

Guided modes in photonic crystal slabs

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We analyze the properties of two-dimensionally periodic dielectric structures that have a band gap for propagation in a plane and that use index guiding to confine light in the third dimension. Such structures are more amenable to fabrication than photonic crystals with full three-dimensional band gaps, but retain or approximate many of the latter's desirable properties. We show how traditional band-structure analysis can be adapted to slab systems in the context of several representative structures, and describe the unique features that arise in this framework compared to ordinary photonic crystals. [S0163-1829(99)00832-2]

I. INTRODUCTION

The discovery of photonic crystals, periodic dielectric materials with a photonic band gap, has opened up new methods for controlling light, leading to proposals for many novel devices.¹ Straightforward application of these results to three dimensions requires a structure with a three-dimensional band gap. Fabricating such structures, however, has been a challenge because they tend to have complex three-dimensional connectivity and strict alignment requirements.²⁻⁵ Such designs have been the subject of many recent developments.⁶⁻¹⁰ An alternative system, the photonic crystal slab, has been proposed¹¹⁻¹⁸ that promises easier fabrication using existing techniques. This is a dielectric structure that has only two-dimensional periodicity and uses index guiding to confine light in the third dimension. Photonic crystal slabs retain or approximate many of the desirable properties of true photonic crystals, but at the same time are much more easily realized at submicron lengthscales. We present in this paper a novel band-structure analysis of photonic crystal slabs, providing a systematic understanding of many important features of these systems.

In many ways, photonic crystal slabs are analogous to two-dimensional photonic crystals, such as those depicted in Fig. 1, and this analogy aids greatly in the visualization and analysis of slab systems. Two-dimensional calculations, however, cannot be applied directly to three-dimensional slab structures. In particular, the band structure computed for a two-dimensional structure, as shown in Fig. 2, applies in three dimensions only to a structure that is infinitely "extruded" in the third dimension. Moreover, these two-dimensional bands correspond only to states that have no wave-vector component in the vertical direction (perpendicular to the plane of periodicity). The inclusion of vertical wave vectors produces a continuum of states depicted by the shaded region in Fig. 2, destroying the band gap of the two-dimensional structure. The restriction of a slab to finite height recreates the band gap in the guided modes of a slab, but also forces a new analysis of the system that is fundamentally three-dimensional and distinct from the two-

dimensional calculations. New issues such as slab thickness, index contrast with the substrate, and mirror symmetry assume a prominent role in determining the properties of photonic crystal slabs.

The paper is structured as follows. We first outline the numerical methods that were used in our calculations. We then introduce slab band structures for two characteristic systems, the slab analogues of Fig. 1, suspended in air. The selection of an appropriate slab thickness is discussed, and an estimate for the optimal slab thickness is derived using a variational approach. Finally, the effects of different backgrounds, the regions above and below the slab, are examined in the context of the two example structures. Band structures are given for solid, periodic, and symmetry-breaking backgrounds.

II. COMPUTATIONAL METHOD

The computation of a slab band structure is performed in two stages. First, the states of a slab are computed in a periodic cell. Then, the light cone is calculated and overlaid as an opaque region on the band diagram. The resulting nonobscured bands are the guided modes of the system, as described in the following section.

The eigenstates of the slab are computed using preconditioned conjugate-gradient minimization of the Rayleigh quo-

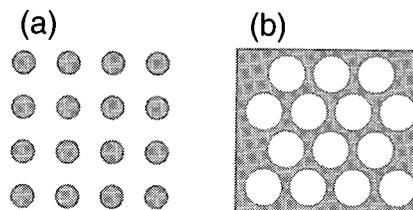


FIG. 1. Two-dimensional photonic crystals. (a) Square lattice of dielectric rods in air, with lattice constant a and radius $0.2a$. (b) Triangular lattice of air holes in dielectric, with lattice constant a and radius $0.45a$. In both cases, the dielectric constant of the high-index material is 12.

