Dynamical Diffraction Area Applicability in Case of 1D Photonic Crystals with Sinusoidal Permittivity Profile

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Abstract: Bragg reflection and transmission spectra of the 1D photonic crystals characterized by a spatially sinusoidal profile of permittivity are studied as a function of the crystal-plate thickness. Applicability of the dynamical theory of diffraction in describing such spectra is considered. In the framework of the dynamical theory, we (i) calculated and analysed the reflection and transmission spectra for oblique incidence of polarized light, (ii) computed the spectra making use of the transfer matrix technique, and (iii) compared quantitatively the results of the two approaches. As a result, the analytical dynamical theory of diffraction is found to be correct in calculating the Bragg spectra in the vicinity of single photonic band-gap when the plate thickness is equal to the integer number of the spatial periods, or the permittivity is symmetric about the middle plane of the structure.

1 INTRODUCTION

Optical research of new artificial structures, studying their properties and applying them to modern technological devices is a trend in science nowadays. Photonic crystals belong to a large class of such structures (Joannopoulos *et al*., 2008; Sibilia *et al*., 2008). The photonic crystal (PhC) is a spatially periodic structure which permittivity is a spatially periodic function with the period equal-order to electromagnetic wavelength. In semiconductors, electronic properties are governed by the presence of allowed and forbidden energy bands for electrons. In the case of PhC one can control properties and propagation of electromagnetic waves. This unique feature of PhC can be utilized in various applications: photonics, lasers, optoelectronics, etc.

Propagation of light in PhC is very similar to propagation of X-rays in ordinary crystals for which the dynamical theory of diffraction is widely used to study optical properties (Cowly, 1995). Therefore it is of interest to apply the dynamical theory approach to PhCs taking into account high spatial modulation of the PhC dielectric function (Sel'kin, 2004).

In this work, we discuss the model of the opal-like PhC characterized by the one-dimensional (1D) periodicity of permittivity $\varepsilon_s(z)$. As an example, we consider the permittivity of an opal-like PhC averaged along all the crystallographic directions except for [111]. In this case (Bazhenova *et al*., 2007; Gajiev *et al*., 2005)

$$\varepsilon_s(z) = \varepsilon_a f_s(z) + \varepsilon_b\left(1 - f_s(z)\right), \tag{1}$$

where ε_a and ε_b are the permittivities of spheroidal particles that constitute the PhC and interparticle space, respectively, and $f_s(z)$ is the effective filling function (Figure 1).

It should be noted that the effective filling function can be approximated well by the harmonic one. It allows us to suppose that the dynamical theory can be applicable when describing Bragg reflection and transmission spectra of opal-like PhCs. The model proposed is of principal interest because it is closely associated with the previously performed theoretical and experimental studies (Bazhenova *et al*., 2007; Fedotov *et al*., 2011; Gajiev *et al*., 2005) of the opal-like PhCs and allows one to answer the question why the dynamical theory of diffraction is applicable to the PhC with relatively high dielectric contrast.

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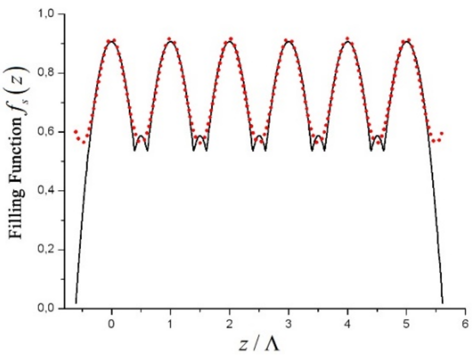

Figure 1: Effective filling function $f_s(z)$ of opal-like PhC along [111] direction. Solid line is given by exact calculation; dashed line corresponds to harmonic approximation.

The main purpose of our study is to elucidate the validity limits of the dynamical theory of diffraction, in particular, to find a minimum slab thickness that provides rather good numerical agreement between the analytical and full-electrodynamic computations of Bragg reflection and transmission spectra.

