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Physica B 338 (2003) 178–181

PHYSICA B

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Photonic crystal slabs

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Abstract

The dispersion relation, density of states, and wave functions of the electromagnetic guided modes of a free standing photonic crystal slab are computed. The solution of Maxwell's equations are obtained from a self-consistent matrix eigenvalue problem solved by a fast computer routine. Comparison is made with experiments on an electrically injected photonic crystal microcavity light source.

PACS: 42.55.Tv; 42.70.Qs; 42.55.Sa; 42.60.Da

Keywords: Photonic crystals; Band structure; Density of states

Recently there has been great interest in the properties of photonic crystal slabs [1–6]. These are dielectric slabs that exhibit a two-dimensionally periodic dielectric constant in the plane of the slab. A number of experimental and theoretical (simulation) studies of these structures have appeared, along with suggestions of potential technological applications [1–6]. In this paper, an analytical treatment is presented for the waveguide modes of a photonic crystal slab embedded in a uniform homogeneous dielectric medium. The method is based on reducing the equations for the electric field to a self-consistent matrix eigenvalue problem in which the matrix of the eigenvalue problem depends on its own eigenvalue. The resulting problem is solved by standard methods using an iterative routine which converges to a self-consistent solution.

A photonic crystal slab is located in the region $-d < x_3 < d$ and formed from a periodic array of cylinders with dielectric constant ε_a and radii R which are embedded in a background of dielectric constant ε_b. The axes of the cylinders are parallel to the x_3-axis and lie in the x_1–x_2 plane on a hexagonal lattice at sites given by $\mathbf{x}_{\parallel}(l) = l_1\mathbf{a}_1 + l_2\mathbf{a}_2$, where $\mathbf{a}_1 = a\hat{x}_1$, $\mathbf{a}_2 = a(\frac{1}{2}\hat{x}_1 + \frac{\sqrt{3}}{2}\hat{x}_2)$, l_1 and l_2 range over the integers, and a is the lattice constant. The dielectric constant outside of the slab ($x_3 > d$ or $x_3 < -d$) is uniform and isotropic and denoted by ε_0.

Eliminating the magnetic field between Ampere and Faraday laws and assuming a time-dependent electric field of the form $\mathbf{E}(\mathbf{x};t) = \mathbf{E}(\mathbf{x}|\omega)\exp(-\mathrm{i}\omega t)$ gives

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{x}|\omega) = \varepsilon(\mathbf{x})\left(\frac{\omega}{c}\right)^2 \mathbf{E}(\mathbf{x}|\omega) \qquad (1)$$

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doi:10.1016/S0921-4526(03)00482-4

for the wave equation of the electric field inside and outside the photonic crystal slab. (Here $\varepsilon(\mathbf{x})$ is the position-dependent dielectric constant.) To determine the eigenvalues and eigenvectors of the system in Eq. (1), $\mathbf{E}(\mathbf{x}|\omega)$ is represented by a series of linearly independent functions based on the modes of the uniform slab waveguide. The coefficients in the expansion are determined by substitution in Eq. (1).

Let us summarize the forms of the modes for a waveguide described by Eq. (1) with $\varepsilon(\mathbf{x}_{\|}) = \varepsilon_j$ for $-d < x_3 < d$ and $\varepsilon(\mathbf{x}) = \varepsilon_0$ otherwise (see Ref. [7] for details). The TE waveguide modes are of the form

$$E_i(\mathbf{x}|\omega) = \hat{t} f^{(l)}(\mathbf{k}, s, x_3)\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_{\|}} \tag{2}$$

where $i = 1$ or 2, $\hat{t} = [1/(k_1^2 + k_2^2)^{1/2}](k_2, -k_1)$, and $l = \mathrm{e}$ or o indicates the even or odd symmetry functions in x_3. For the even TE modes

$$f^{(\mathrm{e})}(\mathbf{k}, s, x_3) = \begin{cases} \cos q_s x_3 & \text{if } -d < x_3 < d, \\ \cos q_s d \mathrm{e}^{-q(x_3-d)} & \text{if } x_3 > d, \\ \cos q_s d \mathrm{e}^{q(x_3+d)} & \text{if } x_3 < -d, \end{cases} \tag{3}$$

where $q(\mathbf{k}) = [k_1^2 + k_2^2 - \varepsilon_0\,\omega^2/c^2]^{1/2}$ and $q_s \tan q_s d = q$. For odd TE modes

$$f^{(\mathrm{o})}(\mathbf{k}, s, x_3) = \begin{cases} \sin q_s x_3 & \text{if } -d < x_3 < d \\ \sin q_s d \mathrm{e}^{-q(x_3-d)} & \text{if } x_3 > d \\ -\sin q_s d \mathrm{e}^{q(x_3+d)} & \text{if } x_3 < -d \end{cases} \tag{4}$$