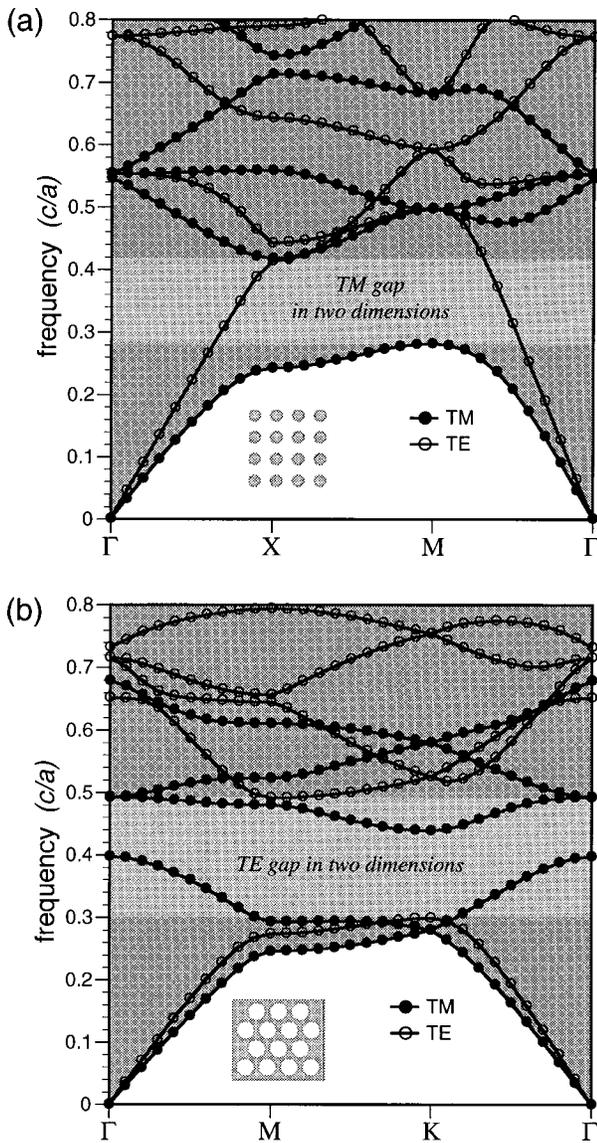


FIG. 2. Band diagrams for the photonic crystals from (a) Fig. 1(a) and (b) Fig. 1(b). The shaded region indicates the frequencies of states introduced when vertical propagation (i.e., perpendicular to the plane of periodicity) is permitted.

tient in a plane-wave basis.¹⁹ Such a computation requires a periodic cell. The slab is already two-dimensionally periodic, and we impose a three-dimensional periodicity by assuming a periodic sequence of slabs separated by a sufficient amount of background region. Because the guided modes are localized within the slab, the addition of periodic slabs at large intervals does not affect their frequencies noticeably. The nonguided modes are affected, but since they fall inside the light cone their exact frequencies are inconsequential.

The light cone is a continuous region indicating all possible frequencies of the bulk background. It is sufficient to compute only the lower boundary of the light cone, since all higher frequencies are automatically included. In the case of a uniform background region, the boundary is simply the wave vector divided by the index. For a periodic background, the boundary is the lowest band of the corresponding two-dimensional system, as is discussed in a later section, and is computed using the two-dimensional version of the

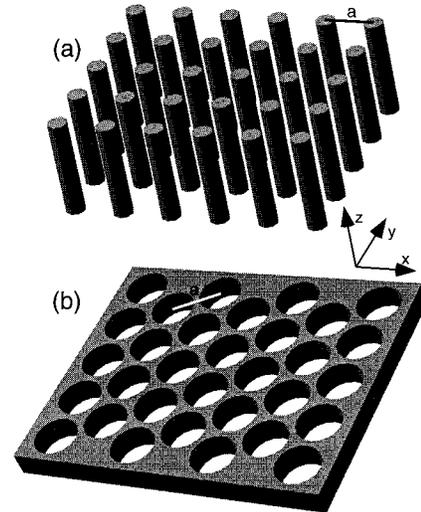


FIG. 3. Photonic crystal slabs analogous to the two-dimensional structures from Fig. 1. (a) Square lattice of rods in air with height $2.0a$. (b) Triangular lattice of holes in a dielectric slab with thickness $0.6a$. (Other parameters are as in Fig. 1.) Both slabs are suspended in air.

method in Ref. 19. In all cases, the light cone is depicted with a uniform shading that does not reflect the varying density of states in this region.

III. PHOTONIC CRYSTAL SLAB BAND STRUCTURES

Shown in Fig. 3 are the photonic crystal slab analogues of the two-dimensional structures from Fig. 1. These two systems, a square lattice of dielectric rods in air and a triangular lattice of air holes in a solid dielectric slab, embody the two basic topologies of two-dimensional crystals, and are characteristic of many possible slab structures. [An air-bridge structure similar to Fig. 3(b) was fabricated in Ref. 18.] As seen from Fig. 2, in two dimensions the rod structure has a band gap in the TM modes (magnetic field in plane) and the hole structure has a band gap in the TE modes (electric field in plane). (The hole structure also has a small band gap in the TM modes, but we focus here on the more robust TE gap, which is larger and separates the lowest two TE bands.)

The corresponding projected band structures for the three-dimensional slab structures are shown in Fig. 4. These graphs, whose computation was discussed in the previous section, illustrate many features that are common to all photonic crystal-band diagrams.

Perhaps the most important feature of the projected band diagram, the element that distinguishes slabs from ordinary photonic crystals, is the light cone, a continuum of states indicated by a shaded region in the plot. The light cone consists of states, or radiation modes, that are extended infinitely in the region outside the slab; we refer to this region as the “background.” Guided modes, which are states localized to the plane of the slab, can only exist in the regions of the band diagram that are outside the light cone. The primary interest in the radiation modes lies in how they interact with and constrain these guided modes.

