FDTD Simulations on periodic perforated slabs

Bachelor thesis
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1 - Introduction

Nowadays, materials can be engineered that prohibit propagation of light or allow propagation only in certain directions at certain frequencies. Such materials, called photonic crystals, contain a periodic arrangement of dielectric materials on a wavelength scale.

Photonic crystals (see ref[1] for an introduction) are best known for their special known optical properties. When made from materials that have a large non-linear coefficient these non-linear photonic crystals can be used for non-linear optical effects. Here the special linear optical properties enable phase-matching conditions that make the non-linear effect (e.g. second harmonic generation) "efficient".

To observe these effects experimentally crystals need to be made out of material with a large non-linear coefficient, such as GaAs. Understanding the non-linear properties requires a good understanding of the linear optical properties. This can be done by measurements on these photonic crystals (transmission / reflection) combined with theory and/or simulations that complement these measurements.

In this thesis we simulate the reflection of a dielectric slab with a periodic array of slits (1-D) or holes (2-D). We will first discuss the finite-difference time-domain technique in chapter 2 and test results for well-known structures in chapter 3. Chapter 4 contains results for periodic structures that show sharp resonances in the reflectivity. We describe the Fano line shape of these resonances and present a simple waveguide model that allows predicting the presence and frequency of the resonances.

2 - FDTD simulation for electromagnetism

2.1 - The finite-difference time-domain (FDTD) method

Maxwell's equations in differential form relate the time derivative of the E-field to the curl of the H-field. This can be used to implement the basic finite-difference-time-domain (FDTD) step. At every point in space the new value of the E-field is dependent on the old value of the E-field and on the difference of the H-field on either side of the point in space. The H-field can be found in a similar manner.

Today, many different computer codes exist that implement this FDTD method. All of them generate a computational grid and evolve the E and H fields over time by taking small time steps. The FDTD technique is a very useful tool to calculate transmission and reflection spectra of the photonic crystal structures that we study. In addition, FDTD methods can find resonant modes, frequencies and field patterns.

For our calculations we have made use of Meep, the free FDTD code from MIT[2].

2.2 - MIT Electromagnetic Equation Package (Meep).

Figure 1 shows two setup types for simulation in two dimensions. Type A shows the setup for simulating the reflectance of a continuous wave source for a layer on a substrate. Type B shows a setup for simulating the frequency dependent reflectance and transmittance using a Gaussian pulse source on a layer with a periodic slit. The computational cell contains a source-region that produces the fields, and flux regions that keep track of the fields. Bloch Periodic or Perfectly Matched Layer boundary conditions are applied at the edges of the cell.

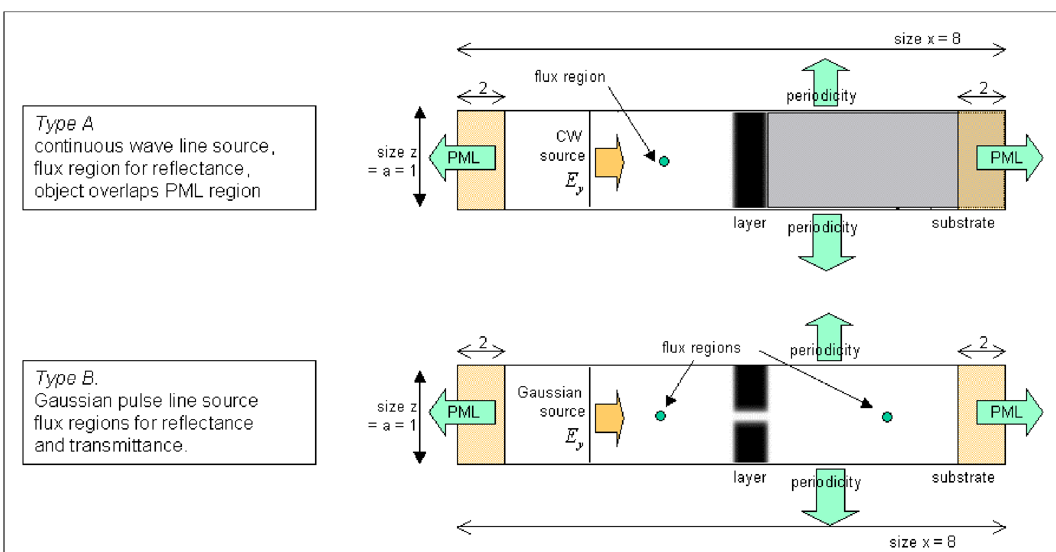


figure 1 – Meep 2 dimensional simulation set-up examples

The Meep manual and reference guide gives further guidance for the setup of a Meep simulation. To obtain accurate numerical results it is important to have enough grid-points in the cell. Typically, 20 points per wavelength is sufficient. The calculation of resonant phenomena (as presented in chapter 4) requires a simulation to run for a sufficient amount of optical cycles. We used 400 cycles for the resonances, while approximately 40 cycles is enough for non-resonant phenomena (as presented in chapter 3).

Source regions and Flux regions

Meep allows to calculate the reflectance (transmission) as a function of frequency in a single run, by Fourier transforming the response to a short pulse. Every function f(t) can be expressed as $f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega) e^{i\omega t} d\omega$, where $F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt$ is the Fourier Transform of $f(t)$. We used a continuous wave $f(t) = e^{-i\omega_0 t}$ with well-defined frequency ω_0. The Fourier Transform is given by the Dirac delta function: $F(\omega) = 2\pi\delta(\omega - \omega_0)$. A spectrally broad pulse can be created by using a Gaussian pulse $f(t) \sim e^{-(t^2/2\sigma^2)}$ with a Fourier Transform $F(\omega) \sim e^{-\omega^2\sigma^2/2}$. Short pulses in time (small temporal width σ) represent a broad spectrum (broad pulse in frequency), and vice versa.

In the defined flux regions, Meep keeps track of the fields and their Fourier transforms. This is used to compute the flux of electromagnetic energy as a function of frequency.

Meep units

Maxwell's equations are scale invariant. Multiplying the dimensions of an object by a constant factor is the same as dividing the frequency by that factor. Therefore it is convenient in electromagnetic problems to choose **scale-invariant units**. In practice, that means that we use some characteristic scale of length in the system, *a*, and use that as our unit of distance. For numerical convenience Meep also sets constants, such as ε_0, μ_0, c, and 4π to 1. As a consequence, the numerical value of the time and distance units is equal and frequency $\omega = 1/\lambda = 1/T$. Frequency ω is expressed in units of $2\pi c/a$.

For example an experiment with a lattice constant of 800 nm, for light with a vacuum wavelength of 400 nm, uses Meep units: a = 1, λ = 0.5, and ω = 2. A run for 100 wave periods has to run for 50 time units.

Boundary conditions

Since our computational cell is finite (and the simulated world usually is not) we have to make use of boundary conditions for the computational cell. Meep supports several:

- *Bloch Periodic* – is a generalization of ordinary periodic boundaries: $u(\vec{r} + \vec{L}) = e^{i\vec{k}\vec{L}} u(\vec{r})$ for a Bloch wave-vector k;

- *Perfectly Matched Layer (PML),* is defined inside our computational cell, and absorbs all fields in a specified direction, without reflection. In a discretised system it has some finite reflections that makes it imperfect. For this reason one has to give the PML layer some thickness, in which the absorption gradually “turns on”.

We set a PML with thickness 2 on both ends of our computational cell in the x direction (the direction of the wave propagation) and a Bloch Periodicity on the z (and in 3D: y) direction, which makes our scattering object periodic. Our computational cell contains just one unit cell of a periodic structure.

Output

At each time, the *field pattern* can be generated. For example, figure 2 shows the E_y field of a y-polarized plane wave, that propagated in vacuum and is partly transmitted from a material with index n=4.5. A sequence of such field patterns allows one to construct a movie.

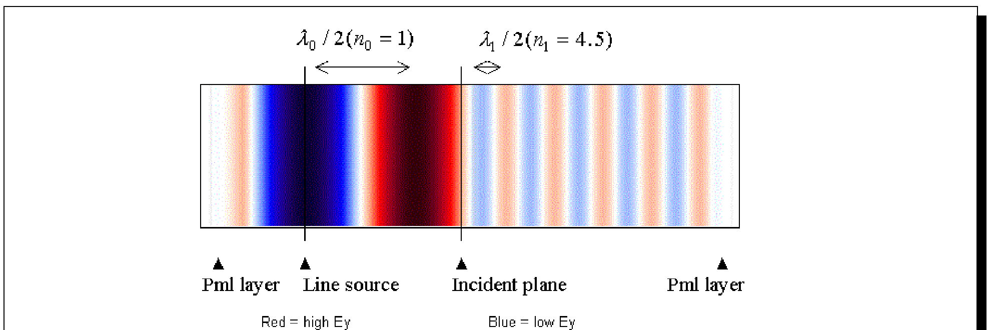


figure 2 – E_y field distribution of continuous line source with a single incident plane (n=4.5)

Reflectance (transmittance) spectra are obtained by dividing the reflected (transmitted) flux by the incident flux.

