_1 = 1 \\ n_2 = 2 \end{cases}$$





TM & TE angular transmittance

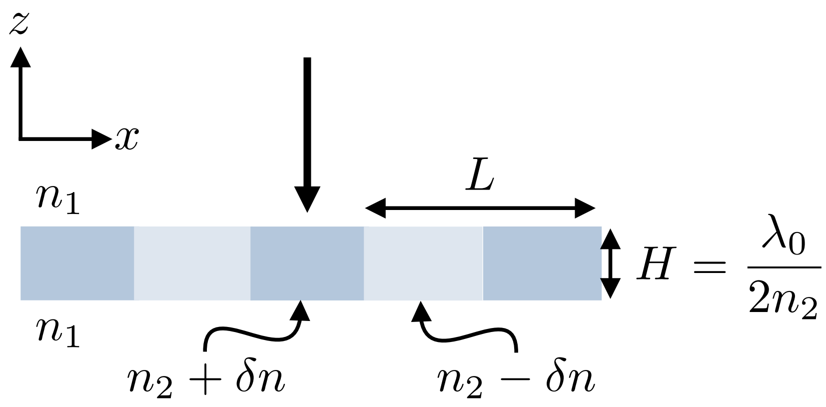




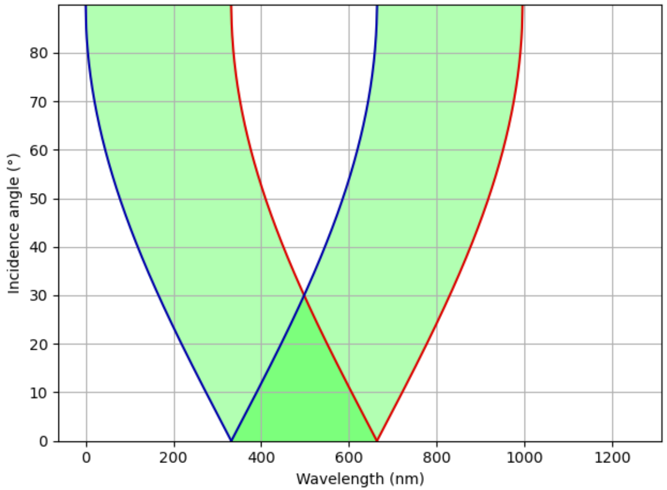
GMR Design Example

Parameters

$$\begin{cases} \lambda_0 = 550 \text{ nm} \\ H = 137.5 \text{ nm} \\ n_1 = 1 \\ n_2 = 2 \\ \delta n = 0.1 \\ L = 332 \text{ nm} \end{cases}$$