Any state that lies below the light cone in the band diagram cannot couple with modes in the bulk background. Thus, the discrete bands below the light cone are guided—

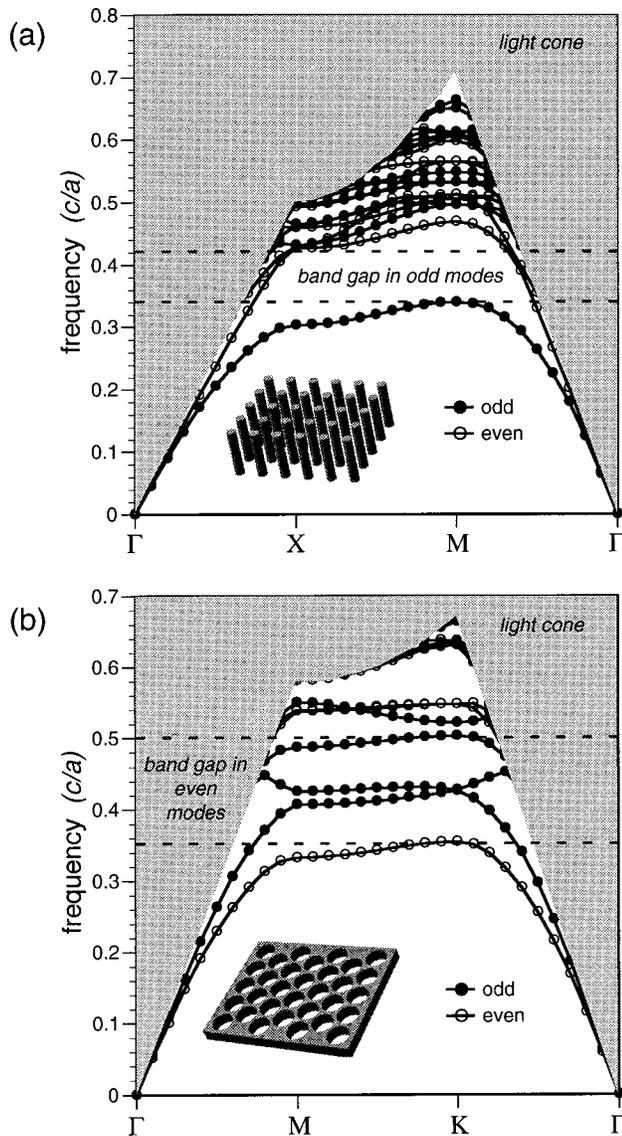


FIG. 4. Projected band diagrams corresponding to the two slabs in Fig. 3. Whether states are even or odd with respect to the horizontal mirror plane of the slab is indicated by open or filled circles, respectively.

the states are infinitely extended within the plane of the slab, but decay exponentially into the background region. This confinement is analogous to total internal reflection, and is due to the guided modes seeing a higher effective index in the slab than in the background regions (air, in this case). When a guided band reaches the edge of the light cone, it becomes a resonant state: it extends, albeit with low amplitude, infinitely far into the background, and cannot be used to permanently confine light within the slab. We restrict our discussion, and our use of the term “guided modes,” to truly localized states, which grow arbitrarily small as the distance from the slab becomes large.

The reason we refer to these systems as “photonic crystal” slabs is that, like their two-dimensional brethren, they have a band gap—but not of the traditional sort. A “band gap” in this case is a range of frequencies in which no *guided* modes exist. It is not a true band gap because there are still radiation modes at those frequencies. Still, the lack of guided modes in the band gap gives rise to many of the

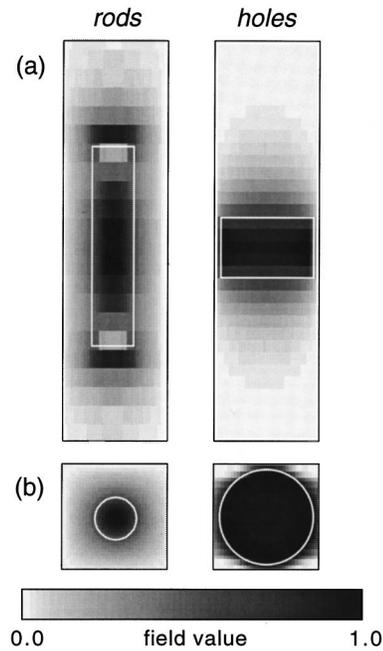


FIG. 5. Lowest-frequency states of the rod and hole structures from Fig. 3 at M and K , respectively, depicted in the unit cell. The shading indicates the z components of the electric and magnetic fields, respectively, which happen to be positive through the unit cell for these states. Outlines of the rods/holes are shown in white. (a) Vertical cross section. (b) Horizontal cross section. In both cases the cross-sections bisect the holes or rods.

same phenomena that occur in two-dimensional crystals, such as the ability to confine light in the plane to waveguides or resonators.¹⁵ (The presence of the radiation modes in the gap has the consequence that resonant cavity modes will eventually decay into the background.) The fact that light in the band gap of the slab is forbidden from propagating in the plane of the slab, and can only radiate into the background, was used in Ref. 13 to design an efficient light emitting diode (LED).

As in two dimensions, one is able to decompose the guided modes into two noninteracting classes. The lack of translational symmetry in the vertical direction, however, means that the states are not purely TM or TE polarized. Instead, due to the presence of a horizontal symmetry plane bisecting the slab, the guided bands can be classified according to whether they are even or odd with respect to reflections through this plane, and are indicated on the band diagram by hollow or filled circles, respectively. As shall be seen below, these even and odd states have strong similarities with TE and TM states, respectively, in two dimensions. (In fact, in the mirror plane itself, the even and odd states are purely TE, and TM, respectively.) It is not surprising, then, that the slab of rods has a gap in its odd modes [Fig. 4(a)], and the slab of holes has a gap in its even modes [Fig. 4(b)].

