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Band Structure Optimization of Two-Dimensional Photonic Crystals in *H*-Polarization

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In the study of photonic crystals, the question arises naturally: Which crystals produce the largest band gaps? This question is investigated by means of an optimization-based evolution algorithm which, given two dielectric materials, seeks to produce a material distribution within the fundamental cell which produces a maximal band gap at a given point in the spectrum. The case of H-polarization in two dimensions is considered. Several numerical examples are presented.

Key Words: periodic structures; band gaps; optimal design.

1. INTRODUCTION

Consider electromagnetic wave propagation in a periodic, dielectric, non-magnetic medium in $\mathbb{R}^2$. We are interested in the case where the magnetic field vector H is polarized orthogonal to the direction of wave propagation. The time-harmonic Maxwell equations then reduce to the scalar equation

$$-\nabla \cdot (\gamma \nabla u) = \omega^2 u, \qquad \text{in } \mathbb{R}^2, \tag{1}$$

where $\gamma(x) = 1/\epsilon(x)$, ϵ is the real dielectric coefficient of the medium, u is the out-of-plane component of the magnetic field, and ω is the frequency. The structure is assumed to be periodic with respect to the integer lattice $\Lambda = Z^2$, $Z = \{0, \pm 1, \pm 2, \ldots\}$. In other words,

$$\gamma(x) = \gamma(x + n) \qquad \text{for all } n \in \Lambda, \text{ and } x \in \mathbb{R}^2.$$

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An interesting feature of structures of this type is that, for certain functions γ, *band gaps*, i.e., intervals of frequencies in which waves cannot propagate in the medium, appear. This was proved in the case of certain high contrast structures by Figotin and Kuchment [7, 8], and has been observed both computationally and experimentally in many other cases. See [1, 9] for an introduction to photonic crystals, computational methods, and applications. In two dimensions, band gaps can occur both in the H-polarization case, as modeled by (1), and in the E-polarization case, for which the model is $-\Delta u = \omega^2 \epsilon u$. In a previous paper [5], considering the E-parallel polarization case, the question was studied: Which periodic structures, composed of arbitrary arrangements of two given dielectric materials, produce the largest band gaps? The question was formulated as an optimization problem, and approximate solutions were obtained through numerical computations. In the present paper, our aim is to carry out a similar program of investigation for the H-parallel polarization model (1). The H-parallel problem is more difficult both theoretically and computationally, due to the fact that the unknown coefficient γ is now present in the differential operator. Further, a primary deficiency of the approach of [5] was that it required an initial guess which already had a band gap. Here, a new evolution algorithm is presented which allows structures with gaps to be produced without knowledge of an initial structure with a gap.

The outline of this paper is as follows. In the next section we introduce the family of Bloch eigenproblems associated with problem (1). We then formulate in Section 3 the problem of maximizing band gaps about a given reference function and calculate the generalized gradient of the objective. In Section 4. the evolution algorithm is described. Finally in Section 5 the results of several numerical experiments are presented.

2. EIGENPROBLEMS

The standard procedure for analyzing problem (1) over $\mathbb{R}^2$ is to reduce it to a family of subproblems over the periodic domain (torus)

$$\Omega = \mathbb{R}^2/\Lambda,$$

which can be identified with the unit square $(0, 1)^2$ with periodic boundary conditions. Defining the first Brillouin zone $K = [-\pi, \pi]^2$, we seek eigenfunctions u of (1) in the form of Bloch modes (see, e.g., [11]),

$$u(x) = e^{i\alpha \cdot x} u_\alpha(x),$$

where the quasimomentum vector $\alpha \in K$, and the function u_α is periodic.

If ω^2 is an eigenvalue corresponding to the Bloch mode u with $\alpha \in K$ given, it follows formally that the pair (ω^2, u_α) should satisfy

$$-(\nabla + i\alpha) \cdot \gamma(\nabla + i\alpha) u_\alpha = \omega^2 u_\alpha \qquad \text{in } \Omega. \tag{2}$$

Conversely, eigensolutions of (2) yield Bloch mode solutions for problem (1). The transformation from problem (1) to the family (2) can also be viewed as an application of the Floquet transform [10]. We are interested in the family of problems (2) as α ranges over K.

