The modelling of high-contrast photonic crystal slabs using the novel extension of the effective index method

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This paper presents a new approach to determination of the band structure in two-dimensional (2D) photonic crystal slabs using the enhanced effective index approximation. The proposed method remains valid in the wide frequency range even for high-index contrast heterostructures.

Keywords: photonic crystal slabs, effective index method.

1. Introduction

Determination of the photonic band structure in photonic crystals (PCs) is one of the crucial steps in numerical simulations of all PC devices including two-dimensional photonic crystal slabs, which are of particular interest because of their easy fabrication and suitability for a wide range of applications. While exact numerical modelling of such PC slabs requires fully vectorial 3D calculations, it can often be reduced to the simpler 2D ones using the effective index method (EIM) [1, 2]. Such an approach has recently proved to be well suited for low-index-contrast heterostructures [2]. However, in high-contrast heterostructures, the effective index varies significantly with frequency and hence the classical techniques for PC band structure determination, in which permittivity is assumed to be constant, can only be used for the narrow frequency range.

In our work, the classical frequency-domain finite-difference method for 2D PCs analysis is enhanced to allow for a strong refractive index dispersion which consequently makes it possible to analyse properly photonic crystal slabs with high-index-contrast heterostructures. Moreover, the same technique can be straightforwardly used for dispersive materials, as they only introduce the small variation for effective index.

2. Computational method

As some authors [2, 3] have shown, the guided modes in symmetric photonic crystal slabs can be divided into quasi-TE and quasi-TM ones which correspond to H and E

modes of the two-dimensional PC structure. Therefore, it is possible to use a 2D approximation in photonic band computations by means of several techniques among which the EIM is the most popular.

In this method, the 3D profile of refractive indices in a multilayer slab is replaced with a single effective index of unperturbed waveguide. When the contrast ratio between all waveguide layers is low, the effective index varies no more than a few percent for a large frequency range, which allows us to use the finite-difference time-domain (FDTD) method or any technique in which the frequencies are obtained as eigenvalues of the structure-dependent matrix. The latter approach includes plane-wave method, finite element method or the finite difference method, which is used in our calculations.

2.1. Finite difference method

Take the photonic crystal slab and introduce the Cartesian coordinate system where the periodicity is introduced in the *xy* plane (Fig. 1).
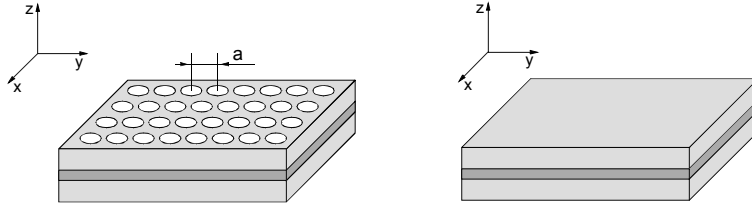

Fig. 1. Photonic crystal with rectangular 2D lattice and the unperturbed slab.

In order to determine eigenfrequencies for a fixed effective index we utilise the two-dimensional decoupled Maxwell equations [4]

$$-\left\{ \frac{\partial}{\partial x}\, n_{\mathrm{eff}}^{-2}\, \frac{\partial}{\partial x} + \frac{\partial}{\partial y}\, n_{\mathrm{eff}}^{-2}\, \frac{\partial}{\partial y} \right\} H_z(x,y) = \frac{\omega^2}{c^2} H_z(x,y) \tag{1}$$

$$-n_{\mathrm{eff}}^{2}\left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right\} E_z(x,y) = \frac{\omega^2}{c^2} E_z(x,y) \tag{2}$$

where Eq. (1) corresponds to quasi-TE and Eq. (2) to quasi-TH modes, to which we apply the Bloch theorem by expressing the field components as

$$E_z(x,y) = \Psi_k(x,y)\exp(ik_x x + ik_y y) \tag{3}$$

$$H_z(x,y) = \Phi_k(x,y)\exp(ik_x x + ik_y y) \tag{4}$$

where the functions Ψ_k and Φ_k are periodic in the x and y directions. After substituting (3) and (4) into (2) and (1) we obtain the eigenmode equations with ω^2/c^2 as the eigenvalue and $\Psi(x, y)$ and $\Phi(x, y)$ as the eigenmodes. Then, we convert them using central finite-differences into the non-Hermitian matrix, whose eigenvalues are the squared frequencies of the effective-index modes.

It is important to realize that the proposed finite-difference approach is only an example and the enhanced effective index method presented below can be as well applied when using different computation techniques (*i.e.*, plane wave expansion or FDTD). Thus, in the two-dimensional plane all the properties of this technique (*e.g.*, periodic boundary conditions of plane-wave expansion or possibility to handle the non-rectangular lattices) are retained.