A note on working with angles

All simulations in this thesis are done for normal incidence.

In principle, producing incident beams under an angle is possible by adding an amplitude phase to the line source, along the axis of the source. Field patterns produced with a continuous wave line source ($\omega = 0.5$ turned on at t=0) and with a Gaussian pulse source (around $\omega = 0.5$) both demonstrate that we indeed produced a plane wave under an angle. However, the reflectance spectrum for a beam on a single incident plane (tested with a Gaussian pulse source, with $\omega = 0.05$ and frequency width $1/\sigma = 0.2$) does not match with theory. This might be because the definition of the phase is incompatible with the use of periodic boundary conditions, or it may be that the definition of flux (Poynting vector) should be modified in this case.

2.3 - Reflectance and Transmittance spectra with the FDTD method

One main purpose of FDTD simulation is to plot reflectance or transmittance spectra as function of frequency.

Reflectance is defined as the Intensity of the reflected beam divided by the Intensity of the incident beam. Intensity per unit area is defined as the (time) average of the energy flow given by the Poynting vector $\vec{S} = \varepsilon_0 c^2 \vec{E} \times \vec{H}$:

$$I = \left\langle \left| \vec{S} \right| \right\rangle = \varepsilon_0 c^2 \left\langle E_0 H_0 \sin^2(\vec{k} \cdot \vec{r} \pm \omega t) \right\rangle = \frac{1}{2} \varepsilon_0 c^2 E_0 H_0 = \frac{1}{2} \varepsilon_0 c E_0{}^2 \qquad (1.1)$$

Meep first accumulates the Fourier transforms of E and H for every point in the flux-plane via summation over the (discrete) time steps. It then calculates the power over these Fourier transformed fields (in Meep units):

$$I(\omega) = \mathrm{Re}\left[\vec{n} \cdot \int \vec{E}_\omega(x)^* \times \vec{H}_\omega(x) d^2 x \right] \qquad (1.2)$$

To get the reflectance / transmission spectrum, the intensity $I(\omega)$ is divided by the incident power at each frequency. Therefore, each simulation is run twice: once with only the incident wave for normalization, and once with the scattering structure.

This principle works for transmittance but is more involved for reflection spectra, since measuring the intensity in the backwards direction would give us the sum of the reflected and the incident power. Therefore we need to subtract the Fourier transformed incident fields $E_\omega^{(0)}(x)$ and $H_\omega^{(0)}(x)$ from the total fields before calculating intensity:

$$I(\omega) = \mathrm{Re}\left[\vec{n} \cdot \int \left[\vec{E}_\omega(x) - \vec{E}_\omega^{(0)}(x) \right]^* \times \left[\vec{H}_\omega(x) - \vec{H}_\omega^{(0)}(x) \right] d^2 x \right] \qquad (1.3)$$

These calculations are part of the standard functionality of Meep and are controlled via the script of the simulation (see appendices for example scripts).

3 - Simulation Test

In this chapter we compare the output of Meep to three simple cases for which analytical expressions exist for the reflectance and transmittance[3]. We compare our result to the Fresnel coefficients for normal incidence on a single interface as function of the refractive index (A); reflectance as function of frequency for normal incidence on a dielectric slab (parallel plate, B); and reflectance as function of frequency for a dielectric slab on a substrate (C).

A - Fresnel coefficient for a single interface

The reflectance R (reflected power) at normal incidence is given by:

$$R = \frac{I_r}{I_i} = r^2 = \left(\frac{1-n}{1+n}\right)^2 \qquad (1.4)$$

where n is the refractive index and r is the Fresnel reflection coefficient for the E-field.

The simulation setup is explained in chapter 2 and depicted in figure 1, type A, with refractive index of the layer equal to that of the substrate). Figure 3 shows the Reflectance simulated by Meep (symbols) for different values of the refractive index, at a fixed frequency of $\omega = 0.15$ Meep units. The result (drawn line in figure 3) agrees well with Eq. 1.4.

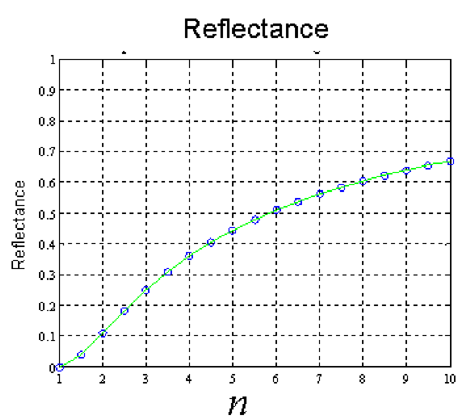


Figure 3 – Reflectance as function of refractive index.
The Meep simulation (symbols o) agree with Eq. 1.4 (line)

B - Reflectance of a dielectric slab, as function of frequency

Figure 4 shows a ray optics picture of multiple reflections inside a dielectric slab. The reflectance (transmittance) of a dielectric slab can be calculated by considering all possible multiple reflections (transmissions). The calculation sums all contributions and takes into account the amplitude and phase of the E field of all the reflected (transmitted) beams. For a slab in air ($n_0 = n_s = 1$), the reflectance is given by:

$$R = \frac{I_r}{I_i} = \frac{2r^2(1-\cos 2\delta)}{1+r^4-2r^2\cos 2\delta} \quad (1.5)$$

This is a periodic function with periodicity $2\delta = 2kn_1 d\cos\theta_{t1}$, dependent on refractive index n_1 and thickness d of the layer. k is the wave number of the incident ray. The amplitude of this periodic function is dependent on the Fresnel coefficient for a beam travelling from air to the layer (which for normal incidence reads $r = 1-n_1/1+n_1$) and hence on the index of the layer.

The transmittance is given by:

$$T = \frac{I_t}{I_i} = \frac{(1-r^2)^2}{1+r^4-2r^2\cos 2\delta} \quad (1.6)$$

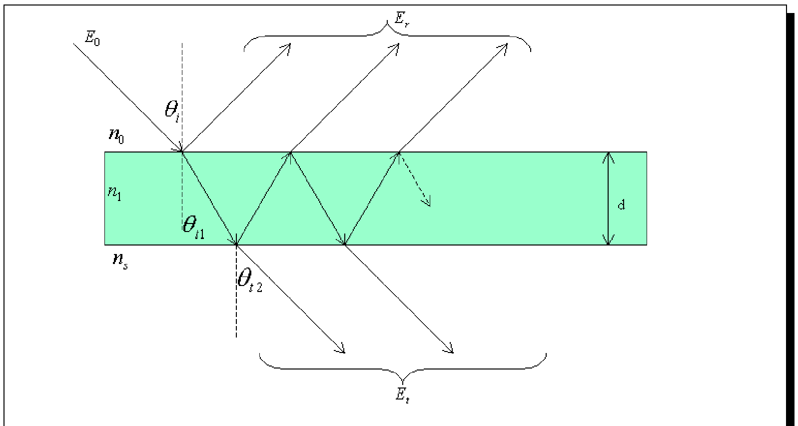


figure 4 – Multi beam interference for a dielectric slab

To simulate this situation, we used setup type B in figure 1, without the periodic grating in the slab. We used a Gaussian input pulse with a frequency width $1/\sigma = 2$ around a frequency $\omega = 1$ (Meep units).

Figure 5 shows the simulated Reflectance and Transmittance as function of frequency. The Meep result (symbols) agrees well with Eq. 1.5 and 1.6 (lines).