Let us rewrite (2) as

$$A(\gamma, \alpha)u = \lambda u, \qquad \alpha \in K, \tag{3}$$

where $A(\gamma, \alpha) = -(\nabla + i\alpha) \cdot \gamma(\nabla + i\alpha)$ and the subscript α has been dropped from u_α. Assuming that γ is real, bounded, measurable, and has strictly positive essential infimum, one can show easily that $A(\gamma, \alpha)$ is symmetric and positive semidefinite, with compact resolvent on $L^2(\Omega)$. It follows that the spectrum of (3) consists of a discrete sequence of nonnegative eigenvalues, each of finite multiplicity. Obviously each eigenvalue λ depends on γ and α. Repeating each eigenvalue according to its multiplicity, we enumerate

$$0 \le \lambda_1(\gamma, \alpha) \le \lambda_2(\gamma, \alpha) \le \lambda_3(\gamma, \alpha) \le \cdots \infty.$$

For a given γ, the Bloch spectrum $\mathcal{B}$ can be defined

$$\mathcal{B} = \{\lambda_j(\gamma, \alpha) : \alpha \in K,\ j = 1, 2, 3, \ldots\}.$$

Frequencies ω such that $\omega^2 \notin \mathcal{B}$ have no associated Bloch modes and do not propagate in the structure. In the next section we formulate an optimization problem to find functions γ which maximize gaps in the Bloch spectrum.

3. OPTIMAL DESIGN PROBLEM

Suppose that we are given two materials, say with dielectric constants ϵ_0 and ϵ_1, such that $\epsilon_0 < \epsilon_1$. We wish to find arrangements of the materials within the fundamental cell Ω which result in maximal gaps in the Bloch spectrum. Let us define a class of admissible designs consisting of arbitrary arrangements of the two materials

$$ad \equiv \left\{ \gamma(x) : \gamma(x) = \frac{1}{\epsilon_0}\chi(x) + \frac{1}{\epsilon_1}(1 - \chi(x)),\ \chi \in S \right\},$$

where S denotes the set of all measurable functions on Ω which are bounded between 0 and 1. We interpret $\chi(x)$ as the volume fraction of material ϵ_0 present at the point x.

Let $q(\alpha)$ be a given real-valued function defined on some subset $K_0 \subseteq K$. The number $q(\alpha)$ represents a squared frequency about which we would like to maximize the distance to any eigenvalue $\lambda_j(\gamma, \alpha)$.

Assume that there exists $\gamma_0 \in ad$ and some index j such that

$$\lambda_j(\gamma_0, \alpha) < q(\alpha) < \lambda_{j+1}(\gamma_0, \alpha), \qquad \text{for all } \alpha \in K_0.$$

We then define

$$g(\gamma, q; \alpha) \equiv \min\{q(\alpha) - \lambda_j(\gamma, \alpha), \lambda_{j+1}(\gamma, \alpha) - q(\alpha)\}, \tag{4}$$

and

$$G(\gamma, q) \equiv \inf_{\alpha \in K_0} g(\gamma, q; \alpha). \tag{5}$$

Holding q fixed, we then consider the optimization problem

$$\sup_{\gamma \in ad} G(\gamma, q). \tag{6}$$

The case where $K_0 = K$ and $q(\alpha) \equiv \omega_0^2$ corresponds to maximizing a band gap of the structure about the center frequency ω_0. The more general case of arbitrary q and K_0 is necessary to implement the evolution algorithm described in a following section and may also be of interest for producing structures with directionally dependent band gaps.

One may rightfully question whether or not problem (6) admits a solution. In fact, similar optimal design problems in mechanics are well known to give rise to optimizing sequences of designs which become highly oscillatory and have no limit within the admissible class. One of two strategies is usually employed to render such a problem well-posed. The first is to constrain the admissible set *ad* to have sufficient compactness properties so that a convergent minimizing sequence is guaranteed. This is often accomplished through some smoothness or perimeter constraint. The second strategy is to "relax" the admissible class *ad*. This is accomplished by studying limiting behavior of minimizing sequences and enlarging the admissible class to include appropriate limits. In the case of (6), such limits would include anisotropic media with certain constraints on the eigenvalues of the dielectric tensors.

Interestingly, in the numerical examples that follow, minimizing sequences showed no tendency to become oscillatory and converged to roughly the same solution regardless of the level of discretization of the problem. Finding the conditions under which existence of a solution can be guaranteed remains an important open problem, but further analysis is beyond the scope of this paper.

