ANALYTICAL AND NUMERICAL CALCULATIONS OF TWO-DIMENSIONAL DIELECTRIC PHOTONIC BAND GAP STRUCTURES AND CAVITIES FOR LASER ACCELERATION*

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Abstract

Dielectric photonic band gap (PBG) structures have many promising applications in laser acceleration. For these applications, accurate determination of fundamental and high order band gaps is critical. We present the results of our recent work on analytical calculations of two-dimensional (2D) PBG structures in rectangular geometry. We compare the analytical results with computer simulation results from the MIT Photonic Band Gap Structure Simulator (PBGSS) code, and discuss the convergence of the computer simulation results to the analytical results. Using the accurate analytical results, we design a mode-selective 2D dielectric cylindrical PBG cavity with the first global band gap in the frequency range of 8.8812 THz to 9.2654 THz. In this frequency range, the TM01-like mode is shown to be well confined.

INTRODUCTION

PBG structures [1] have attracted much attention in recent years because of the large number of promising applications they provide. The distinctive feature of properly designed photonic crystals is the presence of global band gap, such that for a certain range of frequencies electromagnetic waves cannot propagate in the structure for all direction. This feature has found its applications in laser-driven accelerators [2] and microwave generation [3]. For example, metal PBG structures have been used to design selective rf circuit for microwave linear accelerator with successfully suppressed wakefields. Dielectric PBG structures have been proposed to be used in laser-driven accelerator schemes.

Accurate determination of fundamental and high order band gaps is critical in pursuing these applications. Several numerical codes have been developed specifically for PBG structure calculations [4,5]. For these codes the benchmarking and error analysis is an important issue.

In this paper, we consider a 2D dielectric PBG structure in rectangular geometry. For certain specific parameters of the structure an expression for the exact dispersion relation for TM modes is obtained, which allows us to perform the error analysis on certain numerical codes such as PBGSS. In general, our analytical results for the rectangular PBG structure may be used to benchmark other PBG codes that have been or will be developed to solve the dielectric PBG structures.

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ANALYTICAL DISPERSION RELATION FOR TM MODES IN A 2D RECTANGULAR DIELECTRIC PBG STRUCTURE

We consider a 2D periodic PBG structure consisting of rectangular dielectric rods, infinite in the z -direction. The elementary cell for this PBG structure is shown in Fig.1. We are interested in the situation where the component of the wave vector along the rods k_z is equal to zero. In this situation, it is readily shown from Maxwell's equations that the wave fields in the 2D dielectric media can be decomposed into two independent sets of modes, namely, transverse electric (TE) modes and transverse magnetic (TM) modes. The electric field in TE mode is perpendicular to the axis of the rods (i.e. the z axis), whereas in a TM mode the magnetic field is perpendicular to the axis of the rods. All the field components in the TE (TM) mode can be expressed in terms of the longitudinal magnetic (electric) field, which is further denoted by Ψ. The longitudinal field component in each rod satisfies the following Helmholtz equation

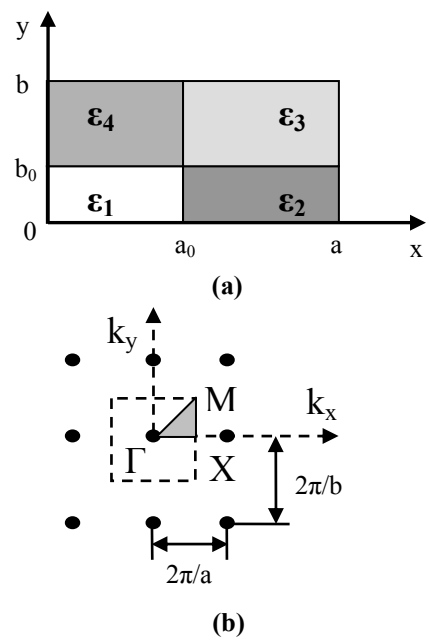

Figure 1. Schematics of a 2D rectangular PBG structure representing (a) elementary cell of the structure and (b) reciprocal lattice and a Brillouin zone with an irreducible Brillouin zone in the shaded region.

$$\nabla_{\perp}^2 \Psi_i(\mathbf{x}_{\perp}) = -k_{i\perp}^2 \Psi_i(\mathbf{x}_{\perp}), \quad (1)$$

where index i refers to the i - type of the dielectric rod and $k_{i\perp}^2 = \varepsilon_i \omega^2 / c^2$. We use the notation $\Psi_i(\mathbf{x}_{\perp})$ instead of $\Psi_i(\mathbf{x}_{\perp}, \omega)$ assuming that the frequency ω is fixed. We specialize to the TM mode in the reminder of the paper.