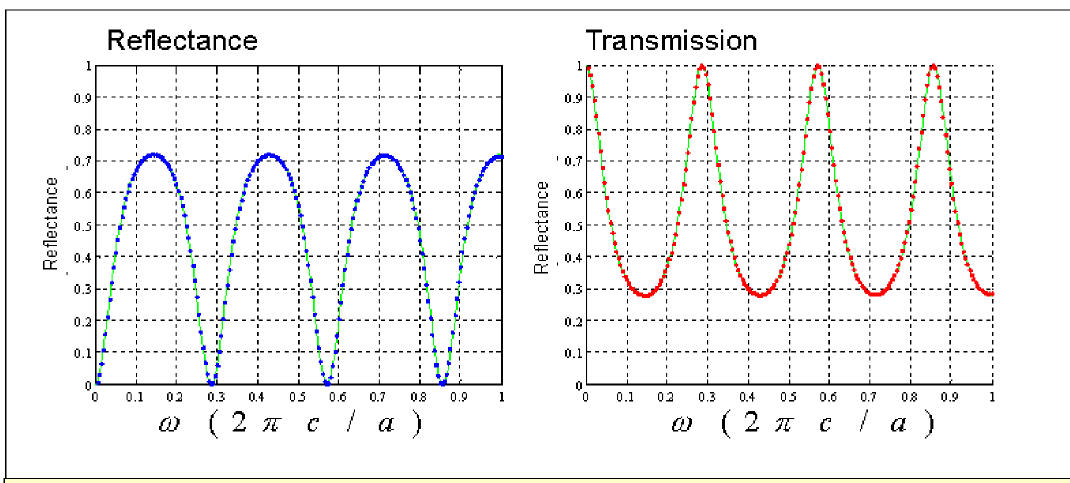


figure 5 – Reflectance and Transmission as function of frequency.
The Meep result (symbols) agrees well with the theoretical prediction (lines)

C - Reflectance of a slab on a substrate as function of frequency

Consider a thin slab of thickness d with index n_1 between a substrate with index n_s and air with index $n_0 = 1$. For normal incidence, the Reflectance is:

$$R = \frac{n_1^2 (n_0 - n_s)^2 \cos^2 \delta + (n_0 n_s - n_1^2)^2 \sin^2 \delta}{n_2^2 (n_0 + n_s)^2 \cos^2 \delta + (n_0 n_s + n_1^2)^2 \sin^2 \delta} \qquad (1.7)$$

This is a periodic function with period $\delta = kn_1 d$ (see figure 4, $\theta_i = 0$). To obtain the reflectance as function of frequency, the simulation setup is analogous to type B in figure 1 (with an extra object to represent the substrate with $n_s = 1.62$ on which the film is fixed). Again, we used a Gaussian input pulse of frequency width $1/\sigma = 2$ around a frequency $\omega = 1$ (Meep units).

In figure 6, the Meep result is compared to Eq. 1.7. for a slab on a substrate with index $n_s = 1.62$. Results are shown for a slab of thickness d=0.5a and refractive index $n_1 = 1.8$ in the left panel of figure 6, and $n_1 = 1.5$ in the right panel of figure 6.

Figure 6 demonstrates that also in this case, FDTD simulations follow theory. For $n_1 = 1.8 > n_s$, the reflectance is higher than the reflectance of a bare substrate, represented by the horizontal dotted line $(1 - n_s / 1 + n_s)^2$, while for $n_1 = 1.5 < n_s$ the reflectance is lower.

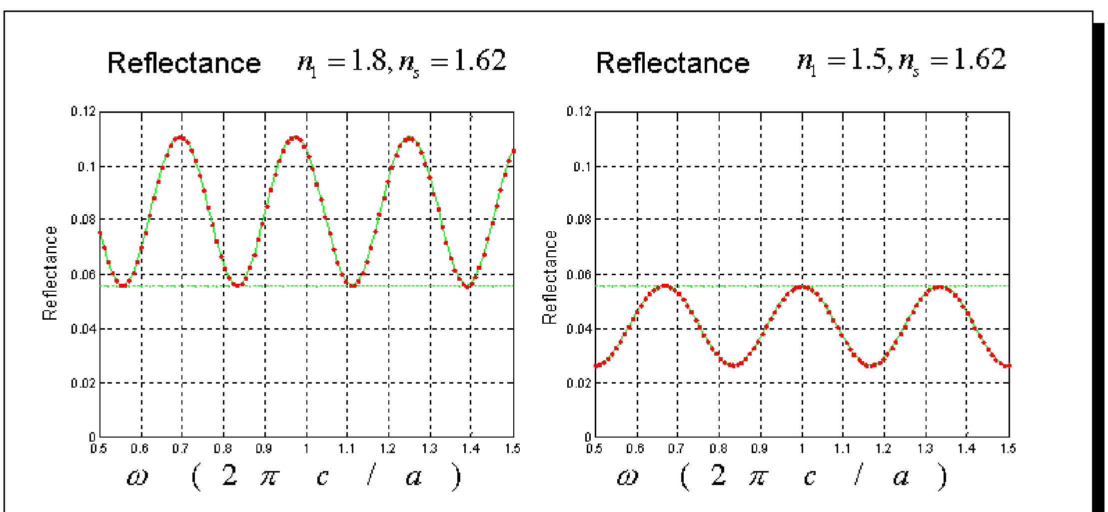


figure 6 – Reflectance as function of frequency for two layer indices

4 - Periodic structures

4.1 - Introduction

In this chapter we will employ the FDTD method that was tested in chapter 3 to study the reflectance of a periodic structure. The basic structure consists of a dielectric slab with refractive index n_1 that is perforated by a periodic array of air scatterers. We distinguish between structures that have air on both sides and structures that have a substrate with index n_s on one side. We elaborate on structures with a periodicity in one direction only and compare the situation for a slab in air (A) to that of a slab on a substrate (B). We also explore the structure with periodicity in two directions (C).

We will first discuss the findings of the numerical simulations in section 4.2. In section 4.3 a simple waveguide model is introduced to predict the resonant frequencies. In section 4.4 we will analyze the shape of the resonances in more detail.

4.2 - FDTD analysis of the guided resonances.

The simulation setup is shown in figure 7. A larger section of the structure is shown on the left, while the unit cell defined in Meep is shown on the right. The top of the figure shows a one-dimensional structure, while the bottom shows a 2-D structure.

The simulation with one-dimensional periodicity (A and B) was done with a slab waveguide of thickness 0.5a and the width of the air scatterer of 0.1a. Aiming to produce a similar spectrum for both one and two-dimensional structures, the fill fraction of air is kept at 10% in both situations. The corresponding diameter of air holes in the two dimensional structure (C) is 0.36a ($r/a = 0.18$).

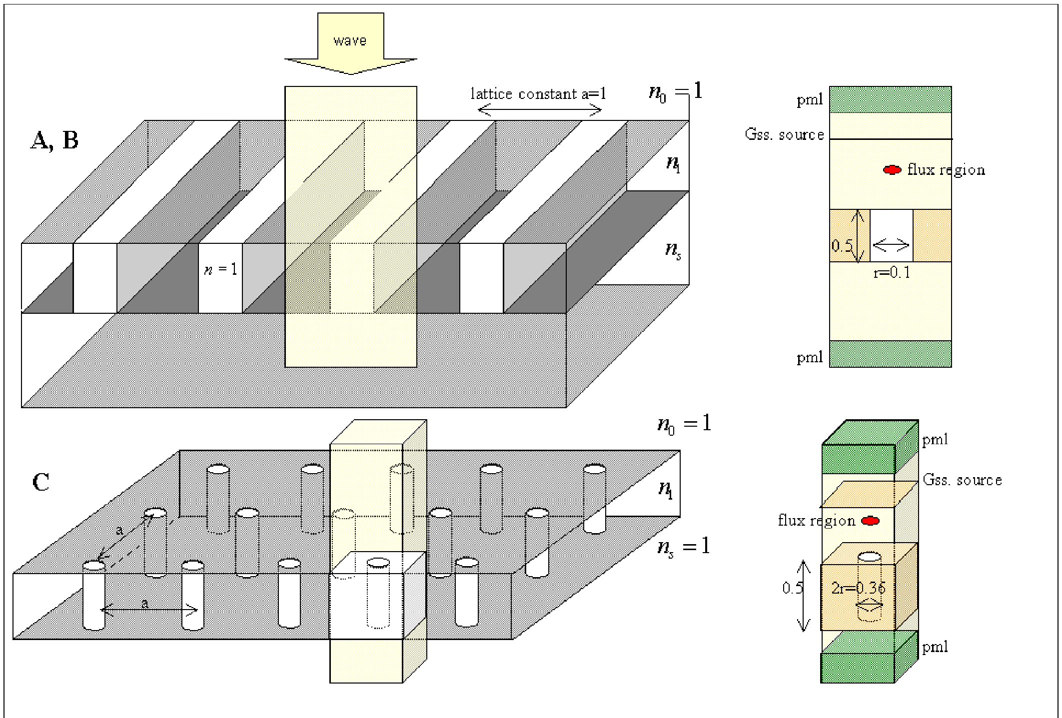


figure 7 – Meep Simulation Set Up for a slab with a 1 dimensional periodic scatterer without (A) and with (B) a substrate and for a slab with (C) a 2 dimensional periodic scatterer