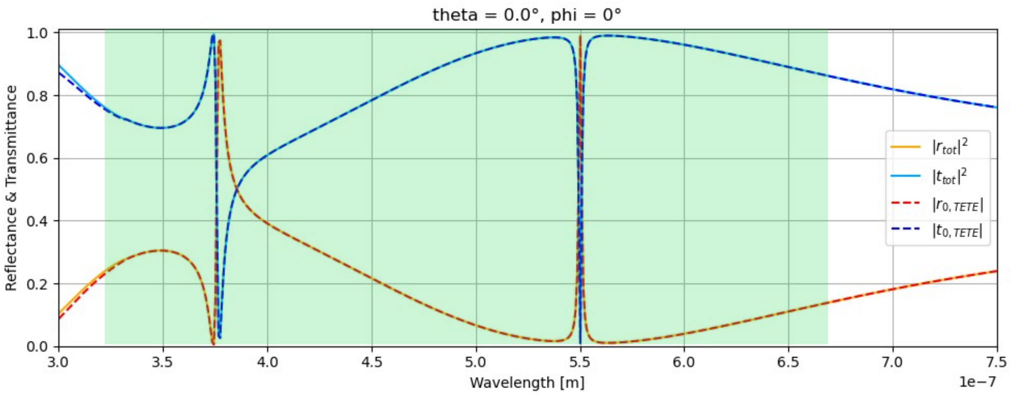


GMR existence condition

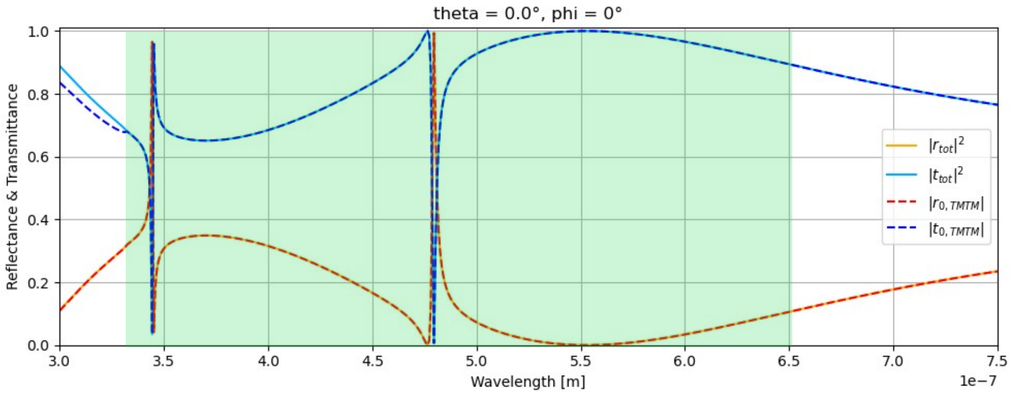


Using RCWA with M = 3 and N = 0

TE polarization

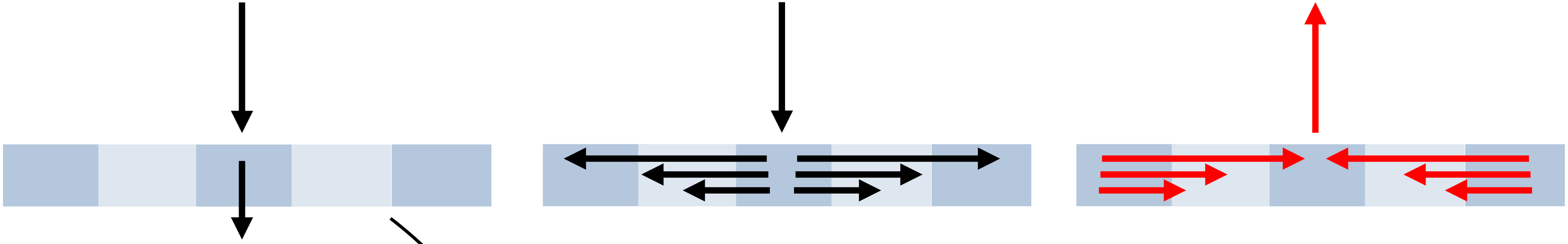


TM polarization



Understanding GMR

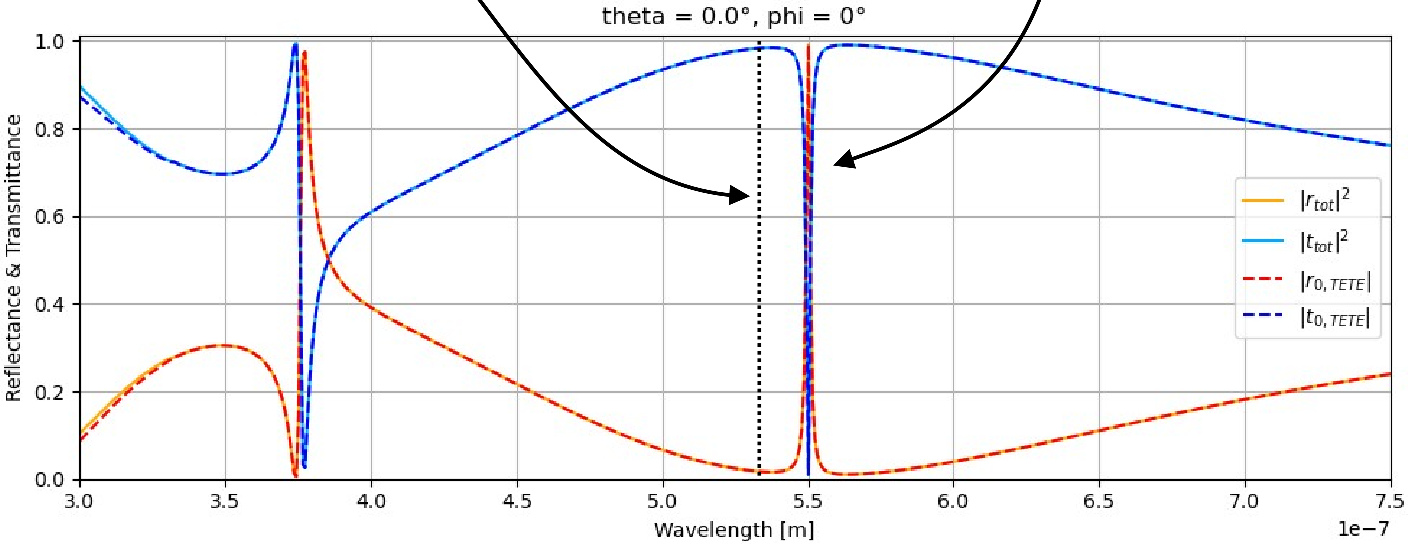
No GMR coupling | **GMR coupling** | **By reciprocity**



