Multiple Bragg diffraction effects in reflection spectroscopy of three-dimensional photonic crystals

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Abstract

We report the results of the theoretical and experimental studies of Bragg reflection spectra for three-dimensional photonic crystals possessing high dielectric contrast, with emphasis on the multiple Bragg diffraction effects. Opal-like photonic crystals made up of polystyrene microspheres are used as an example in our measurements. Numerical calculations of the reflection contours performed on the basis of the dynamical diffraction theory show a good agreement with the experimental data if a uniaxial strain along the sedimentation direction [111] of the opal crystal lattice is accounted for. We also demonstrate theoretically that the multiple Bragg diffraction effects can be observed at any angle of incidence, depending on the magnitude of the strain.

1. Introduction

Photonic band gap (PBG) metamaterials or photonic crystal (PhC) structures are considered to be promising materials for optoelectronics and nanophotonics [1, 2]. Such structures attract also much attention in up-to-date studies due to the fundamental scientific problems which come about in attempting to explain PhC mediated optical phenomena [3]. In this work, the Bragg reflection spectra of three-dimensional (3D) opal-like PhCs are studied taking into account the multiple Bragg diffraction (MBD) [4] and a strain induced anisotropy of the opal crystal lattice. We have suggested a crucially new approach to the analysis and quantitative description of the Bragg reflection complex-shape contour which appears due to the MBD effects. Our method is based on the dynamical multiple diffraction theory generalized to the case of high dielectric contrast of a 3D spatially periodic medium and allows one to calculate and analyze in a simple way the Bragg reflection spectra.

2. Experimental

Experimentally, we studied the opal-like PhC films prepared from monodisperse polystyrene spheres (280 nm in diameter) by sedimentation onto the silica glass substrates. The typical film thickness ranged from 23 to 26 monolayers. The spectra were measured at different incidence angles for *s*-polarized light, the reflecting surface plane being parallel to the (111) planes.

The experimental Bragg reflection spectra for different incidence angles θ are shown in Fig. 1. In general terms, the Bragg reflectance peak position as a function of θ follows from Bragg's law: with increasing θ the peak moves toward the short-wave range. However, as this takes place within the narrow angle range from about 50° to 60°, a doublet structure appears in the reflectance peak. As detailed measurements show, the doublet structure is shaped by the reflectance dip moving toward the long-wave region with increasing θ. The appearance of the doublet structure is indicative of a simultaneous resonant diffraction of light from at least two families of crystal planes non-parallel to each other.

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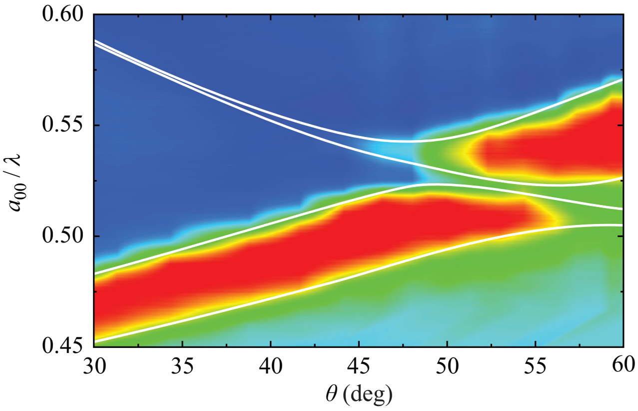

Fig. 1: Experimental spectra of Bragg reflection from an opal-like photonic crystal (made up of polystyrene spheres) with the reflecting surface (111) for *s*-polarized light at different incidence angles θ. The solid curves are the edges of the photonic stop-bands as a function of θ taken from the calculated dispersion curves. $a_{00} = 280$ nm is the distance between the neighboring particles of the structure in the lateral plane, λ is the free-space wavelength of light. Blue and red colors on the contour plot correspond to minimum and maximum values of the reflection coefficient, respectively.

3. Theoretical model

The eigenmode dispersion curves and reflection spectra are calculated using the dynamical multiple diffraction theory within the framework of three-band mixing approximation. Calculations of the reflection spectra are performed with an account of the $\omega(\boldsymbol{K})$ dispersion relations for the electromagnetic modes excited inside a semi-infinite PhC. The Maxwellian boundary conditions of continuity of tangential components for electric and magnetic fields are assumed to be held so that the fields in the surface plane are matched for each spatial Fourier component.

The calculated Bragg reflection spectra for a semi-infinite opal-like PhC at different incidence angles θ are shown in Fig. 2(*a*). Spectral behavior of the peculiarities in the theoretical spectra correlates well with the results of our experiments. The dispersion curves of eigenmodes in the semi-infinite PhC at the incidence angle $\theta = 53°$ are shown in Fig. 2(*b*). As can be seen from Fig. 2(*b*), the dip in the reflection contour arises when additional modes associated with the $(11\bar{1})$ crystal planes (non-parallel to the lateral surface of PhC) are excited.