In Fig. 5, z -components of the electric and magnetic fields are shown for the lowest-order odd and even guided modes from the rod and hole slabs at the M and K symmetry points, respectively. It is apparent from these figures that these states are strongly guided within the thickness of the slab. Moreover, within the slab they are TM- and TE-like, and closely

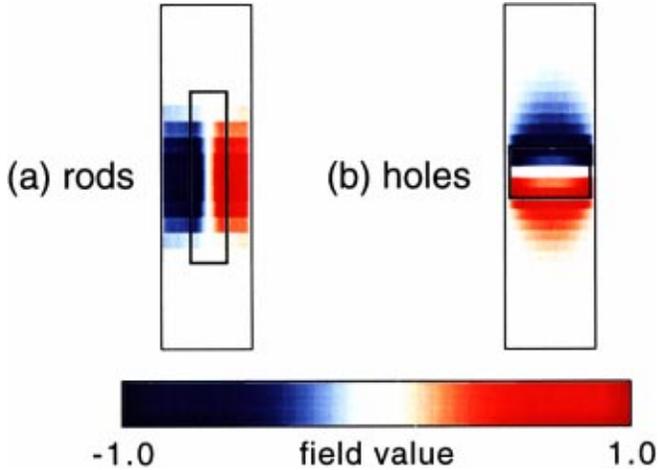


FIG. 6. (Color) (a) Vertical cross section of E_z for the first odd (TM-like) excited state at M in the rod structure from Fig. 4(a). (b) Vertical cross section of H_z for the first TE-like (but odd) excited state at K in the hole structure shown in Fig. 4(b).

resemble the corresponding states in the two-dimensional system.

Higher-order states in the slabs are formed in two ways. First, they can gain additional nodes or other structure in the horizontal plane, corresponding to higher-order states in the two-dimensional system. Second, they can be formed by adding vertical structure such as horizontal nodal planes. In the case of the rods, the lowest higher-order odd state is of the first type, and is depicted in Fig. 6(a). The second odd mode at the M point in the holes slab, as shown in Fig. 6(b), is of the second type—it corresponds to the lowest-order even mode modified by the addition of a single horizontal nodal plane. Note that adding a nodal plane bisecting the slab transforms a state from odd to even and vice versa, so even and odd higher-order modes are not necessarily TE-like and TM-like, respectively.

Higher-order modes of the second type do not correspond to excitations in the two-dimensional system, and are responsible for destroying the gap if the slab becomes too thick, as is discussed in the following section.

IV. EFFECTS OF SLAB THICKNESS

The slab thickness plays an important role in determining whether a photonic crystal slab has a band gap in its guided modes. Shown in Fig. 7 is a graph of the band gap size as a function of slab thickness for the rod and hole slabs from Fig. 3. The existence of an optimal thickness for each slab is easily understood. If the slab is too thick, then higher-order modes can be created with little energy cost by adding horizontal nodal planes. Such modes will lie only slightly above the lowest-order mode, preventing any gap. If the slab is too thin, then the slab will provide only a weak perturbation on the background dielectric constant. Guided modes will still exist, but they will hug the edge of the light cone and be only weakly guided; any gap will be miniscule. Below, we propose a method for estimating slab thicknesses that produces large gaps, and explain the sharp distinction seen in Fig. 7 between the optimal thicknesses for the rod and hole slabs.

We postulate that the optimal thickness will be on the

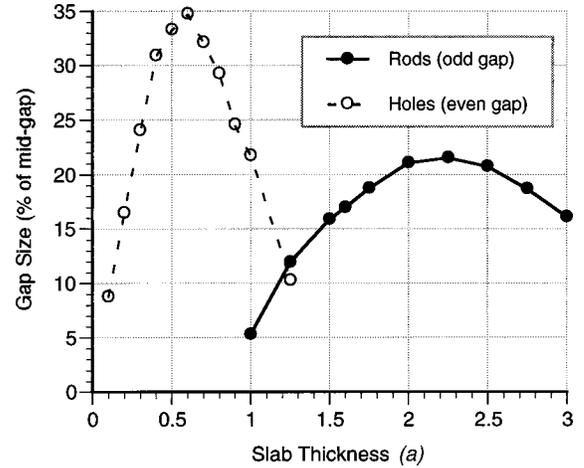


FIG. 7. Gap size (as a percentage of midgap frequency) versus slab thickness for the two slabs from Fig. 3.

order of half the two-dimensional gap-bottom wavelength. The justification for this is based on the fact that the wavelength is the lengthscale for variations in field amplitude at a given frequency. (We use the gap-bottom frequency instead of, say, midgap, because the state at the bottom of the gap is the basis for both the state at the lower edge of the slab gap and the excited states at upper edge.) If the slab thickness is a wavelength or more, then there will be little energy barrier to creating a higher-order state via a nodal plane. If the slab thickness is less than half a wavelength, on the other hand, then the mode cannot be strongly confined within the slab.