The incident light cannot couple to guided waves. It is mostly transmitted

The incident light energy couples to guided waves

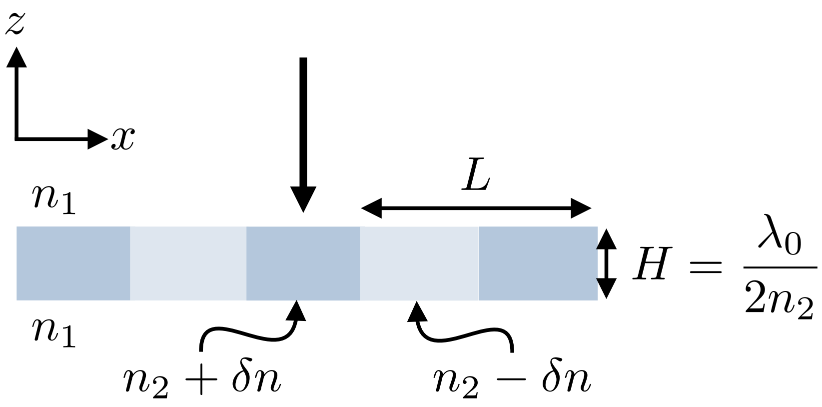
If energy can couple into guided waves, then, by reciprocity, the guided waves can leak out

