Design of two-dimensional photonic crystals with large absolute band gaps using a genetic algorithm

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A two-stage genetic algorithm (GA) with a floating mutation probability is developed to design a two-dimensional (2D) photonic crystal of a square lattice with the maximal absolute band gap. The unit cell is divided equally into many square pixels, and each filling pattern of pixels with two dielectric materials corresponds to a chromosome consisting of binary digits 0 and 1. As a numerical example, the two-stage GA gives a 2D GaAs structure with a relative width of the absolute band gap of about 19%. After further optimization, a new 2D GaAs photonic crystal is found with an absolute band gap much larger than those reported before.

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Much attention has been focused on two-dimensional (2D) photonic crystals since they are much easier to fabricate than 3D photonic crystals[1,2] and have promising applications in, e.g., planar waveguide devices.[3,4] Many applications of photonic crystals are based on photonic band gaps, and it would thus be very interesting to design a photonic crystal with the largest photonic band gap for a given dielectric contrast. Several 2D structures with large absolute band gaps have been found by choosing their geometrical parameters appropriately.[5–8] With the rapid improvement of the speed of modern computers, one may hope that a fast computer could help to design a 2D photonic crystal with a maximal absolute band gap by either scanning all the possible configurations or using an effective global optimization method.

In the present paper, we use a genetic algorithm (GA) to find a 2D photonic crystal with the largest absolute band gap. As an effective global optimization method, a genetic algorithm usually searches for the global maximum in a discrete search space. The idea of the genetic algorithm came from Charles Darwin's theory of evolution (natural selection or survival of the fittest).[9–12] A binary gene is the basic building block in a genetic algorithm. If the range of a parameter is approximately known, one can encode the parameter by a number of genes. In fact, the density of the search grid for a genetic algorithm should not necessarily be very high, since the search results can always be refined by a local adjustment after a point in the vicinity of the global maximum has been found.

We consider a 2D photonic crystal of a square lattice formed by two different materials with dielectric constants ϵ_a and ϵ_b. In order to apply a genetic algorithm, we discretize the unit cell into many rectangular squares (called pixels hereafter) and each square can be filled by one of the two different materials (represented by a binary value, 1 or 0, in the genetic algorithm). The total number of possible structures of 2D photonic crystals increases exponentially with the number of pixels, and a full-space search method would not be practical when the number of the pixels is very large or the pixels are very small. In such a case, a genetic algorithm is expected to be effective. In the genetic algorithm, each binary chromosome corresponds to a 2D photonic crystal formed by ''pixels'' (square rods of dielectric material) and is associated with a value of the fitness (the relative width of the absolute band gap). After ranking, selection, crossover, and mutation in each iteration, the computer finds the global maximum of the fit after a number of iterations (see, e.g., Ref. 10).

Any global optimization method is time consuming (as compared with some gradient-based local search methods), and thus it is essential to find a fast method to calculate the fitness. Fortunately, we have developed a very fast numerical algorithm for calculating the band structure for such a special type of 2D photonic crystal formed by ''pixels.''[13] Therefore, we consider 2D photonic crystals formed by ''pixels'' for the convenience of the application of a genetic algorithm and a fast algorithm for calculating the band structures.

To apply a GA to design a 2D structure with a large absolute band gap, one needs to translate the filling pattern of the unit cell of a 2D photonic crystal into a binary chromosome. GA operators (such as ranking, selection, crossover, and mutation; see, e.g., Ref. 12) are then used in each iteration to find the global maximum of the fitness, which is the relative width of the absolute band gap (i.e., the ratio of the width of the absolute band gap to the midfrequency of the band gap) in the present paper.

The unit cell is divided into $2M \times 2M$ pixels, and each pixel is filled by one of the two dielectric materials. In the present paper we assume that the primitive unit cell (centered at the origin, see Fig. 1) has the primary symmetry of being invariant under the mirror reflection with respect to the xz plane and yz plane and under a 90° rotation around the z axis. Thus, the whole photonic crystal structure can be determined by the pixel-filling pattern of a triangular part of one-eighth of the unit cell (see Fig. 1), which can be represented by a binary number of $M(M+1)/2$ digits. The total number of the possible structures is $2^{M(M+1)/2}$, and even for $M = 10$ there are still more than 3×10^{16} different structures. For such a large searching space, the full-space search method is not practical for finding the best structure. In the