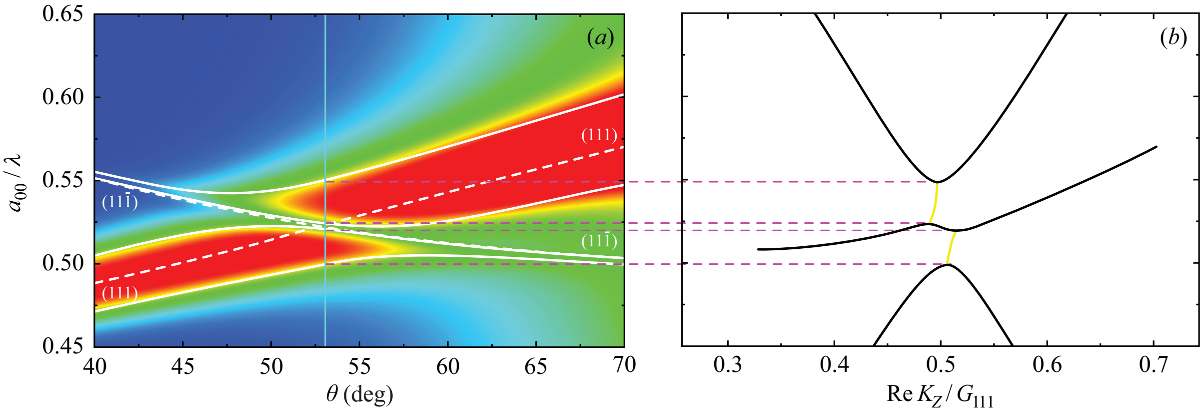

Fig. 2: Calculated are Bragg reflection spectra (*a*), at different incidence angles θ, and the electromagnetic eigenmode dispersion curves (*b*), at the incidence angle $\theta = 53°$, both for a semi-infinite photonic crystal. The solid curves correspond to the edges of the photonic stop-bands taken from the dispersion curves. The dashed curves are calculated within the "empty lattice" approximation using Eq. (1) and Eq. (2). The distance between the neighboring particles of the structure in the lateral plane is $a_{00} = 280$ nm, the average permittivity is $\varepsilon_0 = 2.185$, the coefficient of uniaxial compression is $\eta = 0.94$. λ is the free-space wavelength of light, Re K_Z is the projection of the real part of the mode wave vector onto the normal to the surface, and G_{111} is the length of the reciprocal lattice vector along the [111] direction (*Z* axis).

Spectral position of the dip on the calculated Bragg reflection contour for the face-centered cubic lattice exposed to a uniaxial compression along the [111] direction can be estimated in the limit of very low dielectric contrast (the "empty lattice" approximation) [5],

$$\lambda_{(11\bar{1})} = a_{00}\sqrt{6}\eta(\sqrt{2}\eta\sin\theta + \sqrt{\varepsilon_0 - \sin^2\theta})/(2\eta^2+1)\,, \tag{1}$$

where a_{00} is the distance between the neighboring particles of the structure in the lateral plane, $\varepsilon_0 = \varepsilon_a f + \varepsilon_b(1 - f)$ is the average permittivity of PhC assembled from the spheroids of permittivity ε_a (for polystyrene $\varepsilon_a = 2.522$) and pores with permittivity ε_b (for vacuum $\varepsilon_b = 1$), f is the volume filling factor of the spheroids in PhC, and η is the coefficient of a uniaxial (along the [111] direction) compression. In fact, to the same approximation, Bragg's formula for spectral position of the reflection peak is derived,

$$\lambda_{(111)} = a_{00}\sqrt{8/3}\eta(\sqrt{\varepsilon_0 - \sin^2\theta}) . \tag{2}$$

In the narrow interval of incidence angles the additional electromagnetic mode associated with the oblique $(11\bar{1})$ crystal planes is located within the main photonic stop-band (between the dispersion curves created by the periodicity along the [111] direction). In such a situation, Eq. (1) describes the dip spectral position well. Beyond the main stop-band, the spectral singularity due to light diffraction from the $(11\bar{1})$ planes changes its shape and appears as a peak that decreases in intensity with deflection from the incidence angle at which the MBD is most pronounced. In this case, Eq. (1) gives more precisely the spectral position of the additional peak but it is failed when describing the dip position.

It is worth noting that for the PhCs with a strong uniaxial compression the MBD can be observed at small angles of incidence. In particular, for the case of $\eta = 0.5$ the MBD condition is fulfilled at the normal incidence of light. The reflection spectra calculated for this case are shown in Fig. 3. As we see, the doublet structure is manifested for the angle of incidence $\theta = 0°$.

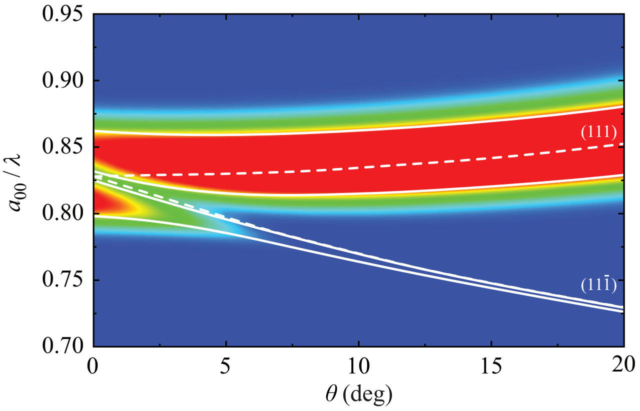

Fig. 3: Calculated are Bragg reflection spectra, at different incidence angles θ, for a semi-infinite photonic crystal with the strong uniaxial compression $\eta = 0.5$. The solid curves correspond to the edges of the photonic stop-bands taken from the dispersion curves. The dashed curves are calculated within the "empty lattice" approximation using Eq. (1) and Eq. (2). Except for the η value, other parameter values are the same as in Fig. 2. λ is the free-space wavelength of light.

4. Conclusion

We have studied the Bragg reflection spectra of opal-like PhCs to clarify the physical mechanisms responsible for the shaping of the spectra when the MBD significantly modifies them. The experimental spectra were analyzed within the dynamical theory of the multiple diffraction of light in the three-band mixing approximation. Numerical calculations of the Bragg reflection contours are performed, and those are compared with the dispersion curves of the electromagnetic field eigenmodes for spatially confined opal-like PhCs. A possibility to observe MBD effects at the normal incidence of light for the opal-like PhCs exposed to a strong uniaxial compression has been demonstrated.

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