In order to find approximate solutions to problem (6), would like to compute the gradient of G with respect to γ. From the definition of G in (4) and (5) we observe three difficulties which may render G nondifferentiable in a classical sense. First, the eigenvalues λ_k may not be smooth functions of γ at points of multiplicity. Multiple eigenvalues cannot be ruled out and in fact are typical for structures with symmetry. Second, the minimum in (4) is not smooth when the two arguments are equal. Finally, in (5), the infimum of a family of functions may not be smooth, even if each function in the family is smooth. Nevertheless the resulting composite function G is Lipschitz continuous (with an appropriate norm on γ), and so the concept of the generalized gradient, as defined by Clarke [2], makes sense.

Taking the domain of definition of G to be the space X of bounded measurable functions of Ω, the generalized directional derivative of G at γ (with respect to the first argument), in the direction η is defined by

$$G^0(\gamma, q)(\eta) \equiv \limsup_{\substack{\tilde{\gamma} \to \gamma \\ t \downarrow 0}} \frac{G(\tilde{\gamma} + t\eta, q) - G(\tilde{\gamma}, q)}{t}.$$

The generalized gradient of G with respect to γ is then defined by

$$\partial_\gamma G(\gamma, q) \equiv \{\xi \in X' : G^0(\gamma, q)(\eta) \geq \langle \xi, \eta \rangle, \text{ for all } \eta \in X\},$$

where X' denotes the dual space of X. Using the calculus of generalized gradients described in [2], and the results of Cox [4], the generalized gradient ∂G (with respect to γ) can be

calculated in a straightforward way. First, following [4], we find

$$\partial_\gamma \lambda_k(\gamma, \alpha) \subset \mathrm{co}\{|(\nabla + i\alpha)u|^2 : u \in \mathcal{E}_k^1(\gamma, \alpha)\},$$

where $\mathcal{E}_k^1(\gamma, \alpha)$ is the span of all eigenfunctions u associated with the eigenvalue $\lambda_k(\gamma, \alpha)$ and satisfying the normalization $\int_\Omega |u|^2 = 1$. Here co denotes the convex hull, i.e., the set of all convex combinations of elements in the given set. From (4) and [2, Proposition 2.3.12], we have

$$\partial_\gamma g(\gamma, q; \alpha) \subset \mathrm{co}\{\partial_\gamma \lambda_{j+1}(\gamma, \alpha), -\partial_\gamma \lambda_j(\gamma, \alpha)\}.$$

Finally, from (5) and [2, Theorem 2.8.2], we find

$$\partial_\gamma G(\gamma, q) \subset \mathrm{co}\{\partial_\gamma g(\gamma, q; \alpha) : \alpha \in \mathrm{Argmin}\, g(\gamma, g; \cdot)\}.$$

Assembling the three previous results,

$$\begin{aligned}\partial_\gamma G(\gamma, q) \subset \mathrm{co}\{&\mathrm{co}\{|(\nabla + i\alpha)u|^2 : u \in \mathcal{E}_{j+1}^1(\gamma, \alpha)\}, \\ &\mathrm{co}\{-|(\nabla + i\alpha)u|^2 : u \in \mathcal{E}_j^1(\gamma, \alpha)\}\} : \alpha \in \mathrm{Argmin}\, g(\gamma, g; \cdot)\}. \quad (7)\end{aligned}$$

Note that ∂G can be computed knowing only the eigenfunctions associated with eigenvalues $\lambda_j(\gamma, \alpha)$ and $\lambda_{j+1}(\gamma, \alpha)$ at the points where minima occur with respect to α in the definition (5). Since these eigenfunctions must typically be computed anyway to evaluate G, obtaining gradient information is essentially no more expensive than computing the value of the function itself.

4. EVOLUTION ALGORITHM

The basic algorithm consists of an inner optimization loop and an outer evolution, or homotopy, loop. The optimization loop is a simple projected generalized gradient ascent method, similar to the scheme described in [5]. We note that many general purpose algorithms exist for extremizing nondifferentiable functions (see, for example, [12]), as well as more specialized methods designed for minimax problems (see, for example, [3]). Any of these algorithms could in principle be substituted for our primitive optimization method. The evolution loop is a simple strategy to homotopically deform the band structure of a given initial design into a desired configuration.