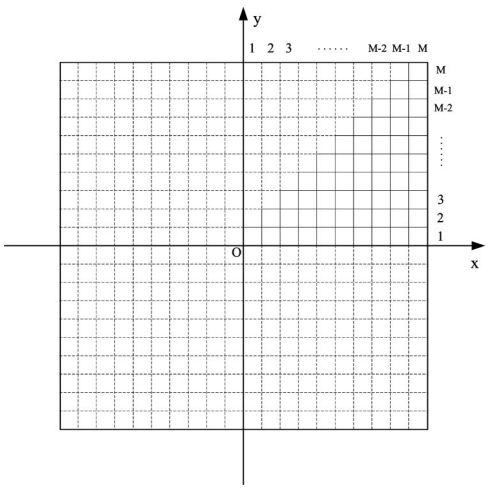

FIG. 1. Division of the unit cell of a 2D photonic crystal (with certain symmetries) of a square lattice. The filling pattern of the pixels (the small squares) with thick, solid line edges in the triangular part of one-eighth of the unit cell determines the whole structure of the photonic crystal.

present paper we show that a genetic algorithm is effective for such cases. The specific genetic algorithm used in the present paper is described as follows.

In step 1, we construct an initial population of N_{pop} chromosomes randomly, i.e., each gene of the N_{pop} chromosomes at the first generation is set by 0 or 1 randomly. In general, a 2D structure corresponding to a randomly produced chromosome has no absolute band gap. To speed up the search, we introduce a special chromosome (as a special seed) in the initial population (the other chromosomes are all randomly produced by the computer). The structure corresponding to the special chromosome is an array of square dielectric columns in air, which has a small absolute band gap when its geometric parameter is properly chosen (the relative width of the absolute band gap is about 5.5% when the dielectric constant of the columns is 12).[14]

In step 2, we evaluate the fitness values for the chromosomes. Note that the fitness of a chromosome is directly defined as the relative width of the absolute band gap of the corresponding structure. In order to maintain the diversity of the chromosomes and avoid a premature convergence of the evolution, we set a small constant (e.g., the value of 0.01) for the fit of any chromosome whose corresponding structure has no absolute band gap. During the evolution process the maximal fitness of the chromosomes of a generation does not always increase. In such a case, we avoid the degradation of the best chromosome. Thus, if this is not the initial population and the maximal fitness of the population decreases, we replace a chromosome (randomly selected) of the current population with the best chromosome (with the maximal fitness) in the previous population (note that each generation has the same size of population, i.e., N_{pop} chromosomes).

In step 3, we create a new population in the following procedure: (i). Select N_{pop} chromosomes from the current population to constitute a mating pool by using the proportional (roulette-wheel) selection scheme (i.e., the parents are chosen with a probability proportional to their fit values). Before the selection, the fitness values of the chromosomes are adjusted with a linear scaling so that the maximum of the scaled fitness is just two times larger than the averaged value of the scaled fitness. This is to avoid any individual taking over a significant selection probability at the start of the GA or the fittest individual making a random walk at the late run of the GA. Note that for the chromosomes in the same generation the averaged value of the fitness is the same before and after the scaling. Also note that some of the selected N_{pop} chromosomes may be identical and this phenomenon occurs more often in the late generations as the evolution tends to become steady.

(ii). Mate the chromosomes randomly from the mating pool, cross over each pair of parent chromosomes to obtain two offspring chromosomes (which inherit combined information from the parent chromosomes), and replace the parent chromosomes. Since the present problem is two dimensional, a one-point crossover is not appropriate. As shown in Ref. 12, a one-point crossover gives too monotonous patterns for a 2D problem. Thus, here we use a uniform crossover to achieve a better performance. We first produce a mask (consisting of 0 or 1 randomly) to label the gene loci, and then cross over the genes of the paired chromosomes at loci labeled with the value of 1.