2 DYNAMICAL THEORY OF DIFFRACTION APPLIED TO PHOTONIC CRYSTALS

Let consider an infinite spatially periodic structure. The corresponding permittivity $\varepsilon(\vec{r})$, the electric, $\vec{E}(\vec{r})$, and magnetic, $\vec{H}(\vec{r})$, fields of an electromagnetic wave can be expanded into Fourier series over the reciprocal-lattice vectors $\vec{G}$. In the vicinity of a Bragg resonance determined by the Laue condition $\vec{k}^2=\left(\vec{k}-\vec{G}\right)^2$ for the wave vector $\vec{k}$ and a specified vector $\vec{G}$, such expansions take the form

$$\varepsilon\left(\vec{r}\right)=\varepsilon_0+\varepsilon_{\vec{G}}\,\mathrm{e}^{i\vec{G}\vec{r}}+\varepsilon_{\vec{G}}^*\,\mathrm{e}^{-i\vec{G}\vec{r}}\,, \qquad (2)$$

$$\vec{E}\left(\vec{r}\right)=\vec{A}_0\,\mathrm{e}^{i\vec{k}\vec{r}}+\vec{A}_{\vec{G}}\,\mathrm{e}^{i\left(\vec{k}-\vec{G}\right)\vec{r}} \qquad (3)$$

$$\vec{H}\left(\vec{r}\right)= =k_0^{-1}\left(\vec{k}\times\vec{A}_0\,\mathrm{e}^{i\vec{k}\vec{r}}+(\vec{k}-\vec{G})\times\vec{A}_{\vec{G}}\,\mathrm{e}^{i\left(\vec{k}-\vec{G}\right)\vec{r}}\right) \qquad (4)$$

where $k_0=\omega/c=2\pi/\lambda$ is the wavenumber of light in vacuum with the circular frequency ω (λ is the wavelength), ε_0 is the average dielectric constant. The amplitudes $\vec{A}_0$ and $\vec{A}_{\vec{G}}$ satisfy a set of equations

$$\begin{cases}\left(\vec{k}^2-k_0^2\varepsilon_0\right)\vec{A}_0-\vec{k}\left(\vec{k}\,\vec{A}_0\right)=k_0^2\varepsilon_{\vec{G}}\vec{A}_{\vec{G}}\\ \left((\vec{k}-\vec{G})^2-k_0^2\varepsilon_0\right)\vec{A}_{\vec{G}}-\\ \qquad(\vec{k}-\vec{G})\left((\vec{k}-\vec{G})\vec{A}_{\vec{G}}\right)=k_0^2\varepsilon_{\vec{G}}^*\vec{A}_0\end{cases} \qquad (5)$$

and are related to an external fields through Maxwell's boundary conditions. On the other hand, the equality to zero of the determinant of equations (5) gives us the dispersion relations $\omega=\omega(\vec{k})$ for eigenmodes. So, the problem of finding the reflection and transmission coefficients for a PhC plate becomes, in principle, quite clear.

3 NUMERICAL CALCULATION AND ANALYTICAL APPROACH

Now examine interaction between a monochromatic plane wave and 1D periodic structure of a thickness L, the permittivity being harmonically varied with the spatial period Λ

$$\varepsilon\left(z\right)=\varepsilon_0+\varepsilon_G\,\mathrm{e}^{iGz}+\varepsilon_G^*\,\mathrm{e}^{-iGz}, \qquad (6)$$

where $G=2\pi/\Lambda$ and $\varepsilon_G^*=\varepsilon_{-G}$. Let the thickness of the slab be

$$L=l_1+N\Lambda+l_2, \qquad (7)$$

with l_1 and l_2 being fractions of Λ at the front and the back of the structure, respectively, and N be the integer number of spatial periods (Figure 2).

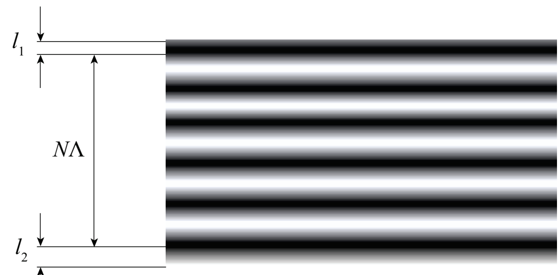

Figure 2: The structure under study: a sinusoidal profile of permittivity includes N periods, Λ, where N is integer and $l_1,l_2\le\Lambda$.

We calculated reflectance and transmittance of such structure with different parameters l_1, l_2, N solving equations obtained from Maxwell's boundary conditions. Two approaches were considered based (i) on the dynamical theory of diffraction and (ii) on the numerical transfer matrix technique, in order to compare them to each other and draw conclusion about validity of the analytical model when describing the reflectance and transmittance spectra.