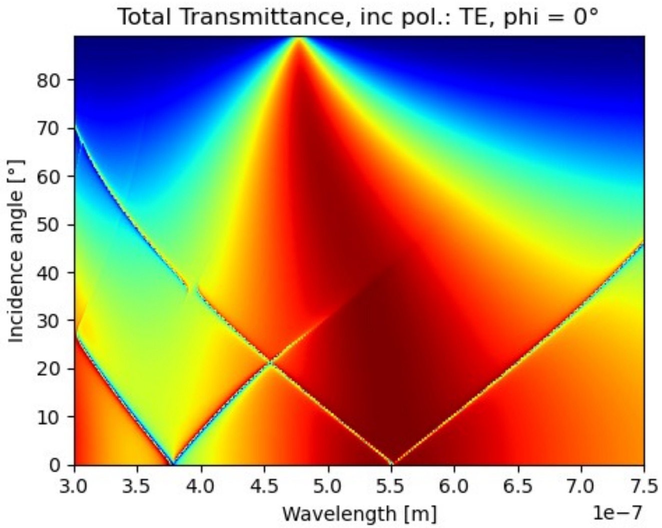


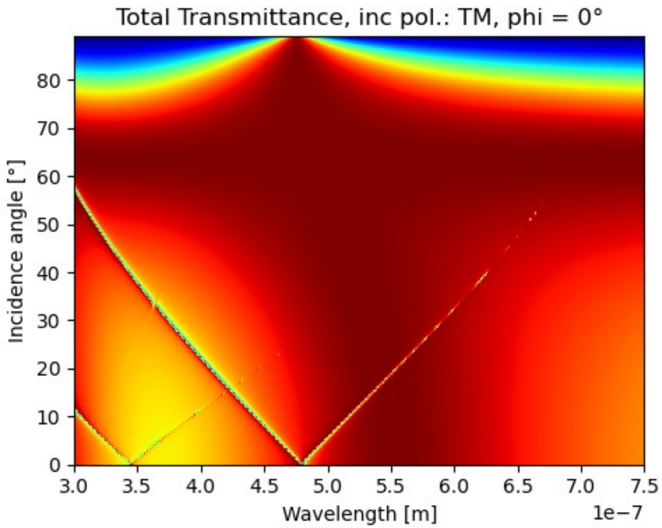
GMR Angular Response

Parameters

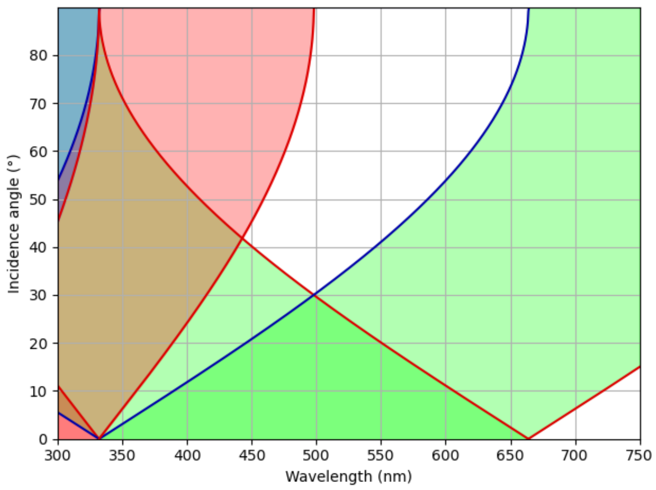
$$\begin{cases} \lambda_0 = 550 \text{ nm} \\ H = 137.5 \text{ nm} \\ n_1 = 1 \\ n_2 = 2 \\ \delta n = 0.1 \\ L = 332 \text{ nm} \end{cases}$$