2.2. Enhanced effective index method for high-contrast heterostructures

For waveguides with a high contrast ratio, the effective index varies strongly with frequency. This adds additional unknown parameters to the problem, making it impossible to use the classical techniques, in which the frequency is determined as an eigenvalue of some matrix. This difficulty can be overcome by determining eigenfrequencies of the 2D photonic crystal as functions of the effective index appearing in Eqs. (1) and (2) (see Fig. 2). As the effective index is a continuous
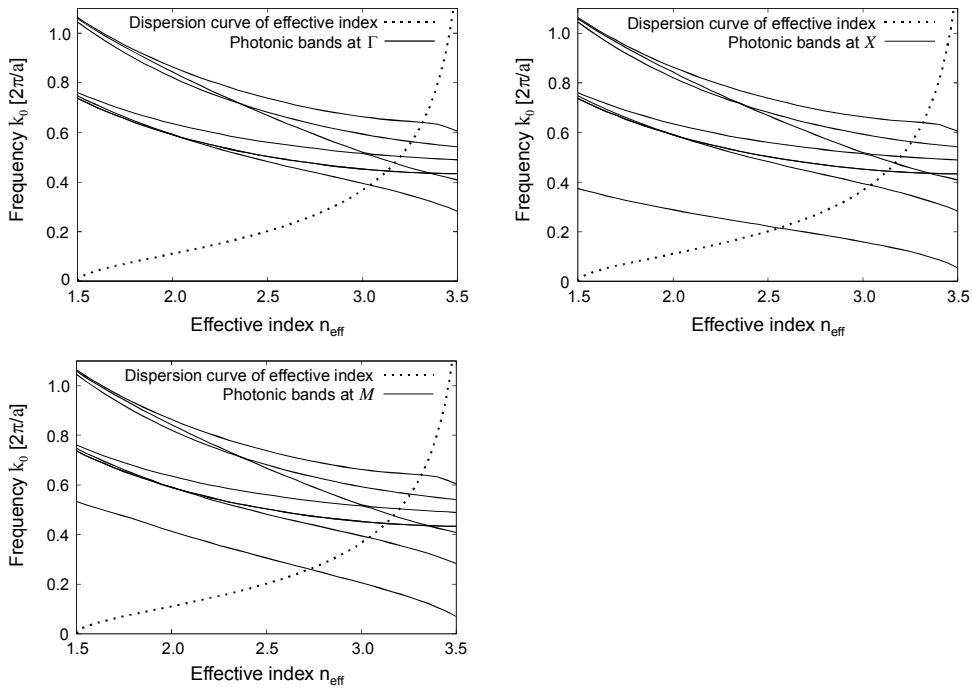

Fig. 2. Dependence of photonic bands on effective index at Γ, X and M and the real effective index–frequency relation for the first-order even modes in $SiO_2/Si/SiO_2$ photonic crystal slab.

function of frequency, we can compute the effective index appropriate for each of the photonic bands by solving the equation

$$\omega_N(n_{\text{eff}}(\omega)) = \omega \qquad (5)$$

where $\omega_N(n_{\text{eff}})$ is the frequency of the N-th photonic band for the two-dimensional photonic crystal, in which the effective index is assumed to be n_{eff} and $n_{\text{eff}}(\omega)$ is the function to the frequency-dependence of effective index.

For more general structures with spacial dependence of the effective index the solution of Eq. (5) is still possible. In such a case, the computational domain must be divided into several sections with different effective indices $n_{\text{eff}}^1(\omega), n_{\text{eff}}^2(\omega), \dots, n_{\text{eff}}^m(\omega)$. Then, the N-th photonic band of the two-dimensional crystal depends on m parameters $\omega_N(n_{\text{eff}}^1, n_{\text{eff}}^2, \dots, n_{\text{eff}}^m)$, which consequently are all functions of frequency. Thus, the problem to solve takes the form

$$\omega_N(n_{\text{eff}}^1(\omega), n_{\text{eff}}^2(\omega), \dots, n_{\text{eff}}^m(\omega)) = \omega \qquad (6)$$

which still is the equation with the single variable ω.

If the structure has only one section with the frequency-dependent effective index and the function $n_{\text{eff}}(\omega)$ is invertible (which is the case, *e.g.*, for the simple three- or four-layer slabs), it is possible to reformulate Eq. (5) into a simpler form

$$\omega_N(n_{\text{eff}}) - \omega(n_{\text{eff}}) = 0 \qquad (7)$$

In our calculations, we have obtained the continuous form of $\omega_N(n_{\text{eff}})$ by determining the PC eigenfrequencies for several arbitrary effective index values and using the third-order spline interpolation to get the continuous function. The solutions of Eq. (7) were found with the Newton–Raphson method [5].

