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MODELING PHOTONIC CRYSTALS WITH COMPLEX UNIT CELLS BY DIRICHLET-TO-NEUMANN MAPS *1)

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Abstract

For a photonic crystal (PhC) of finite size, it is important to calculate its transmission and reflection spectra. For two-dimensional (2-D) PhCs composed of a square lattice of circular cylinders, the problem can be solved by an efficient method based on the Dirichlet-to-Neumann (DtN) map of the unit cell and a marching scheme using a pair of operators. In this paper, the DtN operator marching method is extended to handle 2-D PhCs with complex unit cells and arbitrary lattice structures.

Mathematics subject classification: 78A45, 65Z05.
Key words: Photonic crystal, Periodic structure, Diffractive grating, Dirichlet-to-Neumann map, Operator marching.

1. Introduction

In recent years, photonic crystals (PhCs) have attracted much attention due to their unusual ability to manipulate light [1]. Many applications of PhCs have been proposed and realized in experiments. Numerical simulations are essential to understand the basic properties of PhCs and to design and optimize related components and devices. PhCs give rise to a number of interesting and challenging mathematical problems. For an infinite PhC, it is important to calculate its band structure. For PhCs with point defects and line defects, it is necessary to calculate the defect modes. If the PhC is finite in one direction, we need to solve a scattering problem for each given incident wave. The more general PhC structures, such as waveguide bends and branches, give rise to challenging boundary value problems.

One important problem is to analyze the transmission and reflection of a given plane wave incident upon a PhC of finite size. This problem is usually studied for many frequencies to produce the transmission and reflection spectra. Existing numerical methods developed for diffraction gratings, such as the Fourier modal method [2-7] and the finite element method [8], can be used to solve this problem. Special methods that take advantage of the geometric simplicity of PhCs are often more efficient. The multipole method [9-14] is a semi-analytic method suitable for PhCs composed of a lattice of circular cylinders. The boundary integral equation method [15] also has some advantages, since it only solves the wave field on surfaces of the cylinders. To take advantage of the partial periodicity in the direction where the PhC is finite, the scattering matrix formalism [10] and Floquet mode expansions [12, 13] can be used. In a recent paper [16], we developed a Dirichlet-to-Neumann (DtN) operator marching method for two-dimensional (2-D) PhCs composed of a square (or rectangular) lattice of circular

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cylinders. The method takes full advantage of the geometric simplicity of a typical PhC. It uses a cylindrical wave expansion to construct the DtN map of the unit cell and to march two operators from one side of the PhC to another. A discretization in the unit cell is completely avoided. Compared with the multipole and the boundary integral equation methods, the DtN marching method is simpler, since it does not need sophisticated lattice sums techniques.

In this paper, we extend the DtN operator marching method to 2-D PhCs with general lattice structures and complex unit cells. By a complex unit cell, we refer to a unit cell containing more than one possibly different cylinders. While a complex unit cell can be divided into a few sub-cells each containing only one cylinder, the PhC is not periodic on the scale of the sub-cells. The additional freedom associated with different types of sub-cells can be used to design new devices, such as the photonic crystal resonator arrays in [17]. For PhCs with complex unit cells, we develop a merging technique that computes the DtN map of the complex unit cell from the DtN maps of its sub-cells. We also develop a shifting strategy for arbitrary 2-D lattices. The method works particularly well for the important case of triangular lattices. The efficiency and accuracy of our method are illustrated by a number of numerical examples.

2. The DtN Operator Marching Method

We consider a two-dimensional (2-D) photonic crystal (PhC) that is infinite in the x-direction and finite in the y-direction. The structure is periodic in x with period L and limited in y for $0 < y < D$, where D is the width of the PhC. For $y < 0$ (the bottom) and $y > D$ (the top), we assume that the medium is homogeneous with constant refractive index n_b and n_0, respectively. For an incident wave given in $y > D$, the scattering problem is to calculate the reflected wave in $y > D$ and the transmitted wave in $y < 0$.

For the E-polarization, the z-component of the time-harmonic electric field, denoted by u in this paper, satisfies the following Helmholtz equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k_0^2 n^2\, u = 0, \tag{2.1}$$

where $n = n(x,y)$ is the refractive index function and k_0 is the free space wavenumber. For a plane incident wave, the scattering problem can be formulated as a boundary value problem of Eq. (2.1) in the rectangular domain given by $0 < x < L$ and $0 < y < D$. For $y > D$, we have $u = u^{(r)} + u^{(i)}$, where $u^{(i)}$ and $u^{(r)}$ are the incident and reflected waves given by

$$u^{(i)}(x,y) = e^{i[\alpha_0 x - \beta_0 (y-D)]}, \quad u^{(r)}(x,y) = \sum_{j=-\infty}^{\infty} R_j e^{i[\alpha_j x + \beta_j (y-D)]}, \quad y > D, \tag{2.2}$$

where β_0 is positive and R_j is an unknown reflection coefficient. If we denote θ_0 the angle between the wave vector $(\alpha_0, -\beta_0)$ and the y-axis, then

$$\alpha_0 = k_0 n_0 \sin\theta_0, \quad \beta_0 = k_0 n_0 \cos\theta_0, \quad \alpha_j = \alpha_0 + \frac{2j\pi}{L}, \quad \beta_j = \sqrt{k_0^2 n_0^2 - \alpha_j^2}.$$

For $y < 0$, we have only a transmitted wave given by

$$u = u^{(t)}(x,y) = \sum_{j=-\infty}^{\infty} T_j e^{i[\alpha_j x - \gamma_j y]}, \quad \text{for} \quad y < 0 \quad \text{and} \quad \gamma_j = \sqrt{k_0^2 n_b^2 - \alpha_j^2},$$