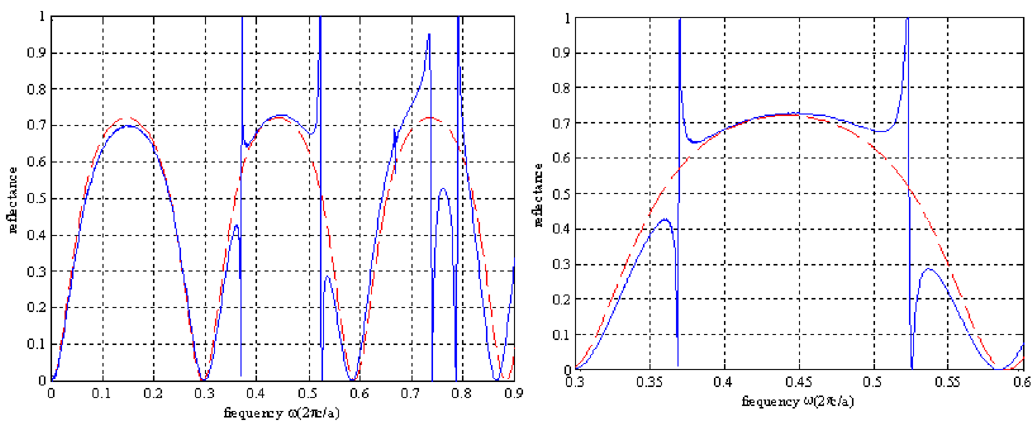
Results of the FDTD analysis

(A) 1-D perforated slab in air.

Figure 8 shows the reflectance for TE polarized light, in the frequency range between 0 and 0.9 (left panel). Two resonances can be seen in the frequency range from 0.3 and 0.6 (right panel) at $\omega = 0.37$ and $\omega = 0.52$. These resonant features are superposed on a "background" spectrum of a homogeneous slab. The same simulation is shown in Fig. 9 for TM polarized light that displays a broader resonance peak around $\omega = 0.47$ (frequency ω in Meep units).

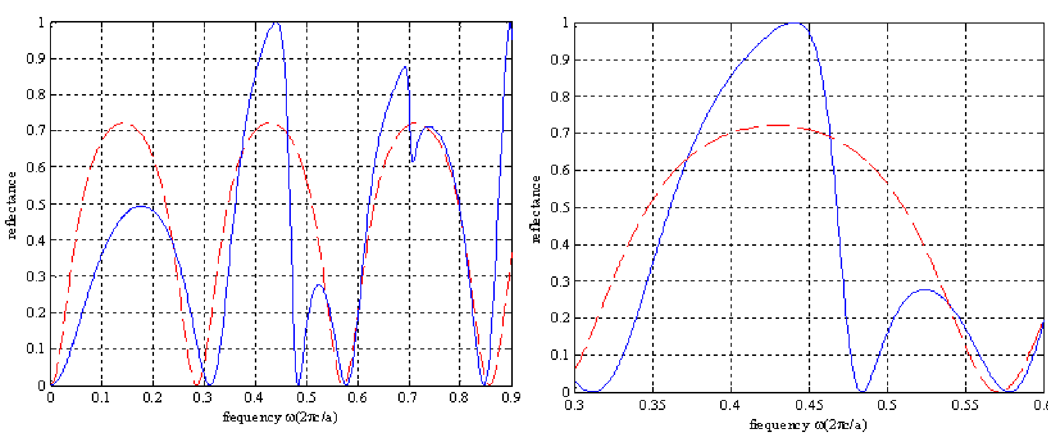
As a reference, the dashed line in figure 8 and 9 show the reflectance of a homogeneous slab following eq. 1.7, with effective thickness $d = 0.485$ and effective index of 3.5, for which values the dashed line fitted best with the simulated "background".

For higher frequencies more resonances are present. We will focus on the two resonances that are lowest in frequency.



solid line = FDTD simulation of perforated layer (A), TE polarization
dashed line = theory for not perforated layer with neff=3.5 and d=0.485

figure 8 – Resonance as function of frequency for perforated slab (A) in air (TE)

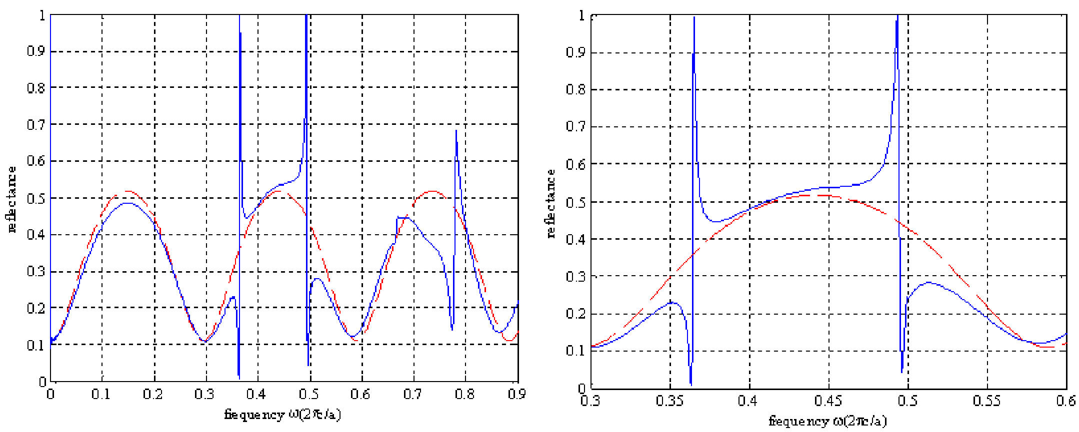


solid line = FDTD simulation of perforated layer (A), TM polarization
dashed line = theory for not perforated layer with neff=3.5 and d=0.485

figure 9 – Resonance as function of frequency for perforated slab (A) in air (TM).

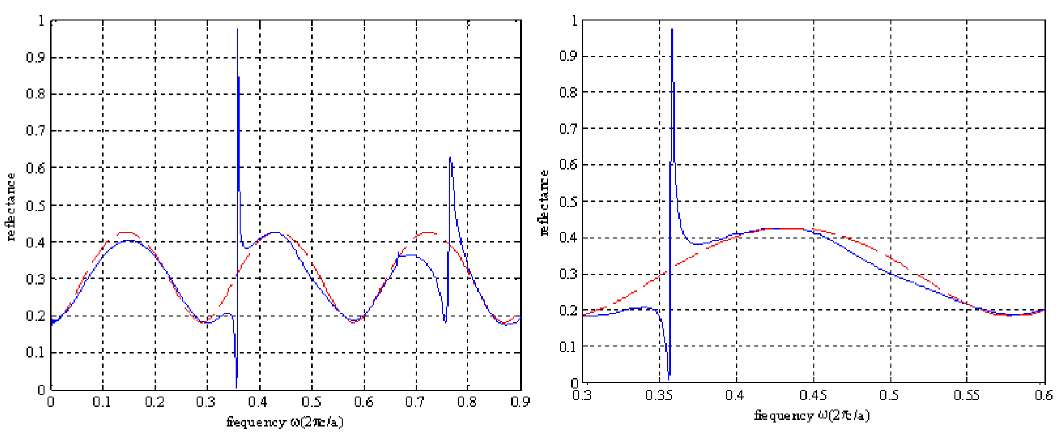
(B) *1-D perforated slab on a substrate.*

Figure 10 shows the reflectance as function of frequency for TE polarized light for a slab with $n_1 = 3.5$ on a substrate with $n_s = 2.0$. Similar resonance features on a background are observed. The background is consistent with the reflectance of a slab on a substrate (dashed line), with well-chosen effective thickness d and effective index of the layer. Figure 11 shows the reflectance for a substrate with $n_s = 2.5$ keeping all other parameters the same. Interestingly the second TE resonance peak at $\omega \approx 0.5$ has vanished, while other resonant peaks in a broader frequency range remain.



solid line = FDTD simulation of perforated layer (A), TE polarization
dashed line = theory for not perforated layer with neff=3.5 and d=0.485

figure 10 – Resonance for perforated slab (B) on substrate with $n_s = 2.0$



solid line = FDTD simulation of perforated layer (A), TE polarization
dashed line = theory for not perforated layer with neff=3.45 and d=0.5

figure 11 – Resonance for perforated slab (B) on substrate with $n_s = 2.5$

(C) 2-D perforated slab waveguide in air.

Figure 12 shows the simulated reflectance for a slab that is perforated by a 2-D square array of holes. The diameter of the holes is 0.36a (with a the lattice vector). The result can be compared to the 1-D simulation of figure 8. Resonances appear at roughly the same frequency, but are now split into a double peaked structure. In addition, the number of modes is larger, which corresponds to resonances that originate from scattering by the different lattice planes ((1,0 and 1,1) in this case). For instance an extra pair of resonances appears for $\omega \sim 0.6$, i.e. at approximately $\omega = 0.4\sqrt{2}$.

