Detailed structure of electromagnetic pulses passing through one-dimensional photonic crystal

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Abstract. The electromagnetic wave propagation in one-dimensional photonic crystals is studied by a finite-difference time domain method. We consider a conventional perfect photonic crystal structures consists of identical alternating layers of high and low refractive indices. When the central frequency is close to the edge of the photonic band gap, the electromagnetic pulse undergoes a large group-velocity dispersion. By using transfer matrix method we examined the transmittance spectrum of terahertz wave filter based on one-dimensional photonic crystals with line defect. We show that is identical structure can be sandwiched between different substrate. Simulation results demonstrate that the terahertz wave filter can achieve a narrow transmission band and high transmission centered at $\lambda_0$, having a flat passband at the central frequency, and sharp edges.

1. Introduction
Photonic crystals (PCs) or photonic bandgap (PBG) materials are a novel class of artificially fabricated structures which have the ability to control and manipulate the propagation of electromagnetic (EM) waves. Properly designed photonic crystals can prohibit the propagation of light, or allow it along only certain directions, or localize light in specified areas. They can be constructed in one, two, and three dimensions with either dielectric or metallic materials. The ability of PCs to control the propagation of light has its origin in their photonic band structure. Just as electron waves traveling in the periodic potential of a crystal are arranged into energy bands separated by bandgapes. We expect the analogous phenomenon to occur when EM waves propagate in a medium in which the dielectric constant varies periodically in space. Photonic bandgap materials are the structures which show such a phenomenon, that is, produce a forbidden frequency gap in which all propagation states are prohibited. It was Yablonovitch who first discovered a dielectric structure containing an absolute gap in the frequency spectrum [1]. Similar gaps can be seen in figure 1, which shows the transmission spectrum of a conventional one-dimensional photonic crystal [2]. A conventional perfect one-dimensional photonic crystal structures consists of identical alternating layers high and low refractive indices. The investigation of these materials is a topic of intensive studies by many groups, both theoretically and experimentally.

The most widely used computer simulation techniques, which can be applied to PCs are the plane-wave (PW) method, the transfer matrix method (TMM), and the finite-difference time-domain (FDTD) method.
Figure 1. The transmission spectrum of a conventional 1D photonic crystal. The transmittance was calculated by TMM. \( (n_1 = 1, 4; n_2 = 2; N=31; n_1d_1 = n_2d_2 = \frac{\lambda_0}{4}) \).

1.1. The PW method
The PW method is used to calculate the \( \omega(k) \) dispersion relation of infinite systems by transforming the problem into an eigenvalue problem [3]. The system must be infinite and frequency independent. Since we study finite systems the PW method is not directly relevant to our work.

1.2. The TMM in one-dimension
The TMM was first used to calculate the band structure of a PC by Pendry and MacKinnon [4]. The simplified TMM for 1D structure is called by TL TMM method [5]. In the transmission line transfer matrix method, the reflection coefficient at the surface of the first layer is obtained by starting the calculations from the last layer using the impedance matching concept. The tangential electric and magnetic field components on the boundary surfaces are continuous. We consider an isotropic and homogeneous multilayered medium as shown in figure 2.

Figure 2. A multilayer dielectric structure (one-dimensional photonic crystal) as a frequency selected surface.

When the light wave normally incident the spectra of TE and TM are the same. Now, we may define \( r \) and \( t \) as the total reflected and transmitted coefficients of structure, respectively,
according to

\begin{align}
 r &= \frac{E_0^-}{E_0^+} \quad \text{in} \quad l = 0, \quad (1) \\
 t &= \frac{E_{N+1}^+}{E_0^+} \quad \text{in} \quad l = N + 1. \quad (2)
\end{align}

Also, we may define reflectance \((R)\), transmittance \((T)\) and absorption \((A)\) as follows:

\begin{align}
 R &= r r^*, \quad (3) \\
 T &= \frac{n_{N+1}}{n_0} t t^*, \quad (4) \\
 A &= 1 - (R + T), \quad (5)
\end{align}

where \(n_{N+1}\) and \(n_0\) are the refractive indices of the \((N + 1)\)'th and 0'th media. The \([I]\) discontinuity transfer matrix of a layer and \([L]\) amplitude transmission matrix may be defined with reference to figure 3.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3}
\caption{Forward and backward traveling waves.}
\end{figure}