Assume we are given a closed subset $K_0 \subseteq K$, a real-valued "target" function q_1 defined on K_0, an initial design $\gamma_0 \in ad$, and a function q_0 defined on K_0 such that

$$\lambda_j(\gamma_0, \alpha) < q_0(\alpha) < \lambda_{j+1}(\gamma_0, \alpha), \qquad \text{for all } \alpha \in K_0.$$

Thus $G(\gamma_0, q_0) > 0$. For $0 < t < 1$, define $q_t(\alpha) = tq_0(\alpha) + (1-t)q_1(\alpha)$. Define the projection operator $P : L^1(\Omega) \to ad$ by

$$(Pf)(x) = \begin{cases} 1/\epsilon_1 & \text{if } f(x) < 1/\epsilon_1, \\ 1/\epsilon_0 & \text{if } 1/\epsilon_0 < f(x), \\ f(x) & \text{otherwise.} \end{cases}$$

The basic algorithm proceeds as follows.

1. Set $t := 0, k := 0,\ flag = 0$.
2. While $G(\gamma_k, q_t) < tol_1$ and $flag = 0$,
   - *a*. Choose a direction $s_k \in \partial G(\gamma_k, q_t)$ and a step size β_k to yield an increase in G,
   - *b*. Set $\gamma_{k+1} = P(\gamma_k + \beta_k s_k)$.
   - *c*. Set $k := k + 1$.
   - *d*. If step is sufficiently small then stop.

   end
3. If $t < 1$, increase t by tol_2,
   else set $flag := 1$.
4. Go to step 2.

The *while* loop in Step 2 constitutes the optimization. Step 2a in the inner loop is accomplished by solving a small subproblem via linear programming, as described in [5]. By increasing the objective $G(\gamma, q_t)$, eigenvalue bands are "pushed away" from q_t. When all eigenvalues are sufficiently far away (controlled by tol_1) from the current q_t, the outer loop moves the current q_t linearly toward the target q_1, by an amount tol_2 (Step 3). The two tolerances tol_1 and tol_2 are kept fixed and must be selected beforehand. The value of tol_1 is not crucial and can be chosen to be any relatively small number. The parameter tol_2 must then be chosen such that

$$tol_2 < tol_1 / \max_{\alpha} |q_0(\alpha) - q_1(\alpha)|,$$

so that the condition

$$\lambda_j(\gamma_k, \alpha) < q_{t+tol_2}(\alpha) < \lambda_{j+1}(\gamma_k, \alpha), \qquad \alpha \in K_0$$

holds for the next iteration. Provided that each inner optimization is successful, the outer loop gradually moves q_t toward the target q_1, until finally it is reached. At this point, a flag is set (Step 3) which allows the optimization to proceed without further stops to update q. Convergence is checked in Step 2d according to step length. Note that the usual necessary condition for optimality $0 \in \partial G$ (see Clarke [2]) may not hold in this setting due to the constraints on γ.

5. NUMERICAL RESULTS

The algorithm described in the previous section was implemented in a discrete setting using a finite element method coupled with a preconditioned subspace iteration for computation of the eigenvalues. The method employed for eigenvalue computation, and references to several other methods for band structure calculations, can be found in [6]. The number of eigenvalue computations carried out at each step in the optimization can be greatly reduced by considering only designs with some symmetry. In particular, we assume that $\gamma(x)$ is invariant under the transformations

$$(x_1, x_2) \mapsto (-x_1, -x_2), \qquad (x_1, x_2) \mapsto (-x_1, x_2) \qquad (x_1, x_2) \mapsto (x_1, -x_2).$$

In this case, it follows easily [5] that all possible eigenvalues must occur in the triangular subset of the Brillouin zone

$$T = \{(\alpha_1, \alpha_2) : 0 \le \pi, 0 \le \alpha_2 \le \alpha_1\}.$$

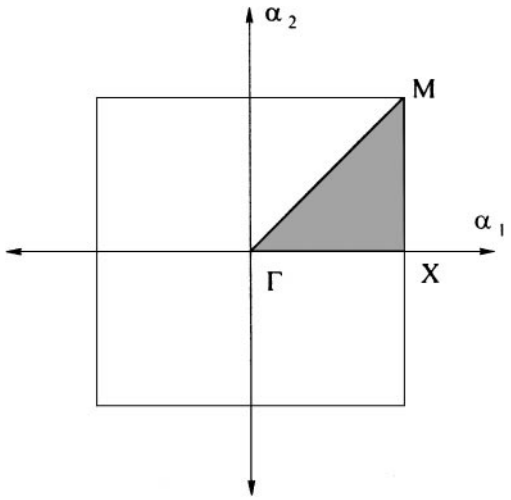

FIG. 1. Brillouin zone, with labels for symmetry points.