As a result, it was found that the dynamical theory of diffraction describes correctly the spectra in the vicinity of a single photonic band-gap as compared with the computations based on the transfer matrix technique, if

$$l_1 + l_2 = \Lambda \text{ or } l_1 = l_2 . \quad (8)$$

In all other cases, conspicuous contradiction between analytical and numerical approaches takes place. It was shown analytically that

$$R + T = 1 + F(l_1, l_2), \quad (9)$$

where R is reflectance, T is transmittance and

$$F(l_1, l_2) \sim [\cos(Gl_1) - \cos(Gl_2)] \quad (10)$$

Figures 3 and 4 show, as an example, some results of computations of the reflectance and transmittance, respectively, when normal incidence of light on the plane surface of the structure is considered. The parameter values are taken close to that for an opal-like polystyrene PhC ($\varepsilon_0 = 2.127$, $|\varepsilon_G| = 0.135$) (Bazhenova *et al.*, 2007). It can be noticed that at the conditions (8) both approaches give practically the same results (Figure 3) independent on N, among them the value $N = 0$. If permittivity is symmetric with respect to the middle plane of the structure ($l_1 = l_2$), this conclusion is valid at any thickness L of the slab including the limiting case $L \to 0$.

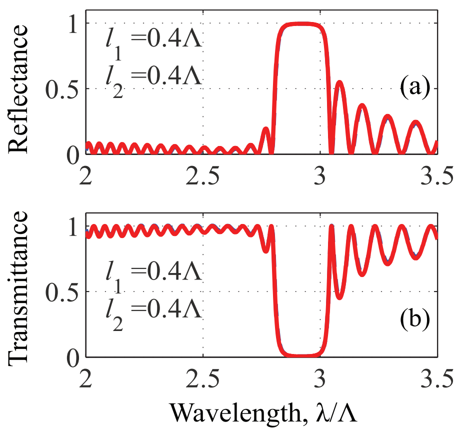

Figure 3: Reflectance and transmittance spectra at normal incidence of light on the PhC-plate (the number of the spatial periods, Λ, is N=30): (a,b) $l_1 = l_2$, (c,d) $l_1 + l_2 = \Lambda$. Red solid curves correspond to the dynamical model; blue dotted curves are computed with the transfer matrix technique.

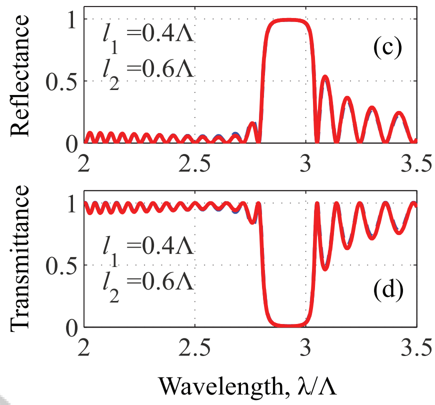

Figure 3: Reflectance and transmittance spectra at normal incidence of light on the PhC-plate (the number of the spatial periods, Λ, is N=30): (a,b) $l_1 = l_2$, (c,d) $l_1 + l_2 = \Lambda$. Red solid curves correspond to the dynamical model; blue dotted curves are computed with the transfer matrix technique (cont.).

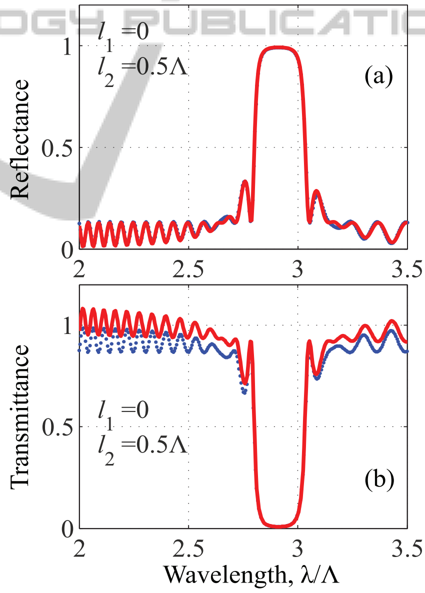

Figure 4: Reflectance (a) and transmittance (b) spectra at normal incidence of light on the PhC-plate (the number of the spatial periods, Λ, is $N = 30$): here the conditions (8) are not satisfied. Red solid curves correspond to the dynamical model; blue dotted curves are computed with the transfer matrix technique.

When the conditions (8) are not fulfilled, the analytical approach does not agree well with the numerical one (Figure 4), which is most pronounced in the case of transmission spectra. Moreover, the transmittance exceeds unity on some frequencies, which is in contradiction with the energy balance principle.

4 CONCLUSIONS

The reflectance and transmittance spectra have been calculated within two approaches based on the dynamical theory of diffraction as applied to 1D photonic crystals and on the numerical modeling using the transfer matrix technique. The dynamical theory is shown to be correct if a photonic crystal plate is symmetric in its dielectric properties about plate boundaries or the thickness of the plate is a multiple of the spatial period of the structure. The conditions obtained are consistent with the energy balance and time-reversal symmetry considerations.

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