The \(E^\pm\) and \(E'^\pm\) are the forward and backward traveling waves at the end and beginning of each layer, respectively, \([I]_{(l+1)}\) is the transmission matrix of the discontinuity between the \(l\)'th and \((l + 1)\)'th layer. \([L]_{(l+1)}\) is the wave amplitude transmission matrix of the \((l + 1)\)'th layer

\begin{align}
 \begin{bmatrix}
 E'^+_{(l+1)} \\
 E'^-_{(l+1)}
 \end{bmatrix}
 &= [I]_{(l+1)} [I]_{(l+1)} \begin{bmatrix}
 E^+_{l+1} \\
 E^-_{l+1}
 \end{bmatrix}, \quad (6) \\
 \begin{bmatrix}
 E^+_{(l+1)} \\
 E^-_{(l+1)}
 \end{bmatrix}
 &= [L]_{(l+1)} \begin{bmatrix}
 E'^+_{(l+1)} \\
 E'^-_{(l+1)}
 \end{bmatrix}. \quad (7)
\end{align}

Therefore

\begin{equation}
 \begin{bmatrix}
 E^+_{(l+1)} \\
 E^-_{(l+1)}
 \end{bmatrix}
 = [L]_{(l+1)} [I]_{(l+1)} [I]_{(l+1)} \begin{bmatrix}
 E^+_{l+1} \\
 E^-_{l+1}
 \end{bmatrix}, \quad (8)
\end{equation}

and the transfer matrix of a layer may be defined as:

\begin{equation}
 [T]_{(l+1)} = [L]_{l+1} [I]_{(l+1)} [I]_{(l+1)}, \quad l = 0, 1, \ldots, N - 1. \quad (9)
\end{equation}
Consequently, the waves on the two outer sides of the multilayered medium between the 0’th and \((N + 1)’th\) layers are related as:

\[
\begin{bmatrix}
E^+_{(N+1)} \\
E^-_{(N+1)}
\end{bmatrix}
= [T]_{(N+1)0}
\begin{bmatrix}
E^+_0 \\
E^-_0
\end{bmatrix},
\] (10)

where the total transfer matrix can be obtained by multiplaying all individual transfer matrixes in sequence

\[
[T]_{(N+1)0} = \prod_{N+1}^0 [L][I] = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}.
\] (11)

Now, equation (10) is divided by \(E^+_0\)

\[
\begin{bmatrix}
t \\
0
\end{bmatrix} = [T]_{(N+1)0}
\begin{bmatrix} 1 \\ r \end{bmatrix},
\] (12)

which is expressed in terms of \(r\) and \(t\) according to the definitions of equations (1) and (2). The outer half space is assumed matched (\(E^-_{N+1} = 0\)).

\[
\begin{bmatrix}
t \\
0
\end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}
\begin{bmatrix} 1 \\ r \end{bmatrix}
\] (13)

The reflection responses and the transmission coefficient will satisfy the recursions:

\[
r = -\frac{T_{21}}{T_{22}},
\] (14)

\[
t = T_{11} - T_{12} \frac{T_{21}}{T_{22}}.
\] (15)

If the media is lossless and nonmagnetic the \([L]\) matrix can be written in the following forms:

\[
[L]_{(l+1)} = \begin{bmatrix}
\exp\{-j \frac{2\pi}{\lambda} \sqrt{\mu_r \varepsilon_r} h_r\} & 0 \\
0 & \exp\{j \frac{2\pi}{\lambda} \sqrt{\mu_r \varepsilon_r} h_r\}
\end{bmatrix} = \begin{bmatrix}
\exp\{-j \frac{2\pi}{\lambda} n_r h_r\} & 0 \\
0 & \exp\{j \frac{2\pi}{\lambda} n_r h_r\}
\end{bmatrix},
\]

where \(n_r = \sqrt{\varepsilon_r}\) is the refractive index of the layer. It should be mentioned that the optical thicknesses are typically chosen to be quarter-wavelength long, that is, \(n_r h_r = \frac{\lambda_0}{4}\) at operating wavelength \(\lambda_0\). The \([I]\) matrix is given by

\[
[I]_{(l+1)}l = \frac{1}{1 - r_{(l+1)}l}
\begin{bmatrix}
1 & -r_{(l+1)}l \\
-r_{(l+1)}l & 1
\end{bmatrix},
\]

where

\[
r_{(l+1)}l = \frac{\eta_{(l+1)}l - \eta_l}{\eta_l + \eta_{(l+1)}};
\]

and \(\eta_l, \eta_{(l+1)}\) the wave impedance of the \(l\)’th and \((l + 1)’th\) layer.
1.3. The FDTD method in one-dimension