Applying the boundary conditions on the interface of the dielectric rods and the periodic boundary conditions on the boundaries of the elementary cell, we derive analytical dispersion relation for a special case when the dielectric constants of the rods satisfy the algebraic condition

$$\varepsilon_1 + \varepsilon_3 = \varepsilon_2 + \varepsilon_4 . \quad (2)$$

In this case, we can obtain the following analytical dispersion relation for the TM modes with $k_z = 0$:

$$\begin{aligned} D(\omega, k_x, k_y) \equiv\ & 2\cos(k_x a) - 2\cos(k_{1x} a_0)\cos[k_{2x}(a - a_0)] \\ +\ & \left(\frac{k_{1x}}{k_{2x}} + \frac{k_{2x}}{k_{1x}}\right)\sin(k_{1x} a_0)\sin[k_{2x}(a - a_0)] = 0 \end{aligned}, \quad (3)$$

where the functions $k_{1x} = k_{1x}(k_y, \omega)$ and $k_{2x} = k_{2x}(k_y, \omega)$ are implicitly defined by the relations

$$\begin{aligned} & 2\cos(k_y b) - 2\cos(k_{1y} b_0)\cos[k_{3y}(b - b_0)] \\ & + \left(\frac{k_{1y}}{k_{3y}} + \frac{k_{3y}}{k_{1y}}\right)\sin(k_{1y} b_0)\sin[k_{3y}(b - b_0)] = 0, \end{aligned} \quad (4)$$

$$k_{1x}^2 + k_{1y}^2 = \frac{\varepsilon_1 \omega^2}{c^2}, \quad (5)$$

$$k_{2x}^2 + k_{1y}^2 = \frac{\varepsilon_2 \omega^2}{c^2}, \quad (6)$$

$$k_{2x}^2 + k_{3y}^2 = \frac{\varepsilon_3 \omega^2}{c^2}. \quad (7)$$

There are a number of useful applications of the analytical dispersion relation. First, it allows for benchmarking the existing numerical codes for PBG calculations. Second, it enables us to perform a rigorous error analysis and establish error tolerance in a PBG simulation code. Third, it allows for an accurate determination of global band gaps, especially very narrow ones which are required in order to design an oversized PBG cavity or waveguide with a single transverse mode. Fourth, it allows us to study the attenuation of the mode which has a frequency in the global band gap and therefore it is trapped in the defect of the structure.

COMPARISON BETWEEN THEORY AND NUMERICAL SIMULATIONS

In this section, we present results of the comparison between the analytical calculation and the numerical calculations using our PPGSS code [4] and the MIT Photonic-Bands (MPB) package [5]. Our PBGSS code uses the real-space finite-difference method [4], whereas the MPB package uses preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a plane wave basis [5].

Results of the calculations of the first six bands are presented on Fig. 2 for a PBG structure with the following parameters: $a_0/a = 0.7$, $b_0/b = 0.7$, $a/b = 1.0$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = \varepsilon_4 = 5.0$ and $\varepsilon_3 = 9.0$. In the PBGSS code, the fundamental unit cell is covered by square mesh with $(2N+1)\times(2N+1)$ mesh points. In our calculation, we use the value of $N = 8$. For the MPB code, we use the value of resolution (grid points per lattice constant a) equal to 32. We can see that the numerical simulations agree well with the analytical solution.

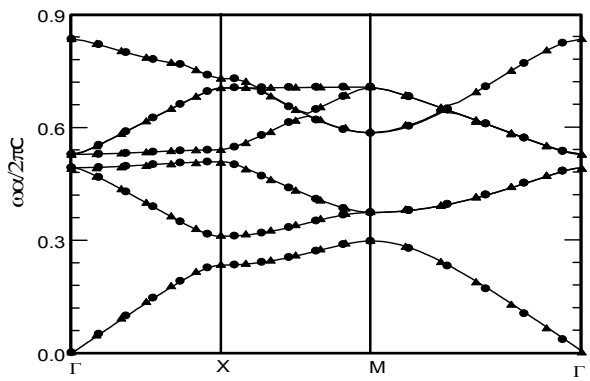

Figure 2. Plots of the normalized frequency $\omega a/2\pi c$ for the first six bands versus the wave vector $\mathbf{k}_{\perp}$ for TM modes as $\mathbf{k}_{\perp}$ varies from Γ to X, X to M, and M to Γ [see Fig. 1(b)]. Solid curves are analytical results; triangles, PBGSS simulation results; dots, MPB code simulation results.

As discussed previously, the analytical dispersion relation can be used to test different numerical codes. To this end, we have started the error analysis on the PBGSS code. The results are shown in Fig. 3 for the M point in the irreducible Brillouin zone as the function of N. As one can notice the error is oscillating as N increases. The absolute value of the maximum error is found to scale approximately $\propto 1/N$. We plan to continue working on the error analysis of PBGSS code and to optimize the code in order to improve accuracy.