where $q_s \cot q_s d = -q$. The TM modes are of the form

$$D_i(\mathbf{x}|\omega) = \hat{n}_i \frac{\mathrm{d}h^{(l)}(\mathbf{k}, s, x_3)}{\mathrm{d}x_3}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_{\|}}, \tag{5}$$

where $i = 1$ or 2, $\hat{n} = (\hat{n}_1, \hat{n}_2) = [1/(k_1^2 + k_2^2)^{1/2}](k_1, k_2)$, and

$$D_3(\mathbf{x}|\omega) = -\mathrm{i}|\mathbf{k}|\hat{x}_3 h^{(l)}(\mathbf{k}, s, x_3)\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_{\|}} \tag{6}$$

and $l = \mathrm{e}$ or o indicates even or odd functions x_3. Here for the even TM modes

$$h^{(\mathrm{e})}(\mathbf{k}, s, x_3) = \begin{cases} \cos r_s x_3 & \text{if } -d < x_3 < d, \\ \cos r_s d \mathrm{e}^{-q(x_3-d)} & \text{if } x_3 > d, \\ \cos r_s d \mathrm{e}^{q(x_3+d)} & \text{if } x_3 < -d, \end{cases} \tag{7}$$

where $r_s \tan r_s d = (\varepsilon_j/\varepsilon_0)q$, and for the odd TM modes

$$h^{(\mathrm{o})}(\mathbf{k}, s, x_3) = \begin{cases} \sin r_s x_3 & \text{if } -d < x_3 < d, \\ \sin r_s d \mathrm{e}^{-q(x_3-d)} & \text{if } x_3 > d, \\ -\sin r_s d \mathrm{e}^{q(x_3+d)} & \text{if } x_3 < -d, \end{cases} \tag{8}$$

where $r_s \cot r_s d = -(\varepsilon_j/\varepsilon_0)q$. If ω is the frequency of a waveguide mode, the modal solutions given above are a complete orthogonal set [7].

If ω in Eqs. (2)–(8) is the frequency of a mode in the photonic crystal slab rather than in the waveguide slab, the functions form a linearly independent set. The general form of the solutions of Eq. (1) for the photonic crystal slab are then represented as

$$\vec{E}_{\|}(\mathbf{x}|\omega) = \sum_{\mathbf{G},n} \exp[\mathrm{i}(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}_{\|}]\mathbf{E}_{\|}(\mathbf{k}+\mathbf{G}, n, x_3|\omega), \tag{9}$$

where

$$\begin{aligned} \mathbf{E}_{\|}(\mathbf{k}+\mathbf{G}, n, x_3|\omega) = \Bigg[& \frac{(k_2+G_2)\hat{x}_1 a_1(\mathbf{k}+\mathbf{G}, n) - (k_1+G_1)\hat{x}_2 a_2(\mathbf{k}+\mathbf{G}, n)}{[(k_1+G_1)^2 + (k_2+G_2)^2]^{1/2}} f^{(l)}(\mathbf{k}+\mathbf{G}, n, x_3) \\ & + \frac{(k_1+G_1)\hat{x}_1 b_1^{(a)}(\mathbf{k}+\mathbf{G}, n) + (k_2+G_2)\hat{x}_2 b_2^{(a)}(\mathbf{k}+\mathbf{G}, n)}{[(k_1+G_1)^2 + (k_2+G_2)^2]^{1/2}} \frac{1}{\varepsilon_a'(x_3)} \frac{\mathrm{d}h_a^{(l')}}{\mathrm{d}x_3}(\mathbf{k}+\mathbf{G}, n, x_3) \\ & + \frac{(k_1+G_1)\hat{x}_1 b_1^{(b)}(\mathbf{k}+\mathbf{G}, n) + (k_2+G_2)\hat{x}_2 b_2^{(b)}(\mathbf{k}+\mathbf{G}, n)}{[(k_1+G_1)^2 + (k_2+G_2)^2]^{1/2}} \frac{1}{\varepsilon_b'(x_3)} \frac{\mathrm{d}h_b^{(l')}}{\mathrm{d}x_3}(\mathbf{k}+\mathbf{G}, n, x_3) \Bigg], \end{aligned} \tag{10}$$

and

$$E_3(\mathbf{x}|\omega) = -\mathrm{i}\sum_{\mathbf{G},n} \exp[\mathrm{i}(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}_{\|}] \\ E_3(\mathbf{k}+\mathbf{G},n,x_3|\omega)\hat{x}_3, \quad (11)$$