The FDTD method employs finite differences as approximations to both the spatial and temporal derivatives that appear in Maxwell’s equations [6]. FDTD and related techniques are marching-in-time procedures that simulate the continuous actual electromagnetic waves in a finite spatial region by sampled-data numerical analogs propagating in a computer data space. Time-stepping continues as the numerical wave analogs propagate in the space lattice to causally connect the physics of the modeled region [7]. Although we only have one spatial dimensions, time can be thought of as another dimensions. Thus this is really a sort of two-dimensional problem as it can be seen in figure 4.

\[ \Delta x \] is the spatial offset between sample points and \( \Delta t \) is the temporal offset. The index \( i \) corresponds to the spatial step, while the index \( n \) corresponds to the temporal step. Figure 4 shows the arrangement of the electric and magnetic field sample points, also known as nodes. The electric-field nodes are shown as red circles and the magnetic-field nodes as blue circles. Assume that all the fields below the red line are known—they are considered to be in the past—while the fields above the red line are future fields and hence unknown. The FDTD algorithm provides a way to obtain the future fields from the past field. From the discretized form of Faraday’s law

\[
\mu_0 \mu_r \frac{\partial H_y}{\partial t} \bigg|_{(i+1/2)\Delta x}^{n\Delta t} = \frac{\partial E_z}{\partial x} \bigg|_{(i+1/2)\Delta x}^{n\Delta t} \tag{16}
\]

we obtain an equation for the unknown magnetic fields:

\[
H_y \bigg|_{i+1/2}^{n+1/2} = H_y \bigg|_{i+1/2}^{n-1/2} + \frac{1}{\mu_0 \mu_r} \frac{\Delta t}{\Delta x} \left\{ E_z \bigg|_{i+1}^{n} - E_z \bigg|_{i}^{n} \right\} . \tag{17}
\]

Equation (17) shows that the future value of \( H_y \) depends on only its previous value and the neighboring electric fields. After applying to all the magnetic-field nodes, the dividing line between future and past values has advanced a half-time step. From the discretized form of Ampere’s law

\[
\varepsilon_0 \varepsilon_r \frac{\partial E_z}{\partial t} \bigg|_{i\Delta x}^{(n+1/2)\Delta t} = \frac{\partial H_y}{\partial x} \bigg|_{i\Delta x}^{(n+1/2)\Delta t} \tag{18}
\]
we obtain an equation for unknown electric field:

\[
E_z^{n+1}|_{i} = E_z^{n}|_{i} + \frac{1}{\varepsilon_0 \varepsilon_r} \frac{\Delta t}{\Delta x} \left\{ H_y^{n+1/2}|_{i+1/2} - H_y^{n+1/2}|_{i-1/2} \right\}.
\] (19)

After applying to all the electric-field nodes in the grid, the dividing line between what is known and what is unknown moves forward another one-half temporal step [8].

In most instances one is interested in modelling a problem which exists in an open domain. If we realize absorbing boundary conditions the grid which contain only a finite number of nodes can behave as if it were infinite.

1.3.1. Accuracy and numerical stability

It is worth noting that the FDTD scheme fulfill of four Maxwell’s equation, although only two equations are directly employed. The ratio \( c \Delta t/\Delta x \) is often called the Courant number which plays an important role in determining the stability of a simulation (\( c \) is the light velocity in free space). In FDTD simulations there are restrictions on how large temporal step can be. If the temporal step is too large, the algorithm produces unstable results. The restriction can be expressed \( c \Delta t \leq \Delta x \) or \( S_c \leq 1 \), where \( S_c = c \Delta t/\Delta x \). It turns out that the optimum ratio for the Courant number is also the maximum ratio \( S_c = 1 \) [8], which is called the “magic time step”.

2. Comparison of different numerical techniques

We will discuss the capabilities and disadvantages of the three most successful and widely used numerical techniques [9]. The PW method is usually used to treat infinite periodic systems, giving their dispersion properties. Although it can be applied only in systems with nondispersive components, the PW method is the fastest and easiest to apply. The TMM is able to calculate the band structure of systems with dispersive components but it is less easy to apply than the PW method. Among the most important advantages of the TMM is its ability to treat samples with almost arbitrary internal structure and arbitrary material combinations, giving the complex transmission and reflection amplitudes, that is, magnitude, phase, and polarization information.

Among the drawbacks of the TMM is the necessity of discretization of the unit cell, which introduces some numerical artifacts and some constraints into the shape size of the components inside the unit cell.