Only the frequency, rather than the wavelength, of the gap bottom is known, however. An effective dielectric constant must be determined in order to compute the corresponding wavelength. We accomplish this by constructing an estimate for the slab gap-bottom state using the two-dimensional wave function, and evaluating the dependence of its frequency expectation value on the vertical wavelength. The wave function can be approximated by:

$$|\tilde{H}\rangle = \int \vec{H}_0(x,y) e^{ikz} a(k) dk. \quad (1)$$

Here, \vec{H}_0 is the eigenfunction of the two-dimensional system at the lower edge of the gap. The $a(k)$ amplitudes are assumed to be chosen so that they produce a state strongly localized within the slab. A Fourier basis is used for the z dependence so that the vertical wave vector may be an explicit parameter. We have chosen this wave function based on our experience (e.g., in Fig. 5) that the lowest-order guided band in the slab system is similar in appearance to the corresponding two-dimensional state with the addition of vertical confinement. [We note that the field in Eq. (1) is not divergenceless, however.]

We now evaluate the energy (i.e., frequency) of this state. Since the state is assumed to be localized within the slab, the frequency should not be much affected if we evaluate it in an infinitely thick slab, which can be done exactly. (In the case shown in Fig. 5, more than 90% of the computed wave function's energy was found to lie within the height of the slab.) In this approximation, the frequency is found to be one of

$$\omega_{\text{TM}}^2 = \frac{\langle \tilde{H} | \vec{\nabla} \times \frac{1}{\varepsilon(x,y)} \vec{\nabla} \times | \tilde{H} \rangle}{\langle \tilde{H} | \tilde{H} \rangle} = \omega_0^2 + \frac{c^2 \langle k^2 \rangle}{\bar{\varepsilon}_{\text{TM}}} \quad (2)$$

$$\omega_{\text{TE}}^2 = \frac{\langle \tilde{E} | \vec{\nabla} \times \vec{\nabla} \times | \tilde{E} \rangle}{\langle \tilde{E} | \varepsilon(x,y) | \tilde{E} \rangle} = \omega_0^2 + \frac{c^2 \langle k^2 \rangle}{\bar{\varepsilon}_{\text{TE}}}, \quad (3)$$

where E represents the electric field, and ω_0 is the two-dimensional frequency. Equations (2) and (3) are equivalent only for divergenceless (transverse) fields. In the case of Eq. (1), which is not transverse, we use Eq. (2) for TM fields and Eq. (3) for TE fields, for simplicity of the resulting expression. In both cases, the vertical wavelength is related to frequency simply by an effective dielectric constant that depends upon the polarization of the corresponding two-dimensional state, and is given by

$$\bar{\varepsilon}_{\text{TE}} = \frac{\langle E_0 | \varepsilon | E_0 \rangle}{\langle E_0 | E_0 \rangle} \equiv \langle \varepsilon \rangle_E \sim \varepsilon_{\text{high}} \quad (4)$$

$$\bar{\varepsilon}_{\text{TM}}^{-1} = \frac{\langle H_0 | \varepsilon^{-1} | H_0 \rangle}{\langle H_0 | H_0 \rangle} \equiv \langle \varepsilon^{-1} \rangle_H \sim \varepsilon_{\text{low}}^{-1}. \quad (5)$$

In the TE case, the dielectric constant is weighted by the electric field, which is concentrated in high dielectric for the lower bands,¹ and thus one should get an $\bar{\varepsilon}$ near to the high dielectric constant. For the example of air holes in dielectric [Fig. 1(b)], the topmost state of the bottom TE band in the two-dimensional system gives an $\bar{\varepsilon}$ of 5.06 from Eq. (4). This value, while greater than the uniform-weight mean ε of 3.92, is still far from 12 (the high dielectric), as a result of the structure's dielectric veins being so thin. (This structure has both a TE and a TM gap, but we focus on the TE gap corresponding to the even modes.) In Eq. (5), the TM case, we average the inverse dielectric constant, a mean that favors lower values. Moreover, the mean is weighted by the magnetic field, which tends to be less in the high dielectric than the electric field. (The magnetic field must loop around the electric field in the high dielectric, since the relationship of the magnetic and electric fields is the same as that of a current loop and its magnetic field.) Therefore, the TM average dielectric should be closer to the low dielectric constant. In the case of the dielectric rods in air [Fig. 1(a)], Eq. (5) for the highest-frequency mode of the bottom TM band in two-dimensions produces an $\bar{\varepsilon}$ of 1.25 (versus the uniform-weight inverse mean of 1.13).

From the above calculations, then, an estimate for the optimal slab thickness is given by

$$\text{slab thickness } h \sim \frac{1}{2\omega_{\text{gap-bottom}} \sqrt{\bar{\varepsilon}}}. \quad (6)$$

Here, the frequency is given in units of c/a and the thickness is in units of a . The effective dielectric constant $\bar{\varepsilon}$ can be estimated from the averages in Eqs. (4) or (5), according to whether a TE or a TM gap is of interest, and can use as a weighting factor either the state from a two-dimensional calculation or simply a uniform value.

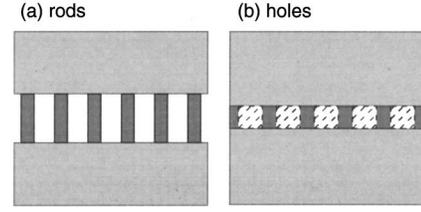


FIG. 8. Side view of the slabs from Fig. 3 with a uniform, low-index background above and below the slabs. (a) is the rod slab and (b) is the hole slab. The background has a dielectric constant of 2.0 and all other parameters are as in Fig. 3.