This region is shown in Fig. 1, along with labels on the vertices. Band structure plots in the figures below show frequencies $\omega/2\pi$ as α moves around the perimeter of T, from Γ, to X, to M, and back to Γ.

Due in part to the crude step size control strategy used in our optimization algorithm, a large number of iterations are typically required before any kind of convergence is observed. For the examples shown below, generally several thousand iterations (the total number of steps in the inner optimization loop) were taken. Fortunately, this is possible with reasonable computational effort since each step is quite inexpensive. With all code written in *Matlab* and running on a 400 MHz Linux PC, a complete run of the evolution algorithm could generally be done overnight. With a more sophisticated optimization algorithm, the computational effort could probably be reduced significantly. All finite element computations were done on a uniform 64×64 grid.

The following examples are computed using two materials with dielectric coefficients $\epsilon_0 = 1$ and $\epsilon_1 = 9$. These values represent high-contrast materials in the optical frequency range. Generally structures with larger gaps can be obtained if one is allowed to use higher contrast materials.

In the first example, we take as an initial guess a low-contrast structure, shown in Fig. 2a, which contains no band gaps. The structure is composed of two materials, with dielectric coefficients $\epsilon = 2.5$ and 5. (The same structure does have a large band gap between the first and second bands with materials $\epsilon_0 = 1$ and $\epsilon_1 = 9$.) We begin the evolution algorithm with $q_0(\alpha) = \lambda_1(\alpha) + \delta$, where δ is a small positive number. This positions q_0 between the first and second eigenvalue bands, as shown in Fig. 2b. The target $q(\alpha)$ is set to a constant, so that the optimized structure should have a band gap. The results are shown in Fig. 3. As can be seen, the optimized structure exhibits a band gap near $\omega/2\pi \approx 0.39$.

In the second example, we take as a starting point the smooth structure shown in Fig. 4a. The volume fraction of high index material in each cell is proportional to the Gaussian $e^{-2\pi|x|^2}$. This structure has no band gap in the lower bands, as shown in Fig. 4b. The goal is to introduce a gap between the third and fourth bands. Similar to the previous example, we take $q_0(\alpha) = \lambda_3(\alpha) + \delta$ and set the target $q(\alpha)$ constant. The optimized structure is shown in Fig. 5a. As can be seen in Figs. 5b and 5c, this structure has a relatively large gap between the third and fourth bands, centered at $\omega/2\pi \approx 0.58$.

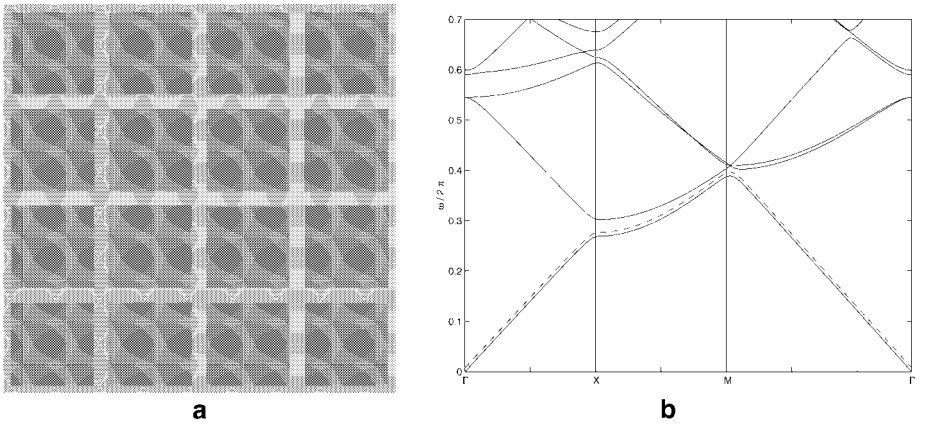

FIG. 2. Starting point for first example. (a) Initial structure. Dark represents $\epsilon = 2.5$, light represents $\epsilon = 5$. (b) Eigenvalue bands. Dashed line is $q_0(\alpha)$. Note that a 4×4 array of cells is illustrated in (a); computations were done on a single cell.