The FDTD method, like the TMM, can also model finite slabs with almost arbitrary internal structure and material combinations. Its main advantages compared to the TMM is that it can give the transmission properties over a wide spectral range with just a single calculation. It also can give time-domain pictures of the fields and the currents over the entire computational domain. Moreover, it can treat defects with no additional computational complications.

Concerning the disadvantages of the FDTD method, part of them stem from the inherent discretizations required. In the case of dispersive materials, though, one encounters additional problems, coming from the time scale that the dispersion model introduces, as the time step of the method (\( \Delta t \)) cannot be much larger than the characteristic time scale of the dispersion model.

Apart from the three methods that we have described, additional methods have been applied to the study of PCs, although less extensively. Some of those are the variations of the PW, TMM, and FDTD methods. Among the existing methods, one worth mentioning is the multiple-scattering (MS) or photonic-KKR method, which is a vectorial extension of the well-known electronic band structure calculation method KKR, and its modification known as the layered-MS method. Their main disadvantages are the heavy formalism, the difficulties in the computational procedure, and the large calculation times.
3. Wave propagation in a one-dimensional photonics crystals

Let us consider a one-dimensional photonic crystal consist of 150 layers (see figure 5). Each layer is isotropic and homogeneous. Furthermore we assume that the material is nonmagnetic. The structure of one-dimensional PCs with linear media and finite length is denoted as $(HL)^{75}$, where $H$ stands for layers with the same high dielectric constant $\varepsilon_h = 9$ and the same thickness $d = 1.5 \times 10^{-5}$ m (15 $\mu$m), while $L$ stands for layers with the same low dielectric constant $\varepsilon_l = 1$ and the same thickness of $d$, respectively, and 75 stands the number of periods. In the one-dimensional FDTD computation used, the computation domain is set as 1000 cells and each cell length is set as $\Delta h = 3 \mu$m. Thus one period of the PC occupy 10 cells. The whole PC is set from cell No. 100 to cell No. 900. The length of the computational domain and the photonic crystal are 3 mm and 2.25 mm. The other domain is free space. The time interval is $\Delta t = \Delta h/c = 10^{-14}$ s (10 fs) ($c$ is the light velocity in free space).

![Figure 5](image_url)

**Figure 5.** Wavelet-shaped DC electric pulse approaches to the entrance of the one-dimensional photonic crystal. The pulse is normally incident from the left.

3.1. Pulse excitation

One of the features of the FDTD technique is that it allows the modelling of broad range of frequencies using a single simulation. Therefore it is generally advantageous to use pulsed sources rather than harmonic source. The Gaussian pulse is potentially an acceptable source expect that it contains a dc component. Source with dc components also have the possibility of introducing artifacts which are not physical. Therefore we consider a different pulsed source which has no dc component. The Ricker wavelet is equivalent to the second derivative of a Gaussian. The operating wavelength and frequency of the wavelet are $\lambda_0 = 9 \times 10^{-5}$ m and $\nu_0 = 3.3 \times 10^{12}$ Hz.

Figure 6 shows temporal-spatial evolution of the electric field. It is clear that, in this case the group-velocity dispersion becomes so large that the pulse entirely disperses. Figure 7, 8, 9, 10 and 11 are the snapshots of the pulse taken at time step 25, 125, 325, 625 and 849.

It should be mentioned that by introducing the Kerr nonlinearity into a PC material, the balance of the large dispersion and the self phase modulation (due to the Kerr nonlinearity) can produce a soliton-like pulse propagating inside the PC structure [10].
Figure 6. Computed electric-field distribution (color map) of a Ricker wavelet as a function of space and time. The dashed lines show the boundaries of the photonic crystal.

Figure 7. Ricker wavelet pulse approaches to the entrance of the photonic crystal.

Figure 8. Ricker wavelet pulse propagating in the photonic crystal.
Figure 9. Ricker wavelet pulse propagating in the photonic crystal.

Figure 10. Ricker wavelet pulse propagating in the photonic crystal.