When applied to the rod and hole systems with the effective dielectric constants computed above, Eq. (6) predicts optimal thicknesses of $1.6a$ and $0.7a$, respectively, compared to the computed gap maxima at $2.3a$ and $0.6a$ from Fig. 7. The estimates come close enough to the optimal values that large gaps are produced (whereas there would be no gap at all if the two estimates were applied to each others' systems). Moreover, this approximation explains how the sharp difference in optimal thickness between the rod and the hole systems derives from the polarizations of the modes exhibiting the gap.

It should be noted that the size of the gap is not necessarily the only consideration in selecting the slab thickness. For example, when localizing states in a resonant cavity, longer decay times can sometimes be achieved by using slightly thicker slabs—this causes the states to be more localized within the slab, and also pulls the frequencies down to where the density of radiation modes is lower (since the density of states in vacuum goes as ω^2). It is often better to tune parameters, such as the slab thickness, based upon the actual phenomenon that is being optimized, rather than indirectly via the size of the band gap. Nevertheless, the approximation in Eq. (6) gives a reasonable starting point for subsequent fine-tuning.

V. SLABS WITH SOLID BACKGROUNDS (SANDWICHES)

So far, we have focused on the idealized system of slabs suspended in air. We now turn to the case where the background regions above and below the slab are occupied by a uniform dielectric material forming a substrate or “sandwich” as shown in Fig. 8. (We focus first on having the same dielectric above and below the slab in order to maintain mirror symmetry; the effects of symmetry breaking are considered in a later section.) The dielectric constant of the substrate is 2, but the holes and the space between the rods continue to be occupied by air. The resulting band structures are given in Fig. 9. The background index remains lower than the effective index in the slab, and hence index guiding is still able to produce the guided bands (and band gap) evident in Fig. 9.

While such a substrate will have a finite thickness in reality, the localization of the guided modes within the slab means that the substrate can be considered infinite as long as it is sufficiently thick. (In this case, a substrate thickness of several wavelengths is sufficient for the guided mode amplitude to be negligible beyond the substrate.) Thus, the light cone states are those of an infinite uniform dielectric, whose frequencies are reduced from those in vacuum by a factor of

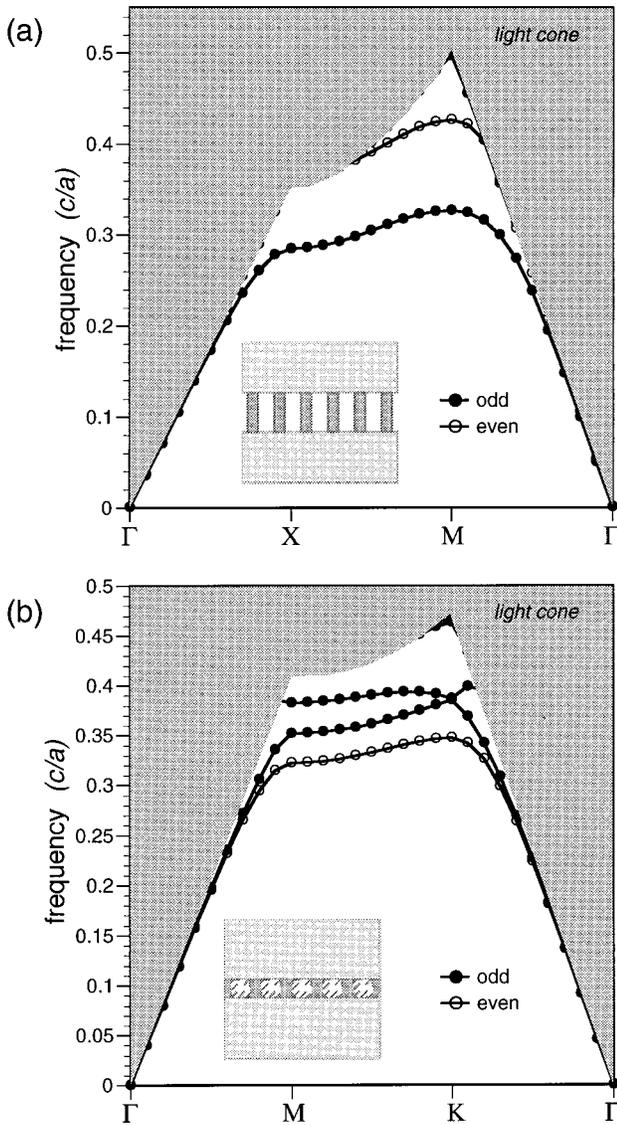


FIG. 9. Projected band diagrams for the structures shown in Fig. 8.

the index. The increased index above and below the slab also has the effect of pulling down the frequencies of the guided modes, allowing them to remain under the now-lowered light cone. In addition, the guided modes are somewhat less localized—for example, 89% of the energy of the lowest band for the hole structure at *K* is within the height of the slab for the solid background, versus 96% for an air background.