(iii). Mutate each gene of a chromosome with a predefined small probability p_m, and a small percentage of the genes may be changed to the opposite values (1 to 0, or 0 to 1). In a genetic algorithm, p_m is a very important parameter. When p_m is too small, the evolution of the chromosomes may converge quickly to a local maximum. On the other hand, when p_m is too large the algorithm tends to search randomly and the average fitness of the population becomes far less than its maximal fitness. Thus, an appropriate choice of p_m is key for balancing the local convergence and the global search. According to the building block hypothesis[9] of the genetic algorithm, the operations (for both the crossover and the mutation) of the algorithm can work effectively in the evolution towards the global maximum when the average fitness has a medium value as compared to the maximal fitness for a generation. Therefore, to keep these operations effective it is necessary to adjust the value of p_m at different stages of the evolution process. In our algorithm, we allow p_m to vary after every certain number (I_{mut}) of generations during the evolution. We choose the following change (Δp_m) of the mutation probability for every I_{mut} generations,

$$\Delta p_m = \begin{cases} -0.0002, & \eta < 30\%, \\ 0, & 30\% \leqslant \eta \leqslant 60\%, \\ 0.0002, & \eta > 60\%, \end{cases}$$

where η is the ratio of the averaged fit to the maximal fit (without scaling) at the last generation of the I_{mut} generations. (iv). Repeat the second step.

The computational time required for the GA to find a structure with the maximal absolute band gap depends on how fast and accurately we can calculate the relative width of the absolute band gap. Therefore, it is necessary to develop a fast and accurate numerical method for calculating the band structure (to evaluate the fitness of each chromosome). Since the material discontinuities of the photonic crystals considered in the present paper are only along either

x or *y* directions, a fast plane-wave expansion method can be developed for these special 2D structures.[15] The fast plane-wave expansion method described in our previous paper[13] is employed in the GA in the present paper.

As a numerical example, we assume that the two dielectric materials forming the crystals are air and GaAs, i.e., $\epsilon_a = 1$ and $\epsilon_b = 11.4$. In order to avoid the obtained structure becoming impractical for fabrication (e.g., having too thin veins or too small holes), we start with $M = 10$ (i.e., the unit cell is divided into 20×20 pixels). In this case each chromosome has 55 gene loci, and we choose $N_{pop} = 100$. The initial value of p_m is set at 0.001, and P_m varies every 100 generations during the evolution in the way mentioned earlier. Plane waves numbering 441 are employed in the fast plane-wave expansion method, and our numerical analysis shows that the relative errors of the obtained absolute band gaps (with a noticeable value) are less than 1%. After a long evolution of more than 10^4 generations, the maximum of the fitness (i.e., the relative width of the absolute band gap) tends to become steady at a value of 16.946%. The obtained optimal structure (with the largest fitness) is shown in Fig. 2(a), and its photonic band structure is shown in Fig. 2(b). This structure has an absolute band gap of $0.132(2\pi c/a)$ at a midfrequency of $0.779(2\pi c/a)$. From Fig. 2(a) one sees that the structure is well composed (GaAs parts are well connected to each other, which favors a large band gap for the *H* polarization[16]) but the interface between the two dielectric materials is quite rough, which is due to the fact that the size of the used pixels is not small enough.

Thus, we divide further the unit cell of the square lattice into 40×40 pixels (i.e., $M = 20$). This time we consider only an improved optimization on the edges of the inclusion (GaAs) for the structure obtained above. We code into a chromosome only those pixels [indicated by the squares with dashed edges in Fig. 3(a) for the triangular part of one-eighth of the unit cell] at the edges of the inclusion, while keeping the remaining pixels unchanged. From Fig. 3(a) one sees that each chromosome contains 56 gene loci now. Note that the pixels located at the internal edges of the thin veins have not been included in the coding since we want the structures to have wide enough veins during the evolution. Here we set the change of the mutation probability as $\Delta p_m = -0.0002$ when $\eta \leqslant 95\%$ and $\Delta p_m = 0.0002$ otherwise. The GA with the new type of chromosomes is then run in a way similar to the one described earlier. Through an evolution of over 1000 generations the maximum of the fit becomes steady at a value of 19.571%. The optimized structure is shown in Fig. 3(b), which has an absolute band gap of $0.1518(2\pi c/a)$ at a midfrequency of $0.7756(2\pi c/a)$.

The structure of Fig. 3(b) naturally suggests a new photonic crystal structure (with smooth circular columns) of Fig. 4(a). This new structure is obtained directly by replacing the staired edges of Fig. 3(b) with straight-line edges or circular edges. Note that two insignificant GaAs pixels [the rightmost pixel of the first row and the topmost pixel of the right column in Fig. 3(b)] are removed. The new structure simply consists of circular, square, and rectangular columns of GaAs linked by three types of thin veins, respectively. The unit cell of the structure is indicated by the dotted square in Fig. 4(a).