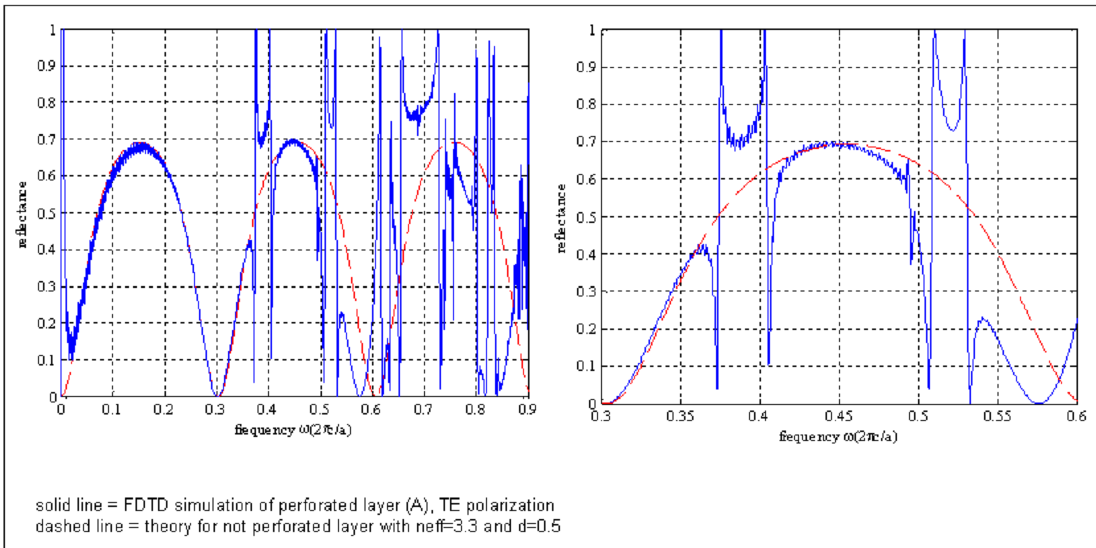


figure 12 – Resonance as function of frequency for slab (C) with 2 dimensional scatterer

4.3 - A simple waveguide model

4.3.1 - Introduction

To understand the spectra shown in section 4.2, two optical modes in a slab are relevant:

a. *propagating modes*
An incident plane wave that exists outside the dielectric slab can be reflected and transmitted by the slab. This leads to the oscillating background in the reflectance spectra.

b. waveguide modes
A wave can be confined to the slab by total internal reflection. These wave-guiding modes exist only if the refractive index of the slab is higher than the refractive index of the surrounding medium. A mode has a unique propagation constant and well-defined field amplitude at each point in space and time.

If the slab is homogeneous, the two effects are strictly separated. However, if the waveguide contains a periodic array of scatterers, a propagating mode can couple to a waveguide mode under appropriate conditions. The coupling is achieved in this case via scattering of the propagating mode on the periodic array.

This coupling is illustrated in the simulation results depicted in figure 13 that shows the E_y field propagation over time. The position of the pulse is shown on the horizontal direction (x), while time progresses in the vertical direction. The results are shown for *homogeneous slab (A)* and a *periodic perforation in the slab* (B). Both figures show multiple reflections of a short pulse on the two interfaces of the slab. In the case of a periodic perforation (B), a waveguide mode is excited that continues to propagate in the slab.

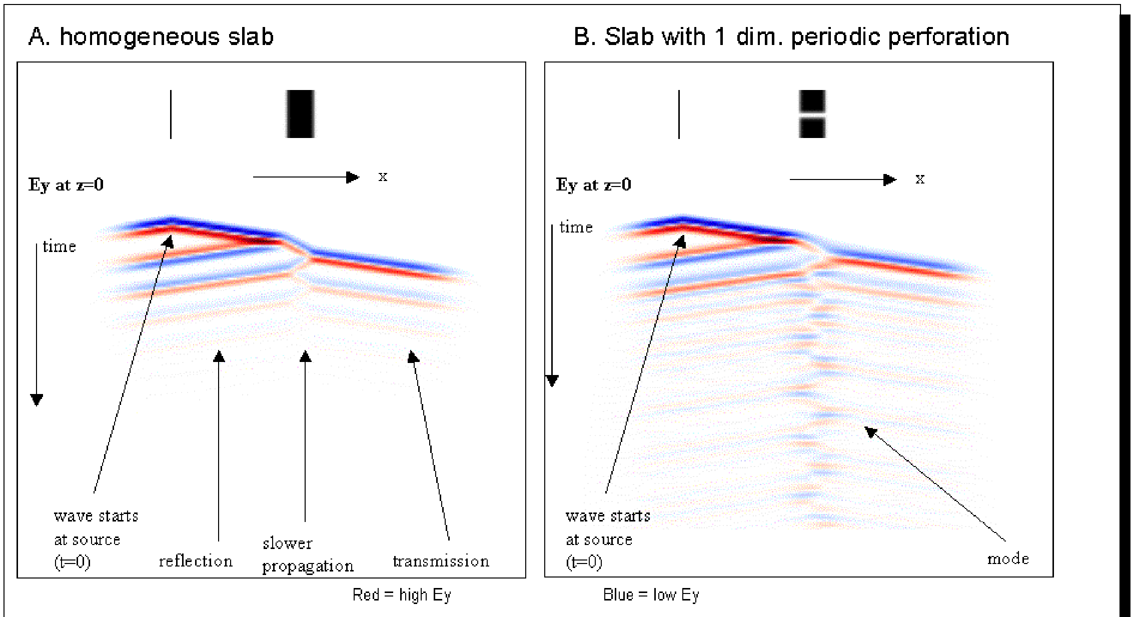


figure 13 – E_y field propagation through a (A) homogeneous and (B) periodic perforated slab

Therefore we will first study the resonant modes of the waveguide in section 4.3.2, the effects of the periodicity of the scatterer in section 4.3.3, and the effects of fixing the slab to the substrate in section 4.3.4.

4.3.2 – Waveguide dispersion

We now consider a homogeneous dielectric slab that supports propagating waves in the z-direction. These modes propagate with a propagating constant k_z. We will focus on the dispersion relation of the waveguide, i.e. the variation of k_z with ω.

To calculate the waveguide dispersion[4], we seek solutions of Maxwell's equations. TE modes have their electric field perpendicular tot the x-z plane (plane of incidence); the TM modes have their magnetic field perpendicular to the x-z plane.

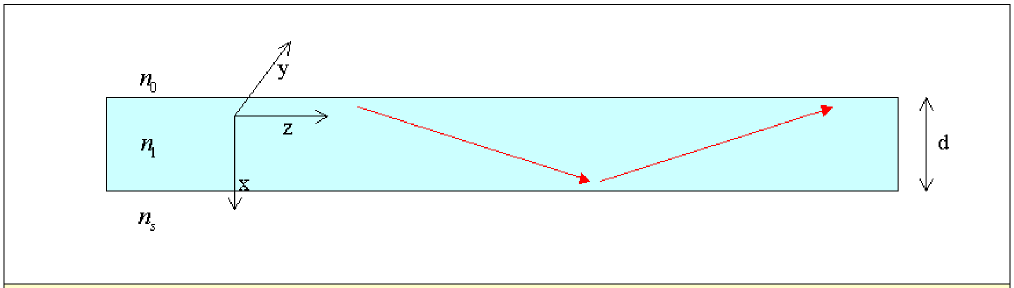


figure 14 – Schematic drawing of a slab wave guide

Consider a slab as depicted in figure 14 with a refractive index n_1 and thickness d, sandwiched between dielectric media of lower refractive index: n_0 and $n_s < n_1$. Since the structure is homogeneous along the z-axis, propagating solutions to Maxwell's equations, for guided TE modes, are of the form:

$$E_y(x, y, z, t) = E_m(x)\exp[i(\omega t - \beta z)], \qquad (1.8)$$

where β is the propagation constant in z-direction ($\beta = k_z$). With this and eliminating H, the Maxwell equations can be written as:

$$\left[\frac{d^2}{dx^2} + \left(\frac{\omega}{c}n\right)^2 - \beta^2\right]\vec{E}_m(x) = 0 \qquad (1.9)$$

The mode function $E_m(x)$ is given as:

$$E_m(x) = \begin{cases} \exp(-qx) & 0 \le x \\ \left[\cos(hx) - \frac{q}{h}\sin(hx)\right] & ,-d \le x \le 0 \\ \left[\cos(hx) - \frac{q}{h}\sin(hx)\right]\exp\left[p(x+d)\right], & x \le -d \end{cases} \qquad (1.10)$$