3. Results

3.1. High-contrast planar waveguide PC

The sample calculations have been carried out for a simple three-layer $SiO_2/Si/SiO_2$ waveguide (Fig. 1). The core and the cladding had refractive indices $n_c = 3.6$ and $n_s = 1.5$, respectively. The PC structure was composed of a square lattice of air holes with the lattice constant a and the hole radius $0.3a$. The Si core thickness was $h = 0.4a$. The computational domain was a single lattice cell implemented with the grid of 1024 nodes under periodic boundary conditions.

We have considered only the fundamental symmetric TE guided mode, but the calculations could be easily generalised to cover every guided mode in the slab. The effective index has been computed assuming the analytical solution in z direction of the form
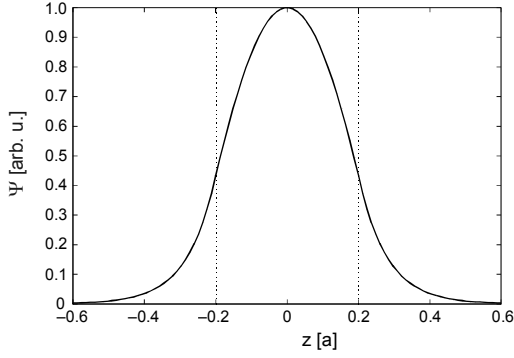
Fig. 3. Distribution of the field along *z* axis for the fundamental mode.

$$\Psi(x, y, z) = \Psi(x, y) \begin{cases} \cos\left(\dfrac{\omega}{c}\sqrt{n_c^2 - n_{\text{eff}}^2}\; z\right) & |z| \leq \dfrac{h}{2} \\[2em] A\exp\left[-\dfrac{\omega}{c}\sqrt{n_{\text{eff}}^2 - n_s^2}\left(|z| - \dfrac{h}{2}\right)\right] & |z| > \dfrac{h}{2} \end{cases} \tag{8}$$

where the constants A and n_{eff} are chosen to ensure the continuity of $\Psi(z)$ and $d\Psi/dz$ at the interface of the layers. The distribution of the field in the z direction for the fundamental mode is presented in Fig. 3.

3.2. Computations

The effective index of the analysed $SiO_2/Si/SiO_2$ waveguide varied from 1.5 to 3.6. In this range, the photonic eigenfrequencies were determined at 9 points for every
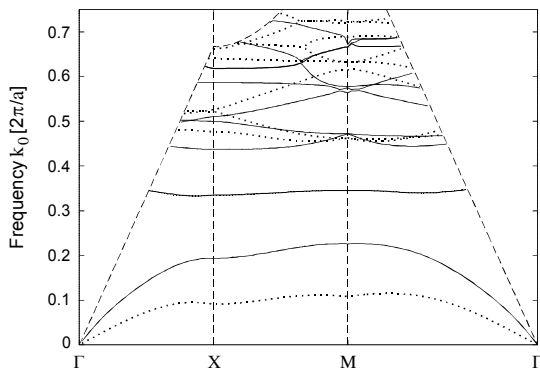

Fig. 4. Photonic bands structure of the first-order even modes in $SiO_2/Si/SiO_2$ photonic crystal slab obtained with our approach (solid lines) compared to the classical effective index method (dashed lines). Note that around the frequency of $k_0 \approx 0.35\,(2\pi/a)$ both methods yield similar results.

wavevector to obtain $\omega_N(n_{\text{eff}})$ relations. They are depicted for Γ, X and M points in Fig. 2 together with the curve representing frequency dependence of the effective index. Only the common points of these two lines are physically meaningful.

3.3. Band structure

Figure 4 presents a photonic band diagram of the sample waveguide (solid lines). For comparison, there is a solution obtained after assuming effective index to have constant arbitrary value 2.95 (dashed lines). As can be seen from the picture, the difference is significant, which shows that in the exact calculation of high-contrast structures the dependence of the refractive index on frequency cannot be neglected.

It is important to notice that when we take the narrow frequency range at any frequency, the method reduces to the classical effective index procedure which has already been verified and proved to be valid [2]. Our approach is merely its generalisation for the wide frequency range.

4. Conclusions

The effective index method is simple, yet often efficient and rationally exact tool for performing band calculations of photonic crystal slabs. The possibility of reducing the problem to 2D allows the computational time to be significantly reduced. One of the major drawbacks of this method was the inability to handle high-contrast waveguides due to the strong dispersion of the effective index.

In this work, we have presented a simple method of photonic band structure computations in such a situation. Although the computational effort in our approach is bigger than in the case of classical methods (the eigenvalues must be determined several times for a single wavevector) it is still much smaller than in the case of full-scale 3D calculations.

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