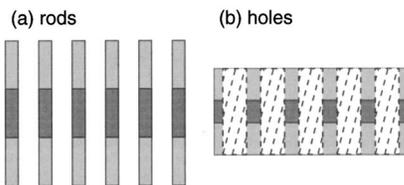


FIG. 10. Side view of the slabs shown in Fig. 3 with a periodic background formed by “extruding” the structures with a low-index material (dielectric constant 2.0). All other parameters are as in Fig. 3.

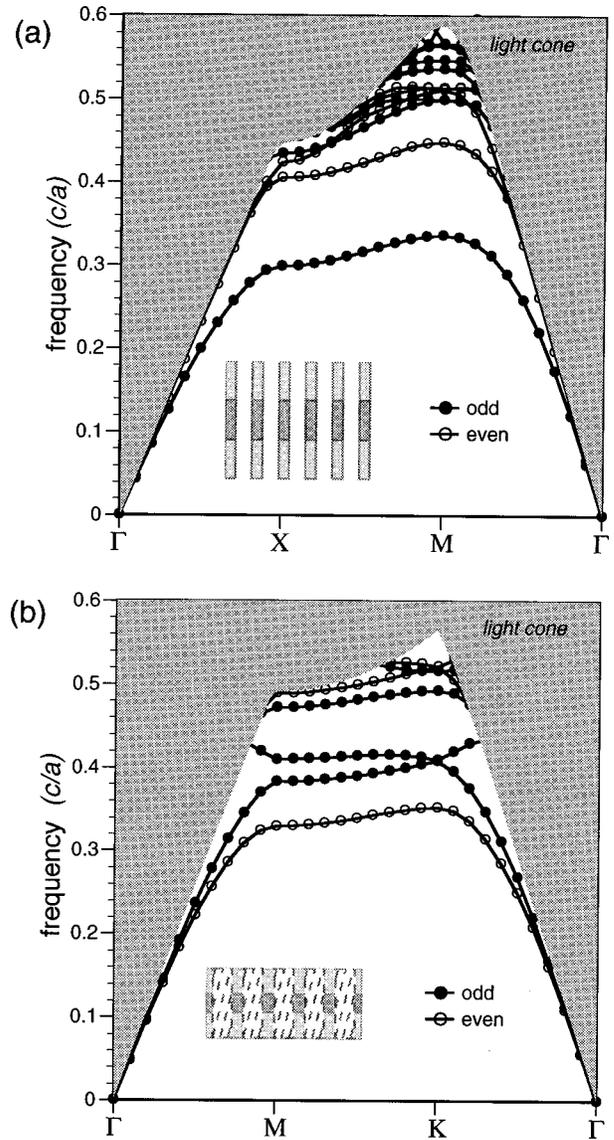


FIG. 11. Projected band diagrams for the structures shown in Fig. 10.

VI. SLABS WITH PERIODIC BACKGROUNDS

The effective index above and below the slab can be reduced from that of a solid background by using an “extruded,” low-index version of the slab, as shown in Fig. 10. For example, in the case of the hole slab, the holes extend through the low-dielectric substrate as well as through the slab. The resulting band structures are shown in Fig. 11, and again demonstrate guided modes and a band gap. Such a structure has advantages both in ease of fabrication (both slab and substrate can be etched at the same time) and in

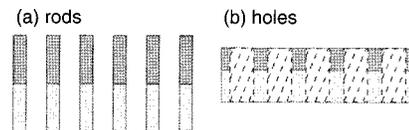


FIG. 12. Side view of the slabs shown in Fig. 10 (extruded backgrounds) with the upper background replaced by air. All other parameters are as in Fig. 10. This background breaks the mirror symmetry of the two photonic crystal slabs.