where

$$E_3(\mathbf{k}+\mathbf{G},n,x_3|\omega) \\ = |\mathbf{k}+\mathbf{G}|\left[b^{(a)}(\mathbf{k}+\mathbf{G},n)\frac{1}{\varepsilon'_a(x_3)}h_a^{(l')}(\mathbf{k}+\mathbf{G},n,x_3) \right. \\ \left. + b^{(b)}(\mathbf{k}+\mathbf{G},n)\frac{1}{\varepsilon'_b(x_3)}h_b^{(l')}(\mathbf{k}+\mathbf{G},n,x_3)\right] \\ + \left(\frac{a^{(a)}(\mathbf{k}+\mathbf{G},n)}{\varepsilon'_a(x_3)} + \frac{a^{(b)}(\mathbf{k}+\mathbf{G},n)}{\varepsilon'_b(x_3)}\right) \\ \times \frac{\mathrm{d}f^{(l)}}{\mathrm{d}x_3}(\mathbf{k}+\mathbf{G},n,x_3) \quad (12)$$

for $(l,l') = (\mathrm{o},\mathrm{e})$ or (e,o), and the expansion coefficients $a_i(\mathbf{k}+\mathbf{G},n)$, $b_i^{(a)}(\mathbf{k}+\mathbf{G},n)$, $b_i^{(b)}(\mathbf{k}+\mathbf{G},n)$ for $i = 1,2,3$ are determined from Eq. (1). Here the subscripts a and b on the h indicate the functions computed from Eqs. (7) and (8) for $\varepsilon_j = \varepsilon_a$ and $\varepsilon_j = \varepsilon_b$, respectively, and $\varepsilon'_j(x_3) = \varepsilon_j$ within the slab but $= \varepsilon_0$ outside the slab. The wave vector $\mathbf{k}$ in the x_1–x_2 plane is restricted to the first Brillouin zone, the sums on $\mathbf{G}$ are over reciprocal lattice vectors, and $n \geqslant 0$ indexes the functions defined in Eqs. (3), (4), (7), and (8). In Eqs. (9) and (11) and Eqs. (2)–(8), $q(\mathbf{k}+\mathbf{G}) = [(k_1+G_1)^2 + (k_2+G_2)^2 - \varepsilon_0\omega^2/c^2]^{1/2}$, where ω is the eigenfrequency of the photonic crystal slab mode being computed.

In Eqs. (9)–(12) the terms involving the functions h are generalizations of the TM modes of the waveguide slab, maintaining the continuity of E_1, E_2, D_3 at the slab surfaces. The terms involving the f functions generalize the TE waveguide slab solutions. In this case, taking $a_1(\mathbf{k}+\mathbf{G},n) \neq a_2(\mathbf{k}+\mathbf{G},n)$ requires the addition to D_3 of terms proportional to $\mathrm{d}f/\mathrm{d}x_3$. This comes from the relation $\mathbf{D} \propto \nabla \times \nabla \times \mathbf{E}$. The f functions and their derivatives maintain the continuity of E_1, E_2, D_3 at the slab surface.

Results for the free standing photonic slab are obtained using the expansions in Eqs. (9)–(12). The $f(h)$ functions have values of $q_s(r_s)$ which cluster about $n\pi/d$ and $(2n-1)\pi/2d$ for n, a positive integer. (Note: The free standing photonic crystal slab, as is also the case with the free standing slab waveguide, has no modal solutions with q_s or $r_s = 0$.) The solutions separate into those written in terms of f functions and those written in terms of h functions. Solutions with q_s clustered about $(2n-1)\pi/2d$ have $\mathbf{E}_{\|}$ (E_3) even (odd) functions of x_3. Solutions with r_s clustered about $(2n-1)\pi/2d$ have $\mathbf{E}_{\|}$ (E_3) odd (even) functions of x_3. For the solutions with q_s and r_s clustered about $n\pi/d$, the symmetry of $\mathbf{E}_{\|}$ and $\mathbf{E}_3$ is reversed.

In Fig. 1, density of states are shown for the $q_s \approx \pi/2d$ and $r_s \approx \pi/2d$ modes in a free standing photonic crystal slab characterized by $\varepsilon_a = \varepsilon_0 = 1$, $\varepsilon_b = 12.6$, $d = 0.438a$, and $R = 0.325a$. These modes have the smallest wave-number component in the x_3 direction. There are many other modes with larger q_s or r_s clustering about $n\pi/d$ or $(2n-1)\pi/2d$ for n, a positive integer. These modes, having more spatial oscillations in the fields along the x_3 directions, are discussed elsewhere. The parameters of Fig. 1 are chosen for a comparison with experiment [6].