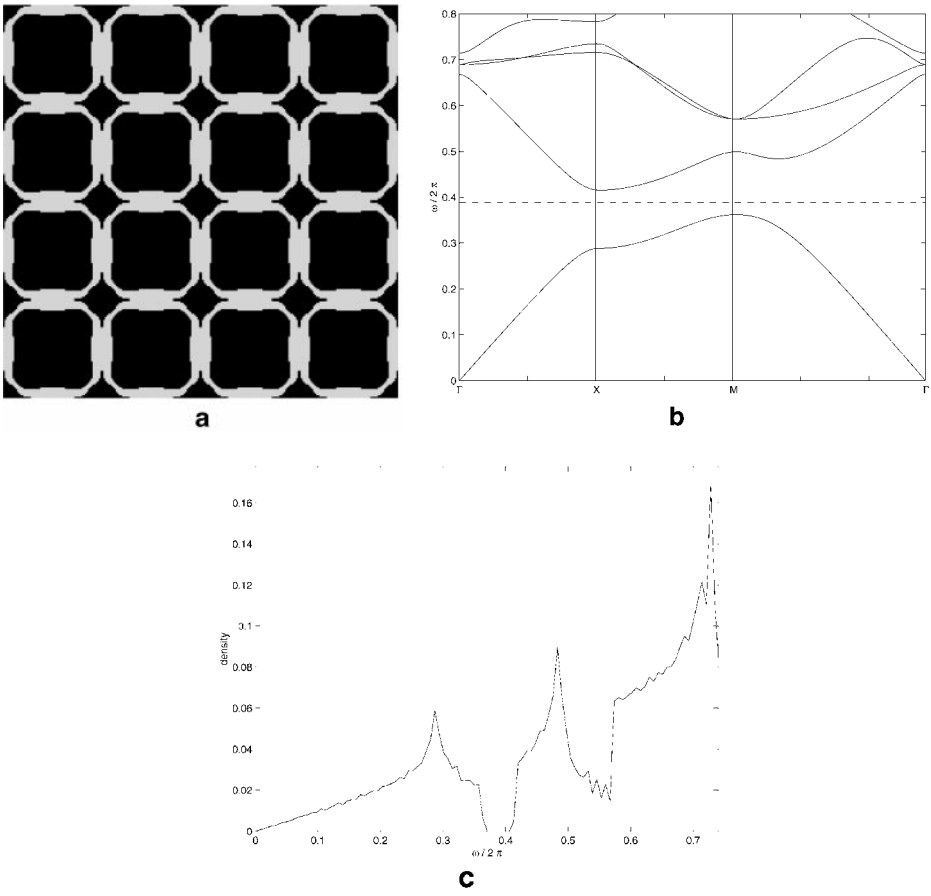

FIG. 3. Optimized structure for first example. (a) Optimized structure. (b) Eigenvalue bands. Dashed line is $q_1(\alpha)$. (c) Density of states, calculated by a sample of 4096 uniformly spaced points in the first quadrant of the Brillouin zone.

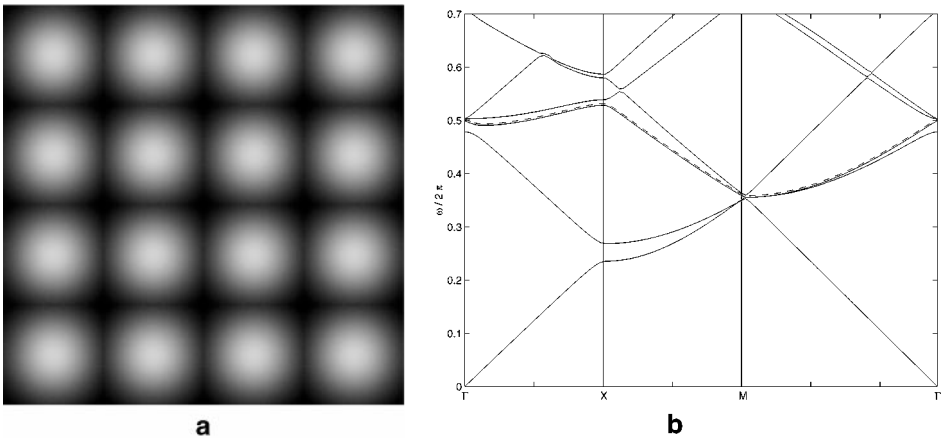

FIG. 4. Starting point for second example. (a) Initial structure. Dark represents $\epsilon = 2$, light represents $\epsilon = 7$. (b) Eigenvalue bands. Dashed line is $q_0(\alpha)$.