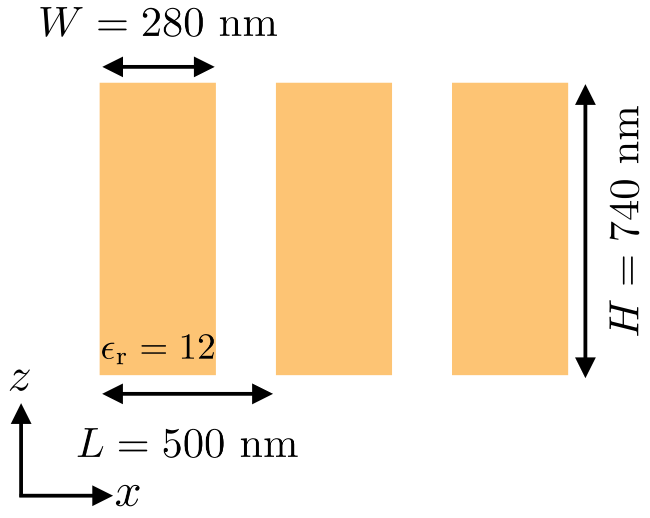




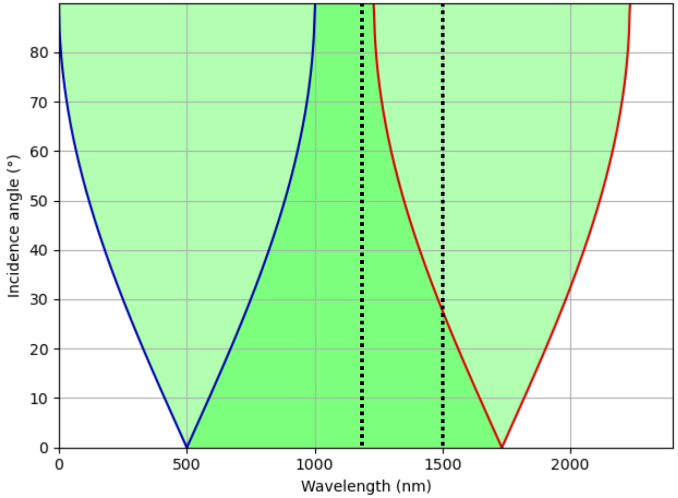
GMR existence condition

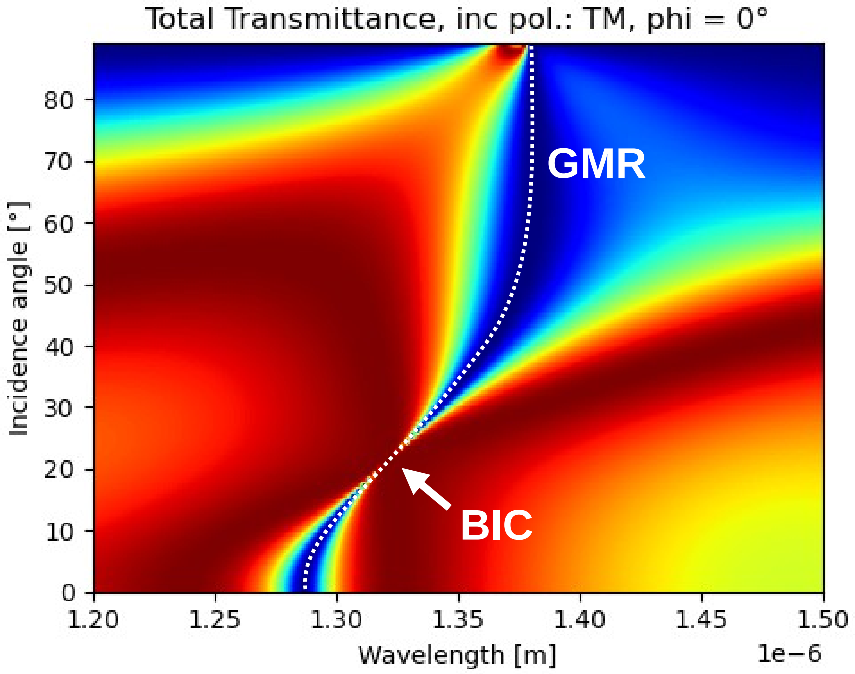


Bound States in the Continuum (BIC)



GMR existence condition





Spatial harmonics

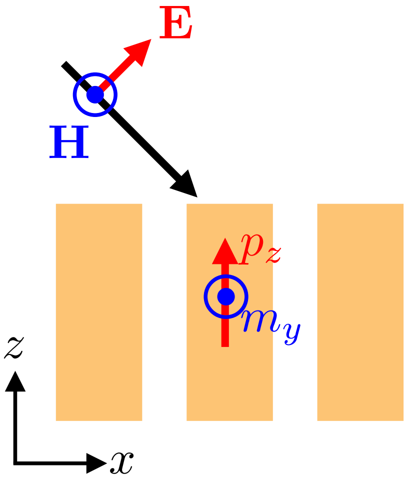
$M = 7$

$N = 0$

Due to the large permittivity of the ridges, GMR are allowed to exist within the entire frequency/angular range. In this special case, the GMR does not split into two lines as before.

The BIC is a point along the GMR where the incident wave is prevented from coupling to the GMR.