The parameters h, p and q are defined as:

$$h = \left[\left(\frac{n_1\omega}{c}\right)^2 - \beta^2\right]^{1/2},$$

$$q = \left[\beta^2 - \left(\frac{n_0\omega}{c}\right)^2\right]^{1/2}, \qquad (1.11)$$

$$p = \left[\beta^2 - \left(\frac{n_s\omega}{c}\right)^2\right]^{1/2}$$

To find a solution, the tangential components of electric field E_y and magnetic field $H_z = (i/\omega\mu)(\partial E_y/\partial x)$ must be continuous at the boundaries. We then get the following mode condition, which can be numerically solved to find $\beta(\omega)$

$$h\sin(hd) - q\cos(hd) = p\left[\cos(hd) + \frac{q}{h}\sin(hd)\right] \qquad (1.12)$$

Similarly, for TM modes:

$$h\sin(hd) - \bar{q}\cos(hd) = \bar{p}\left[\cos(hd) + \frac{\bar{q}}{h}\sin(hd)\right]$$

$$\bar{p} = \frac{n_1^2}{n_s^2}p \qquad (1.13)$$

$$\bar{q} = \frac{n_1^2}{n_0^2}q$$

The solid lines in figure 15 show the waveguide dispersion $k_z(\omega) = \beta(\omega)$ for TE (left) and TM polarization (right). Since waveguide modes have total internal reflection as a necessary condition, these modes can only exist if:

$$n_0\frac{\omega}{c}, n_s\frac{\omega}{c} < k_z < n_1\frac{\omega}{c} \qquad (1.14)$$

For a slab with $n_1 = 3.5$ in air ($n_0 = 1$) the modes exist between the lines $\omega = ck$ and $\omega = 1/3.5\,ck$ (straight lines in figure 15).

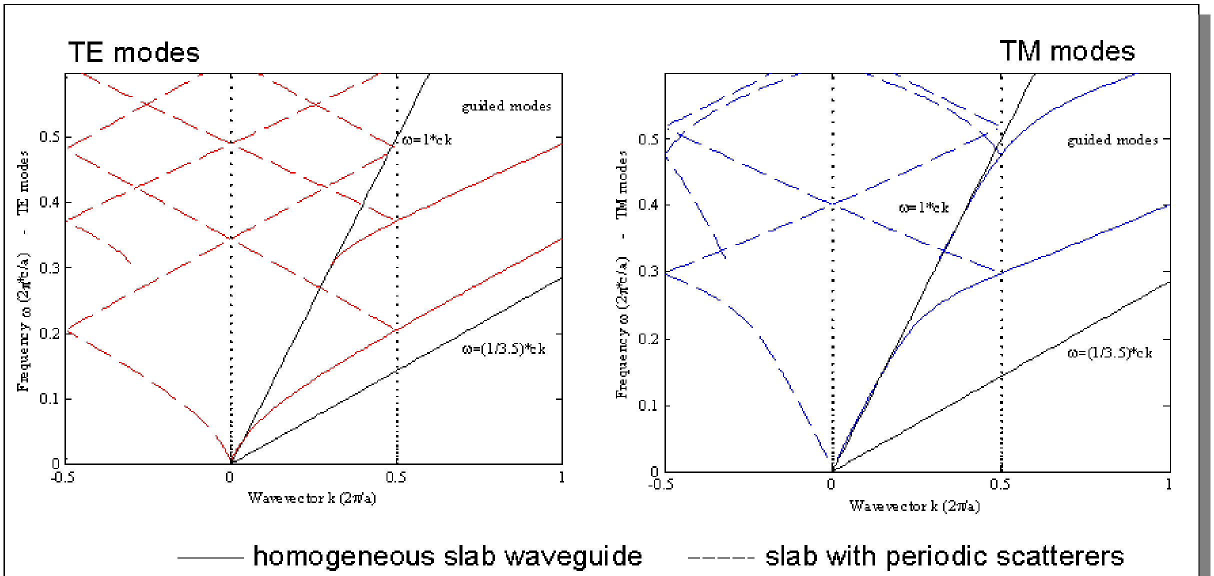


figure 15 – Dispersion for waveguide with thickness 0.5a

An important concept is the cut-off frequency of the m-th mode. A mode cannot exist for frequencies below the cut-off frequency. The cut-off frequencies are given by:

$$\left(\frac{d}{\lambda}\right)_{TE} = \frac{1}{2\pi\sqrt{n_1^2 - n_s^2}}\left[m\pi + \tan^{-1}\left(\frac{n_s^2 - n_0^2}{n_1^2 - n_s^2}\right)^{1/2}\right] \equiv CO_{TE}$$
$$\left(\frac{d}{\lambda}\right)_{TM} = \frac{1}{2\pi\sqrt{n_1^2 - n_s^2}}\left[m\pi + \tan^{-1}\frac{n_1^2}{n_0^2}\left(\frac{n_s^2 - n_0^2}{n_1^2 - n_s^2}\right)^{1/2}\right] \equiv CO_{TM} \qquad (1.15)$$

At the cutoff value: $n_s\omega / c = k_z$, so both ω and k_z are defined by Eq. 1.15.

4.3.3 - Dispersion of a waveguide with a periodic structure

For a periodic structure, a mode with wave vector k can be written in the Bloch form, i.e. a plane wave modulated by a function that shares the periodicity of the lattice ($\vec{L}$ being a lattice vector):

$$\vec{H}_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\vec{u}_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\vec{u}_{\vec{k}}(\vec{r}+\vec{L}) \qquad (1.16)$$

An important feature of these Bloch states is that different values of k do not necessary lead to different modes. Specifically, we can define a reciprocal lattice vector $\vec{G}$, with $\vec{G}\cdot\vec{L} = 2\pi m$. For these vectors, a mode with wave vector $\vec{k}$ and a mode with wave vector $\vec{k}+\vec{G}$ are the same mode. Therefore, we can restrict our attention to k-values in the 1st Brillouin zone, defined as the zone in reciprocal space for which $|\vec{k}| \leq G/2$. Figure 16 shows in orange the Brillioun zone for 1-D periodic slab left and a 2-D square lattice of holes in a dielectric slab.

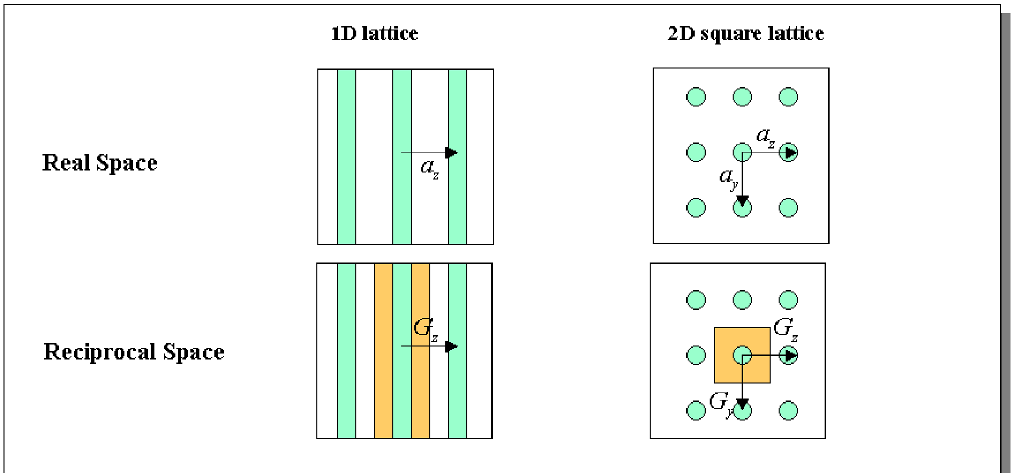


figure 16 – 1st Brillioun zones for 1D lattice and 2D square lattice

If we assume that the presence of the air scatterers does not alter the dispersion, we can “fold” the calculated dispersion of the waveguide to the 1st Brillouin zone. The dashed line in figure 15 shows the “folded” dispersion curve $k_z(\omega)$.

The resonances for normal incidence ($k_z = 0$) as simulated by Meep correspond with intersections of the folded bandstructure with the ω-axis. Based on the folded dispersion relation depicted in figure 15, in the frequency range of $0.3 < \omega < 0.6$ two TE resonance modes at $\omega = 0.34$ and $\omega = 0.48$ (in units of $2\pi c/a$) and one TM resonant mode at $\omega = 0.40$ in units of $2\pi c/a$) can be expected.