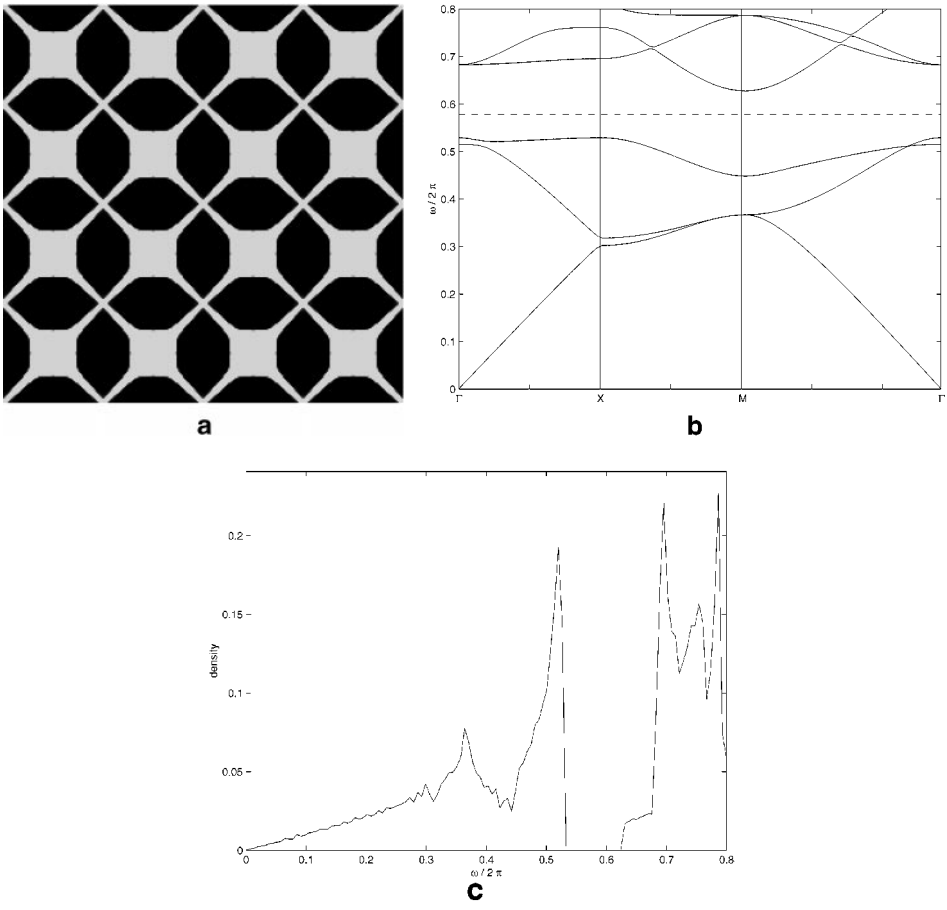

FIG. 5. Optimized structure for second example. (a) Optimized structure. (b) Eigenvalue bands. Dashed line is $q_1(\alpha)$. (c) Density of states.

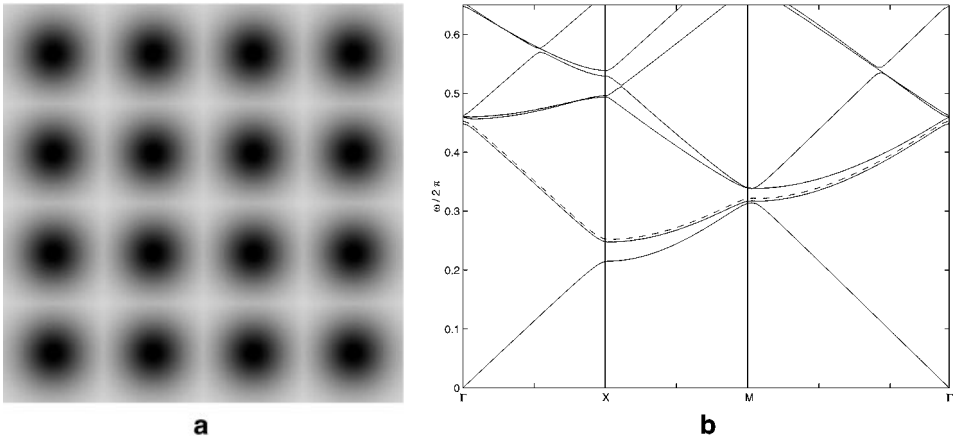

FIG. 6. Starting point for third example. (a) Initial structure. Dark represents $\epsilon = 2$, light represents $\epsilon = 7$. (b) Eigenvalue bands. Dashed lines are initial $q(\alpha)$ functions (the second line is not visible due to proximity with the fourth band).