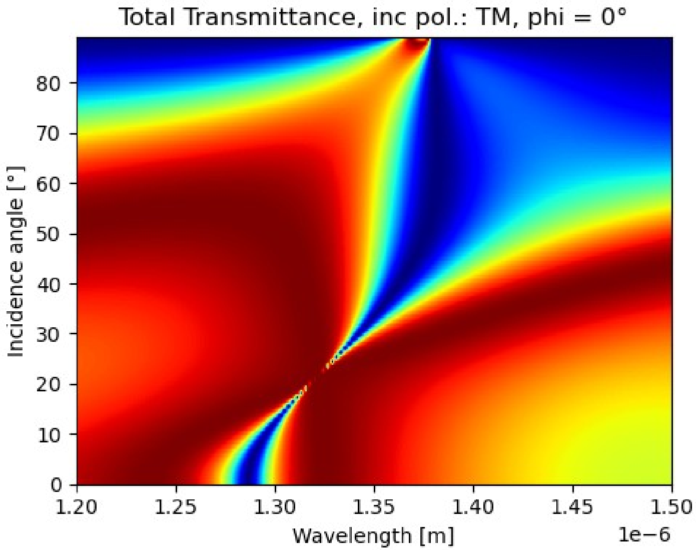
Understanding BIC from a Multipolar Perspective



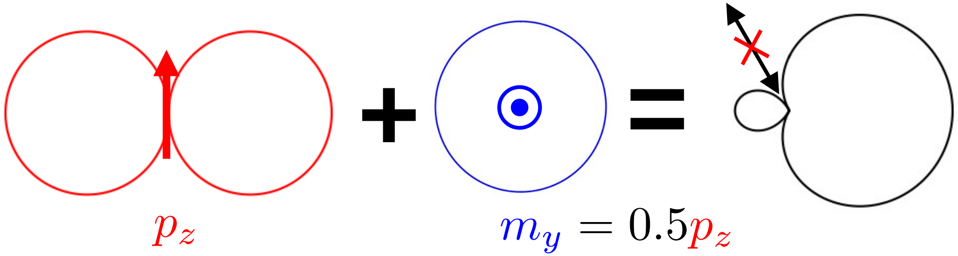
Q factor

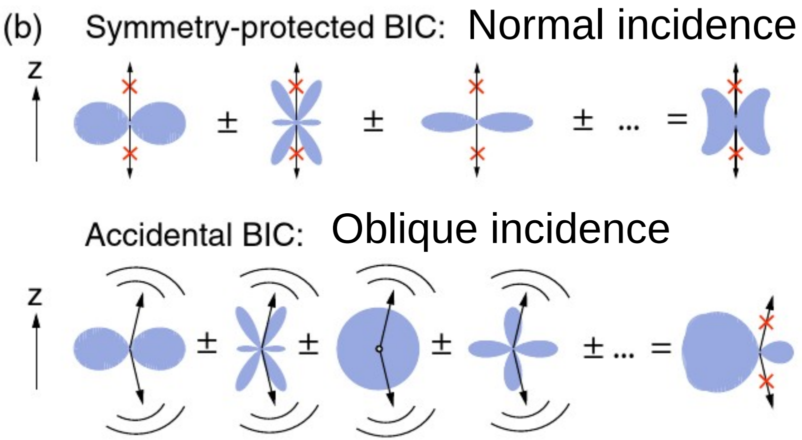
$$Q = \omega \frac{W_\mathrm{e} + W_\mathrm{m}}{P_\mathrm{loss}}$$

For a lossless system, $P_{\mathrm{loss}} = 0$ and $Q \rightarrow \infty$ at the BIC



Simple example with dipoles





The GMR is modeled as an interference between p_z and m_y. In this example, when $m_y = 0.5p_z$, the GMR leakage is suppressed at a specific angle. By reciprocity, we cannot excite a GMR at that angle.

https://doi.org/10.1103/PhysRevB.100.115303

What Have We Learned So Far….

- Guided mode resonances (GMR) are the generalization of Wood anomalies to dielectric structures.
- They exist in periodic structures where they correspond to coupling between propagating waves and evanescent waves.
- Their existence may be easily predicted by considering the grating equation.
- By reciprocity, GMR typically correspond to reflection peaks. This means that to design a GMR filter, we generally start with a low reflection uniform structure. Small spatial modulations are then introduced to create the GMR.
- The lower the modulation amplitude of the spatial variations, the higher the Q factor of the GMR.
- Bound states in the continuum (BIC) are special sets of wavelengths and incidence angles along a GMR where multipolar contributions cancel out by destructive interference.
- The Q factor gets higher the closer we are to the BIC point.