The frequencies found in this section and the Meep-simulated resonance frequencies do not entirely match. The main candidate for explaining the difference is the unknown effective refractive index of the layer. For the waveguide dispersion in figure 15, we have assumed an effective index of 3.5 (as if the layer was homogeneous). It was not possible to predict the value of the effective index with simple analytical formulas, that exist for random arrangements of cylinders.

4.3.4 - Resonance frequencies for slab on substrate

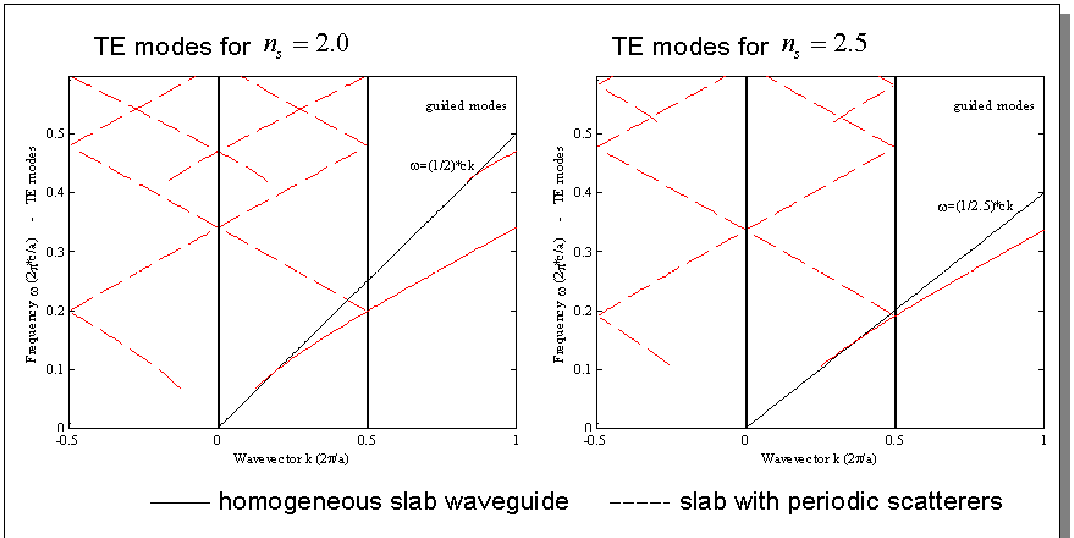


figure 17 – Dispersion for plane wave with thickness 0.5 for (a) ns=2.0 and (b) ns=2.5

Figure 17 shows the dispersion relation folded to the 1st Brillouin zone for a waveguide on a substrate with a refractive index $n_s = 2.0$ (left) and $n_s = 2.5$ (right). For $n_s = 2.0$, the second TE mode crosses the $k_z = 0$ line, but at $n_s = 2.5$, the 2nd TE mode " misses" the $k_z = 0$ line. This is consistent with the results of the FDTD simulation presented in section 4.2, where the second peak in the spectrum has vanished at $n_s = 2.5$.

The calculated dispersion relation reveals that the second resonance disappears because it is beyond cut-off. The peak vanishes for that n_s for which $k_z^{CO} > \vec{G}$, with $k_z^{CO} = 2\pi / \lambda^{CO}$ the cut-off point of the mode and $\vec{G} = 2\pi / a$ the reciprocal lattice vector. This occurs for a substrate index n_s for which $CO_{TE}(n_s) > \dfrac{d}{n_s a}$, with CO_{TE} given by Eq. 1.15. According to this criterion, the resonance of the second TE mode should vanish when $n_s \sim 2.24$. Additional Meep simulations for different substrate indices between 2.0 and 2.5 confirm that the resonance disappears in this range. The exact value of $n_s = 2.24$ is difficult to reproduce because a good analytical estimate of the effective index of the slab is lacking.

4.4 - Resonances in more detail

The resonant peaks in the reflectance spectra have a typical asymmetric Fano line shape, which is known for a wide variety of physical phenomena. In particular, for the case of a dielectric slab with a periodic scatterer, the reflectance is given by[56]:

$$R = \frac{r^2(\omega-\omega_0)^2 + t^2(1/\tau)^2 \mp 2rt(\omega-\omega_0)(1/\tau)}{(\omega-\omega_0)^2 + (1/\tau)^2} \qquad (1.17)$$

This formula represents two channels: the real constants $r = E_r / E_i$ for reflection and $t = E_t / E_i$ for transmission represent the direct reflection and transmission of the slab. The resonant channel has a frequency ω_0, and a lifetime τ. The +/– sign corresponds to the case where the resonant mode is even (odd).

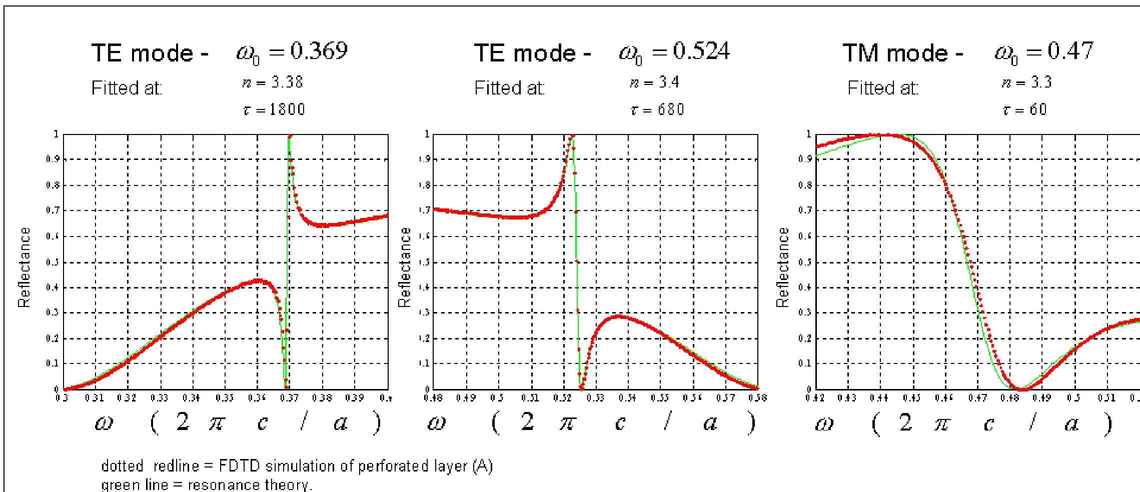


figure 18 – Fano shape of resonance

Figure 18 shows the result of our FDTD method (symbols) for a dielectric slab with lattice constant a=1, thickness d=0.5a and width of the air scatterer equal to 0.1a. (as shown in figure 7A). The solid line is a fit of the data to Eq. 1.17, when we vary effective index n of the layer, center frequency ω_0 and lifetime τ. From the fit we find that the lifetime of the first TE mode ($\tau = 1800$) is longer than that of the second TE mode ($\tau = 680$). The TM mode has a significantly lower lifetime ($\tau = 60$). The first TE mode corresponds to a – sign, while the second TE and the TM mode correspond to a + sign in Eq. 1.17.

5 - Conclusion

The FDTD method as implemented in the Meep software is relatively easy to use, and with the careful definition of source type, boundary conditions, number of grid points and simulation time, it gives a sound prediction of reflectance spectra of the optical systems considered in this thesis.

The simulated reflectance as function of frequency for a slab with a 1-D periodic array of scatterers contains clear resonances. A Fano line shape is seen in many physical phenomena, and can be used to describe our data as well. This analysis allows one to identify a direct channel and an indirect (resonant) channel. When this slab is fixed on a substrate with an increasing refractive index, we found that at a refractive index between 2.0 and 2.5, one of the resonances vanishes.

For the reflectance of such a perforated slab, the "folded" waveguide dispersion gives a good prediction of the resonant frequencies, although we made use of the theoretical dispersion calculated for a *homogeneous waveguide.* For the frequency range between 0 and 0.6 (in terms of $2\pi c$), this model predicts two resonances for TE, and also predicts at what refractive index of the substrate the second peak vanishes. In this model, the vanishing of the peak is related to the cut-off of the first odd TE waveguide mode.

In order to get an exact prediction of the resonance frequencies, some work is left to find an appropriate expression for the effective refractive index of a slab perforated with holes. Currently, it is not known whether such an expression exists.