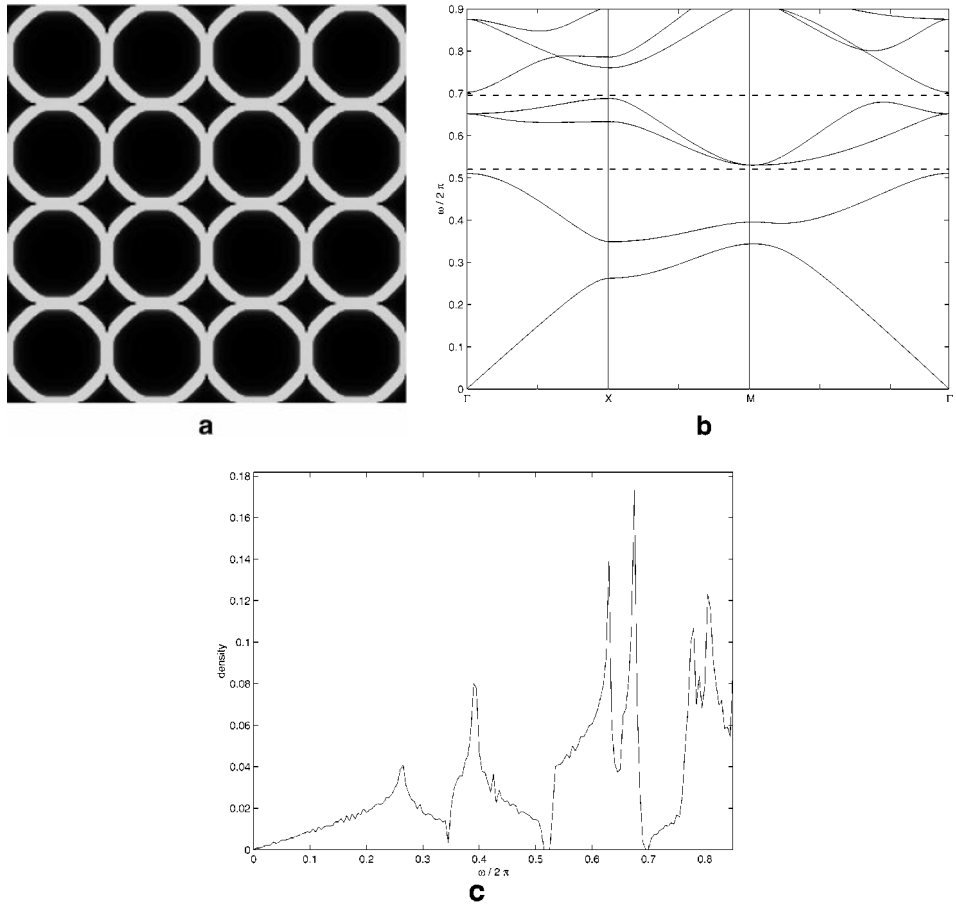

FIG. 7. Optimized structure for third example. (a) Optimized structure. (b) Eigenvalue bands. Dashed lines are target $q(\alpha)$ functions. (c) Density of states.

With an obvious modification, the evolution algorithm can also be used to produce structures with multiple band gaps. Consider for example the smooth starting point shown in Fig. 6a. This corresponds to a Gaussian volume fraction as used in the previous example, but with the high- and low-index materials reversed. The goal is to introduce two gaps, one between the second and third bands, and another between the fourth and fifth bands. We use two $q_0(\alpha)$ functions as shown in Fig. 6b. The optimized structure is shown in Fig. 7a, with very small band gaps near $\omega/2\pi \approx 0.52$, and $\omega/2\pi \approx 0.69$. In other experiments we found that by increasing the material contrast, similar structures with larger gaps can be obtained.

With regard to all of the previous examples, we should note that not all choices of target gaps and initial configurations yielded successful results; in some cases the algorithm terminated without producing a band gap. Indeed it seems clear that with finite contrast materials, some band configurations should be unattainable.

6. CONCLUSIONS

An optimization-based evolution algorithm for producing band gaps in two-dimensional photonic crystals in H-polarization has been presented. Numerical examples illustrate that the algorithm is effective in producing a variety of structures with gaps at various points in the spectrum.

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