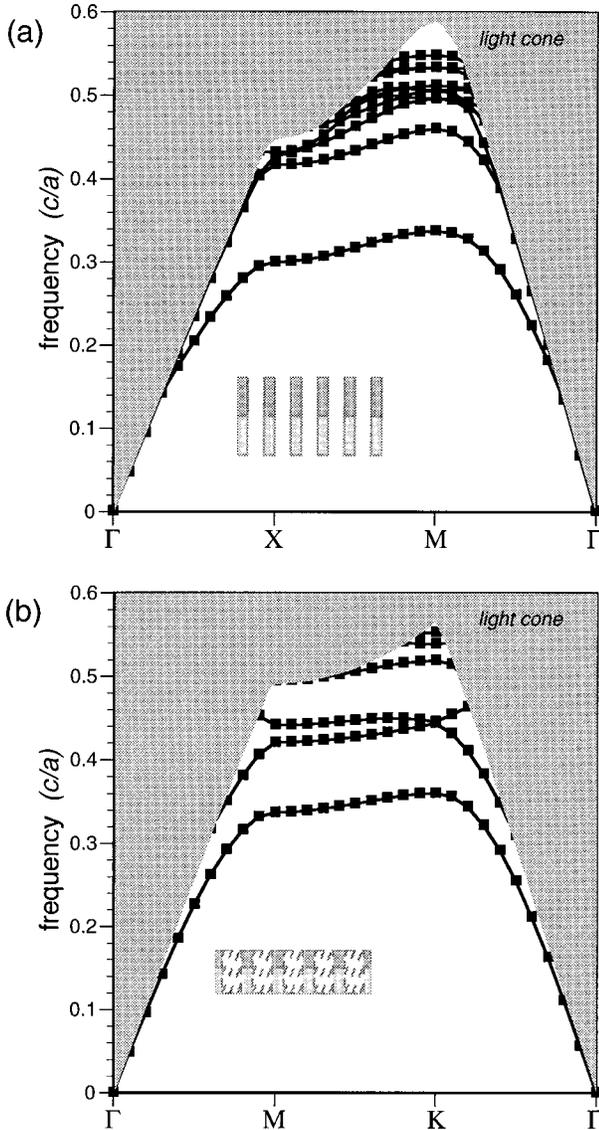


FIG. 13. Projected band diagrams for the structures shown in Fig. 12. The bands can no longer be segregated into even and odd modes, and there is no longer a band gap in the guided modes.

confinement of resonant cavity states (since localized states couple less strongly with a lower-index background). The periodicity of the background does not, however, produce useful photonic crystal slab effects by itself. Even if there were some sort of band gap in the background states, it would lie at higher frequencies than the band gap of the guided modes and would therefore not provide any additional confinement capabilities.

The light cone in this system consists of all the states existing in the bulk background, an infinitely extruded two-dimensional photonic crystal. This is similar to the shaded regions from Fig. 2, except that the material has a smaller index. That is, the lower edge of the light cone is simply the lowest band of the two-dimensional system. The fact that the lowest band of the two-dimensional structure forms a lower bound for the frequencies of the extruded structure in three dimensions may not be immediately apparent, and so we consider it below.

Because the dielectric function of the bulk background, $\epsilon(x,y)$, has translational symmetry in the z direction, any

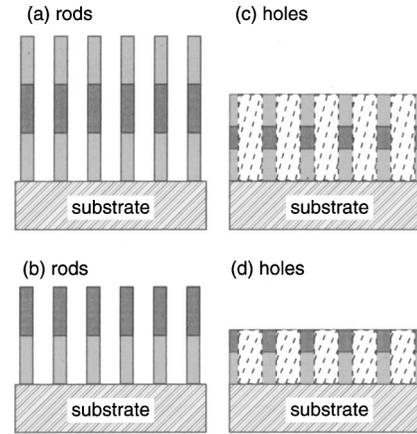


FIG. 14. A solid substrate may lie below a slab without affecting the band structure by being sufficiently far from the slab. (a), (b), (c), and (d) depict such solid substrates below the symmetric and antisymmetric rod and hole structures from Figs. 10(a), 12(a), 10(b), and 12(b), respectively.

background state's magnetic field can be written in the form

$$|H\rangle = \vec{H}(x,y)e^{i(kz - \omega t)}. \quad (7)$$

Such a field is manifestly propagating in the positive- z direction (upwards) for positive k and downwards for negative k . Therefore, the group velocity $d\omega/dk$, which can be expressed as the upwards flux divided by the energy density (using the derivative of the eigenvalue equation), must have the same sign as k . It then follows that the minimum frequency occurs at zero k , at which point the solution $|H\rangle$ is simply the two-dimensional eigenstate. This argument holds at each point in the Brillouin zone, and so the light cone is bounded by the lowest two-dimensional band.

VII. SLABS WITH SYMMETRY-BREAKING BACKGROUNDS

It is also possible to have a background that is not symmetric, for example a substrate below the slab and air above the slab. (Rod and hole slabs with solid substrates have been studied experimentally, e.g., in Refs. 20–22.) The light cone in this case is the union of the light cones for the backgrounds above and below the slab. Such a structure is depicted in Fig. 12, in which the periodic backgrounds from the previous section here lie only below the slabs. The resulting band diagram is given in Fig. 13.

The most important consequence of a symmetry-breaking background is that the guided modes can no longer be classified as even or odd. Thus, there is no longer any band gap in the guided modes, and the photonic crystal properties of the slab are ostensibly lost. If the guided modes are sufficiently localized within the slab, however, so that the background is only a small perturbation, the wave functions may still be approximated as even or odd and some effects of the band gap will persist.

In order to maintain the distinction between even and odd guided modes, it is only necessary to preserve mirror symmetry where the guided modes have non-negligible amplitude. Thus, a solid substrate can be used below the slab (and not above) with no effects on the band gap as long as the

substrate is separated from the slab by a buffer region that is sufficiently thick. Shown in Fig. 14 are examples of how a solid substrate might be used below the structures from the previous two sections without affecting the band structures significantly.

VIII. CONCLUSION

Photonic crystal slabs are an important system in the practical application of photonic crystals, and the band-structure formalism provides a powerful tool in their analysis. Unlike two- and three-dimensional photonic crystals, the band structures for slabs are projected and have the unique feature of a light cone enveloping the states. The presence of the light cone means that a complete band gap is impossible—still, waveguides and resonant cavities are possible.¹⁵ Further-

more, the presence of a band gap in the guided modes is useful in its own right. For example, Fan *et al.* have proposed using slab band gaps to prevent in-plane losses from LED emission.¹³ Perhaps the greatest promise of photonic crystal slabs, however, is that they will allow exciting results from two-dimensional crystals such as waveguide bends²³ and channel-drop filters²⁴ to be implemented easily on optical and infrared lengthscales.

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