Figure 11. Ricker wavelet pulse propagating in the photonic crystal.
4. The transmittance spectrum of the slightly modified Li filter

Terahertz wave, which refers to the frequencies from 0.1 THz to 10 THz, lie in the frequency gap between the infrared and microwave, have received considerable attention during the past decades. Spectroscopy in terahertz radiation could provide novel information in chemistry and biochemistry. Recently developed methods of THz time-domain spectroscopy (THz TDS) and THz tomography have been shown to be able to perform measurements on, and obtain images of, samples which are opaque in the visible and near-infrared regions of the spectrum. The utility of THz-TDS is limited when the sample is very thin, or has a low absorbance, since it is very difficult to distinguish changes in the THz pulse caused by the sample from those caused by long term fluctuations in the driving laser source or experiment. However, THz-TDS produces radiation that is both coherent and spectrally broad, so such images can contain far more information than a conventional image formed with a single-frequency source. A primary use of submillimeter waves in physics is the study of condensed matter in high magnetic fields, since at high fields (over about 15 teslas), the Larmor frequencies are in the submillimeter band. Terahertz radiation could let art historians see murals hidden beneath coats of plaster or paint in centuries-old building, without harming the artwork.

Up to now, some kinds of THz wave filter based on photonic crystal, metamaterial and surface plasmon, have been reported [11],[12]. Recently, a novel terahertz filter has been designed by Li [13]. The device can be called Li filter. A conventional perfect photonic crystal structures consists of identical alternating layers of high ($n_1$) and low ($n_2$) refractive indices.

The configuration of the Li filter using one-dimensional photonic crystal is shown in figure 12.

![Figure 12](image)

Figure 12. Schematic diagram of the terahertz wave filter (Li filter).

It consists of a line defect layer inserted into a periodic structure of alternating layers of high/low index materials. To design a linear defect with specified defect states located at the prescribed frequencies, a quarter-wave layer $n_2$ is implanted in the perfect photonic crystal (namely a quarter-wave layer $n_2$ is inserted between the two groups $(n_1n_2)^N(n_1n_2)^N$, resulting in $(n_1n_2)^Nn_2(n_1n_2)^N$, where $N$ represents the periodicity of the cross, $n_1$ and $n_2$ are the refractive index of the dielectric materials, respectively.) Adding another $n_2$ layer on the right, the structure $(n_1n_2)^Nn_2(n_1n_2)^Nn_2$ will act as $2n_2$, that is, a half-wave absentance layer at $\lambda_0$. Li demonstrated that if identical structure is sandwiched between the same substrate, then it will act as an absentance layer, opening up a narrow transmission window at $\lambda_0$, in the middle of its reflecting band (see figure 13) [13]. The optical thicknesses of the layers are quarter-wavelength long at the operating wavelength $\lambda_0$. The THz frequencies were selected for THz wave wireless communication applications. The frequency is 0.3 THz. The operating wavelength is taken to be $\lambda_0 = 1$ mm. The refractive indices of the layers are selected $n_a = n_b = 1.52$ (glass), $n_1 = 2.1$ (zirconium oxide), $n_2 = 1.4$ (magnesium fluoride). The periodicity of the cross $N$ is equal to 10.
Figure 13. The transmission spectrum of THz wave narrow bandpass filter \((N = 10)\). As Li suggested the filter is sandwiched between the same substrate \((n_a = n_b = 1.52)\).

Simulation results demonstrate that the Li filter can achieve a narrow transmission band and high transmission centered at \(\lambda_0\), having a flat passband at the central frequency, and sharp edges. We will show that is identical structure can be sandwiched between different substrate. The refractive indices of the layers are selected \(n_a = 1\), (air) \(n_b = 2.315\) (titanium dioxide), \(n_1 = 2.1\) (zirconium oxide), \(n_2 = 1.4\) (magnesium fluoride). As can be seen in figure 14, our simulation results show that the slightly modified filter also exhibit good transmission performance at the central frequency.

Figure 14. The transmission spectrum of THz wave narrow bandpass filter \((N = 10)\). The filter is sandwiched between different substrate \((n_a = 1, n_b = 2.315)\).
By the changing of the refractive indices outside the filter the transmission bandwidth remains the same. However, the magnitude of the transmission peak becomes lower, and it is about 85%.

5. Conclusion
We presented a brief review of the three most successful and widely used numerical techniques. We presented the key ideas and equations of the TMM and FDTD method and discussed their capabilities and disadvantages. We have been given several numerical calculations starting from the pulse propagation through one-dimensional photonic crystal and arriving the transmission characteristic of the slightly modified THz wave filter. We have shown the temporal-spatial evolution of the Ricker wavelet pulse within the PC. The effect of the group-velocity dispersion is connected with the center frequency of the electromagnetic pulse: when it is close to the edge of the photonic band gap, the pulse undergoes a large group velocity dispersion. The simulation result has shown that the slightly modified terahertz wave filter preserves the required transmission performance at the central frequency, adjustable bandpass, sharp edges, and good rejection of the sideband frequencies.

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