Recently, an electronically injected photonic crystal microcavity light source has been fabricated based on the photonic crystal slab geometry treated above [6]. The configuration used in the design of the light source does not exactly involve a free standing photonic crystal as the photonic

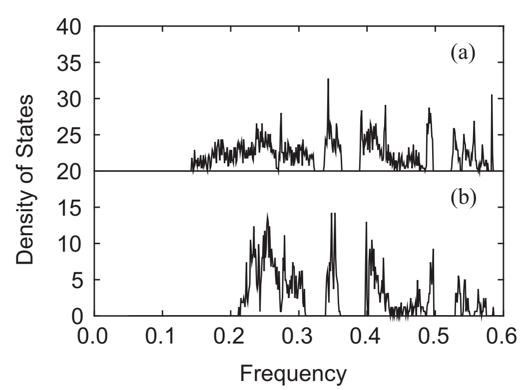

Fig. 1. Density of states versus frequency in units of a/λ of the free standing photonic crystal slab for: (a) $q_s \approx \pi/2d$ modes shifted upward by 20 and (b) $r_s \approx \pi/2d$ modes.

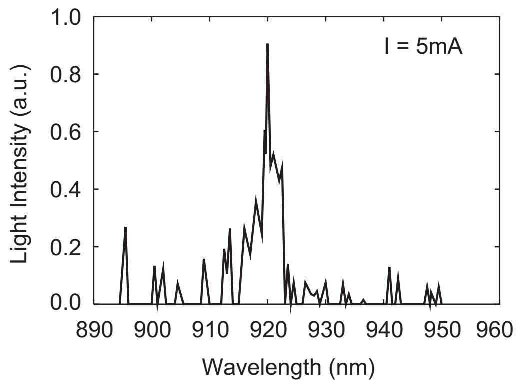

Fig. 2. Measured spectral output of microcavity light source in Ref. [6].

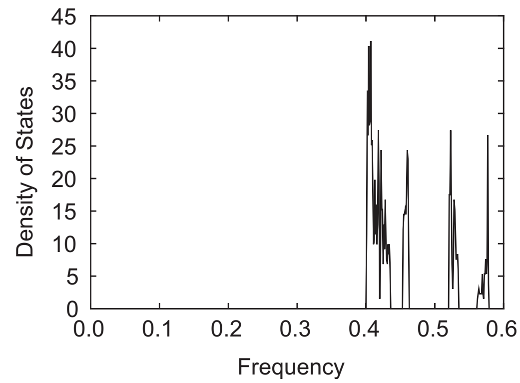

Fig. 3. Density of states versus frequency in units of a/λ of the photonic crystal slab between perfectly conducting plates for $q_s = r_s = \pi/d$.

crystal slab lies on a GaAs substrate, and contains a heterostructure for the generation of light. Nevertheless in the following, a comparison is made between the above theory results and emission measurements on the light source. For details of design and experiment see Ref. [6].

In the light source geometry, light is emitted from the photonic crystal slab along the x_3-axis in a direction away from the GaAs substrate. The light is constrained from propagating in the x_1–x_2 plane by the photonic crystal band gap. At stop gap frequencies either the light cannot propagate in the x_1–x_2 plane or it remains as a leaky wave with a propagation component in the x_3 direction. Fig. 2 shows the intensity emitted from the source as a function of wavelength. The peak at 920 nm corresponds to $a/\lambda = 0.435$ and should be largest in the stop gap of the photonic crystal slab.

In Fig. 1, the results for the free standing photonic crystal slab show a clear gap below $a/\lambda = 0.4$. This is a little off the $a/\lambda = 0.435$ peak in Fig. 2, but in the presence of the GaAs substrate and heterostructure, an upward shift in the band structure is expected. In particular, such a shift is seen in the $\varepsilon_0 \to -\infty$ limit of the theory for modes below the vacuum light cone. This limit corresponds to placing the photonic crystal slab between perfectly conducting plates.

The $\varepsilon_0 \to -\infty$ limit is found to give a good semi-quantitative representation of the gross features of the free standing photonic crystal slab modes below the vacuum light cone. In Fig. 3, the density of states below the light cone in vacuum of the photonic crystal slab between perfectly conducting plates for $q_s = r_s = \pi/d$ is given. A large gap is clearly seen between $a/\lambda = 0.437$ and 0.453, and a downward shift of this gap is expected when a free standing surface is present. If the light from the source is of this mode, the dependence on x_3 is either approximately $\sin(\pi/d)x_3$ or $\cos(\pi/d)x_3$.

Acknowledgements

This work was supported by Army Research Office Grant DAAD 19-01-1-0527 and Office of Naval Research Grant N00014-96-1-0024.

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