References

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Appendix A – Meep script file – rast.ctl

```
; rast.ctl verbeterd op 22 feb. : nu kunnen vierkante herhalende
structuren in 3D worden toegepast.

(define tekst "Start rast.ctl: simulation of Gaussian pulse source")
(display tekst)
(newline)

; parameters

(define-param myres 10)         ; number of grids per distance unit
(define-param mysteps 100)      ; number of simulation steps

(define-param 2dim? true)       ; if false, then 3D;

; a note: if working in 2D, ensure that coordinates in z-direction = 0

(define-param no-inc? true)
; if false, no incident structure (for normalisation)
(define-param TE? true)
; if true polarisation = TE (transverse to plane of incidence), else TM

(define-param wl 2)             ; source wave length
(define-param freq (/ 1 wl))    ; source frequency
(define-param df freq)          ; fr width of gaussian pulse
(define-param fmin (- freq 0.1))
; fr minima en maxima of measured spectrum
(define-param fmax (+ freq 0.1))
(define-param nfreq 100)
; number frequencies at which to compute flux

(define-param kfact 0)          ; angle by phase of size: 2pi*kfact*y

(define-param ind1 1.2)         ; index of layer
(define-param ind2 1)           ; index of subtrate (default=air)
(define-param ind3 1)           ; index of holes in layer (default=air)
(define-param r 0)              ; diameter of hole (default no hole)
(define-param N 1)
; number of holes in computational cell (NxN for 3D
(define-param d 2)              ; distance between center of holes


; structure

(define sy (* N d))
(define sz sy)                      ; sz only used if 3D
(define sx 10)

(set! dimensions (if 2dim? 2 3))    ; default = 2D, 3D works

(set! geometry-lattice (make lattice (size sx sy sz)))

(display "lattice:") (display sx) (display sy) (display sz)
```

```
(newline)

(define-param t1 1)                ; thickness of layer (with ind1)
(define t2 (- (* 0.5 sx) t1))      ; rest of x-space is t2
(display "t2:") (display t2)
(newline)

; objecten, sources and flux planes are defined 3D but work 2D if
dimensions is set to 3

; 2 layer - singlelayer definition possible (if ind2=1)

(set! geometry
      (append
      (list
            (make block
                  (center (* t1 0.5) 0 0)
                  (size t1 infinity infinity)
                  (material (make dielectric
                        (if no-inc?
                              (index 1)
                              (index ind1)))))
            (make block
                  (center (+ t1 (* t2 0.5)) 0 0)
                  (size t2 infinity infinity)
                  (material (make dielectric
                        (if no-inc?
                              (index 1)
                              (index ind2)))))
                                        )
      (geometric-objects-duplicates (vector3 0 d 0) 0 (- N 1)
             (geometric-object-duplicates (vector3 0 0 d) 0 (if 2dim? 0
(- N 1))
                (make cylinder
                        (center (* t1 0.5)
                                (* -0.5 (* (- N 1) d))
                                (if 2dim?
                                        0
                                        (* -0.5 (* (- N 1) d)) ) )
                  (radius (* 0.5 r))
                  (height t1)
                  (axis (vector3 1 0 0))
                  (material (make dielectric
                                (if no-inc?
                                        (index 1)
                                        (index ind3)))) )))
                                        )
                                         )

(display "geometry ready")

; sources met amplitude functie om golven onder een hoek te creeren.

(define (my-amp-function p)
;     (exp (* +1i (/ (* 2 (* pi (* hoekverh (vector3-y p)))) wl))) )
      (exp (* +1i (* 2 (* pi (* kfact (vector3-y p)))) )) )
```

```
(set! sources (list
      (make source
            (src (make gaussian-src
                  (frequency freq)
                  (fwidth df)))
            (if TE?
                        (component Ez)
                        (component Hz))
            (center -2 0 0)
            (size 0 sy sz)
            (amp-func my-amp-function)
            )))

(display "sources ready")

(set! pml-layers (list (make pml (thickness 2)(direction X))))

;(init-fields)                                          ; not well
documented feature:
;(meep-fields-set-boundary fields High Y Magnetic)    ; makes of y
direction perfect magnetic conductor
;(meep-fields-set-boundary fields Low Y Magnetic)       ; tested but
not used for thesis

(set! k-point (vector3 0 sy sz))                ; bloch periodicity
(set! ensure-periodicity true)                  ; should ensure
periodicity

(set! resolution myres)                   ; ensure that minimal 20
pixels per wavelenght

; set flux regions

(define trans                             ; transmitted flux
      (add-flux (* 0.5 (+ fmin fmax)) (- fmax fmin) nfreq
            (make flux-region
                  (center (+ t1 1) 0)
;                 (size 0 sy sz)          ; size is not necessary, then
flux point
                  (direction X))))

(define inc
      (add-flux (* 0.5 (+ fmin fmax)) (- fmax fmin) nfreq
            (make flux-region
                  (center -1 0)
;                 (size 0 sy sz)          ; size is not necessary, then
flux point
                  (direction X))))

(display "inc- and trans-flux-plane ready")
(newline)

; run the simulation, separate reflected from incident fields

(if (not no-inc?) (load-minus-flux "inc" inc))  ; only for reflected
flux
```

```
(if TE?
        (if no-inc?
                (run-until mysteps)
                (run-until mysteps
                        (at-beginning output-epsilon)
;                     (to-appended "ez" (at-every 0.3 output-efield-z))
;                       (at-end output-efield-z)
                        ))
      (if no-inc?
                (run-until mysteps)
                (run-until mysteps
                     (at-beginning output-epsilon)
;            (to-appended "hz" (at-every 0.3 output-hfield-z))
;              (at-end output-hfield-z)
                )))

(if no-inc? (save-flux "inc" inc))
(if no-inc? (save-flux "trans" trans))

(display-fluxes inc trans)

(display "Meep has finished rast.ctl")
(newline)
;(exit)
```

Appendix B – Unix script to call Meep script file - startmeep.sh

```
#!/bin/bash

echo "first the normalisation run..."
meep 2dim?=true no-inc?=true TE?=true myres=40 mysteps=1000 ind1=3.5
ind2=2.3 ind3=1 N=1 d=1 t1=0.5 r=0.1 kfact=0 wl=1 df=5 fmin=0 fmax=1.5
nfreq=5000 rast.ctl | tee rast0.out

echo "then the normal run..."
meep 2dim?=true no-inc?=false TE?=true myres=40 mysteps=1000 ind1=3.5
ind2=2.3 ind3=1 N=1 d=1 t1=0.5 r=0.1 kfact=0 wl=1 df=5 fmin=0 fmax=1.5
nfreq=5000 rast.ctl | tee rast.out


# Some background information:
# As defined on the first line, the script below works with bash shell.

# Change at 11/04/07
# For running meep, PATH and LD_LIBRARY_PATH should have been defined
as below:
# PATH="/home/mdedood/install/bin:$PATH"
# LD_LIBRARY_PATH="/home/mdedood/install/lib:$LD_LIBRARY_PATH"

# To run this script correctly with sun grid engine, use options -cwd
and -V with qmod:
# typically: qmod -cwd -V startmeep.sh

# This script calls with MEEP input file rast.ctl. Twice - first a
normalization run (no objects), then with objects. See meep doc.
# We can define for rast.ctl the input parameters below.

# 2dim? =true or = false        if true 2D, else 3D
# no-inc? =true or = false      if true, then no objects, for
normalization (more precise: all objects get n=1)
# TE? = true or = false         polarization = TE (source Ez) of TM
(source Hz)
# myres                         chosen resolution
# mysteps                       number of steps the simulation runs
# ind1                          index of top layer
# ind2                          index of substrate layer; if not
defined, default is n=1
# ind3                        index of cylinder structure within top
layer (default = air)
# N                             number of holes in cell in 1 dimension.
(so if 3D, N=3 gives 9 holes in cell)
# d                             lattice constant - distance between
center of "holes" - must be larger than r to make sense
#                               ALSO ENSURE THAT N*d = Natural figure
(1, 2, 3, etc).
# t1                            thickness of top layer (and height of
"hole" in top layer)
# r                             diameter (not radius) of hole in top
layer - r must be smaller than d to make sense
```

```
# kfact                         brings angle in source by adding
kfact*2pi/d phase in y direction (to be tested for 3D)
# wl                            wavelength of gaussian source
# df                            frequency width of gaussian source
# fmin                          bottom border of frequency range
(spectrum)
# fmax                          top border of frequency range
(spectrum)
# nfreq                         number of frequencies in spectrum =
number of points measured

# note: if 3D, it may be wise not to produce output-files like ez...,
since they take ages

# .dat files can be imported into Matlab scripts, for producing spectra
(usually reflected/transmitted flux for frequency)

echo "conversie van flux1 naar .dat files ..."
grep flux1: rast0.out > rast0.dat
grep flux1: rast.out > rast.dat

# scipts below produce .prn files, change of scripts is usually
nessecary, if filenames in the scripts change
#(e.g. by changing TE? or mysteps)

echo "conversie naar prn files..."
stepsh5top.sh
stezh5top.sh
```