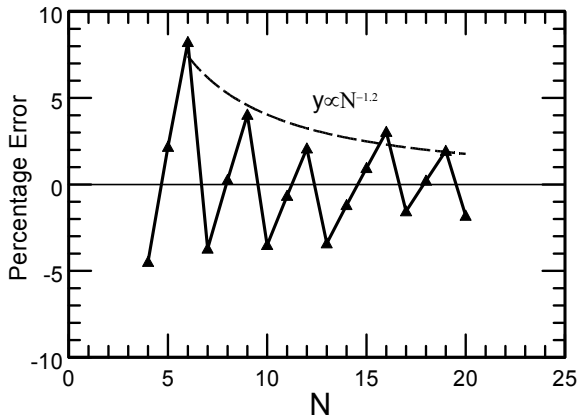

Figure 3. Value of the error in normalized frequency $\omega a/2\pi c$ as a function of N for first TM mode at M point. Dashed line represents the fit for absolute value of the maximum error found.

ATTENUATION OF THE TM MODE WITH FREQUENCY IN A GLOBAL BAND GAP

We make use of Eq. (3) to calculate the attenuation of the evanescent wave in the band gap as a function of angle of the wave vector with respect to $\Gamma - X$ direction in the irreducible Brillouin zone in Fig. 1(b). The results are shown in Fig. 4. The wave attenuates differently in different directions.

From Fig. 4, we estimate the quality factor of a resonator formed by removing part of the PBG structure. For a PBG resonator with a hollow circular cross section with the inner diameter D and the PBG wall thickness L, the quality factor of a TM mode with wavelength λ in the global band gap scales approximately as $Q \propto (D/\lambda)e^{2<\mathrm{Im}k>L}$, where $<\cdots>$ is the averaging over all possible directions of propagation.

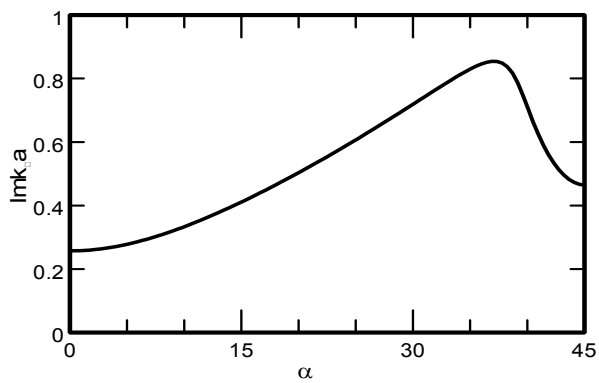

Figure 4. Normalized imaginary part of $k_\perp$ for TM modes with frequency in the global band gap as a function of its angle with respect to $\Gamma - X$ direction in the irreducible Brillouin zone.

We have investigated the confinement of the TM01-like mode in a 2D dielectric cylindrical PGB resonator using High Frequency Structure Simulator (HFSS). The resonator was designed to have inner diameter of $D = 33.5$ μm and a wall thickness of $L = 88.25$ μm. The parameters of the PGB structure are chosen to be $a = b = 10\mu m$, $a_0 = b_0 = 7\mu m$, $\varepsilon_1 = 1.0$, $\varepsilon_2 = \varepsilon_4 = 5.0$ and $\varepsilon_3 = 9.0$. The first band gap for this structure is located between 8.8812 THz and 9.2654 THz. For this resonator a TM_{01}-like mode is found in the band gap at the frequency of 9.0712 THz. The distribution of the electric field magnitude for this mode is shown on Fig. 5. The mode was found to be well confined within a defect.

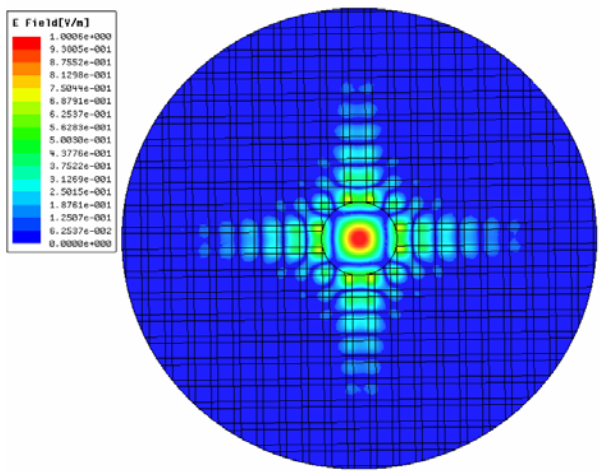

Figure 5. Distribution of the (relative) electric field magnitude for a TM_{01}-like mode in a dielectric cylindrical PBG resonator.

CONCLUSIONS

We found an exact dispersion relation for the TM mode in rectangular 2D dielectric PBG structure with $k_z = 0$ when the dielectric constants of the rods satisfy a certain algebraic condition. We compared the results of our analytical calculations with the results of numerical simulations using PBGSS code and MPB code. The results of numerical calculations were found to be in good agreement with analytical results. We have also estimated the quality factor of the resonator formed by removing part of the PBG structure in long-wave approximation. We performed the error analysis on the PBGSS code.

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