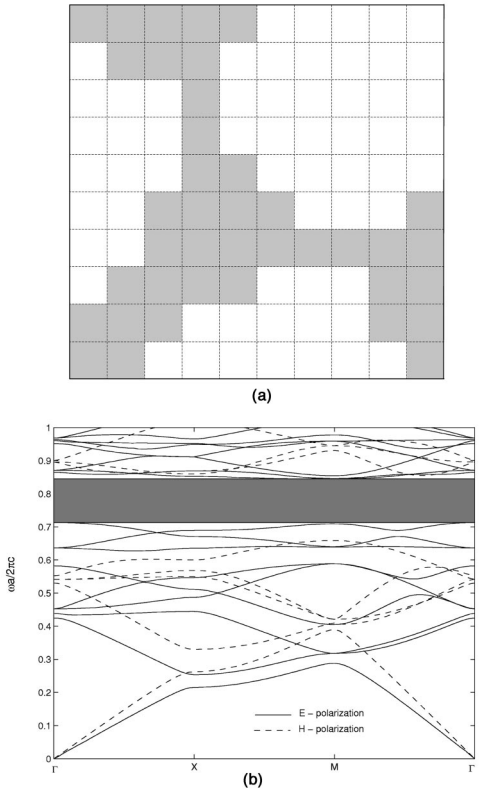

FIG. 2. (a) The best 2D GaAs photonic crystal found with the GA with $M = 10$. (b) The corresponding photonic band structure (the solid lines are for the *E* polarization and the dashed lines for the *H* polarization).

The upright circular column in the unit cell is centered at the point $(\pm 3a/16, \pm 3a/16)$ and has a radius of $7a/80$. The smoothed veins oriented at $\pm 45°$ or $\pm 135°$ in the unit cell have a thickness of $\sqrt{2}a/20$. In order to calculate the band structure of this 2D photonic crystal with the established fast plane-wave expansion method, we divide the unit cell of the structure into 1000×1000 small pixels of same size, and assume that the dielectric permittivity in each pixel takes the value at its center. Our numerical calculation shows that the absolute band gap of this new structure is $0.151(2\pi c/a)$ with its midfrequency at $0.795(2\pi c/a)$ (the relative width of the absolute band gap is about 19%). The number of plane waves used in our calculation is 441. By comparing the obtained results with those computed with more plane waves or smaller pixels (e.g., 2000×2000), it is shown that the relative errors of the numerical results is less than 1%. It is interesting to optimize further the new structure to achieve an even larger absolute band gap. We optimize further the geometric parameters r, w_1, w_2, d_1, and d_2 [see Fig. 4(a) for these notations]. The original values for these parameters are $r = 7a/80$, $w_1 = \sqrt{2}a/20$, $w_2 = a/10$, $d_1 = 3a/20$, and $d_2 = 3a/20$. Note that the symmetries of the structure, the centers of the circular columns, the square column (with a side length of $3a/20$) at the unit center, and the thinnest veins (with width of $a/20$) are fixed in the local optimization. After a smooth search in the neighboring region, we find a larger absolute band gap of $0.157(2\pi c/a)$ at midfrequency of $0.7826(2\pi c/a)$ (the relative band gap increases from 19%

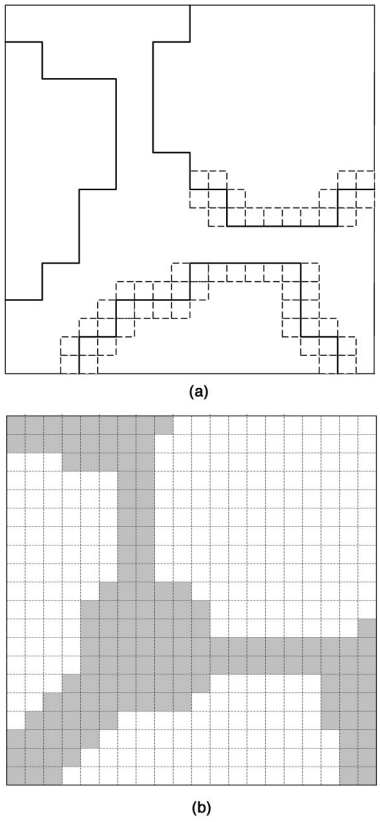

FIG. 3. (a) Further optimization on the edges of the inclusion for the structure of Fig. 2(a). The small, dashed squares at the edges of the inclusion in the triangular part are the pixels to be coded in the second stage of the GA. (b) The best structure of a 2D GaAs photonic crystal found in the second stage of the GA with $M=20$.

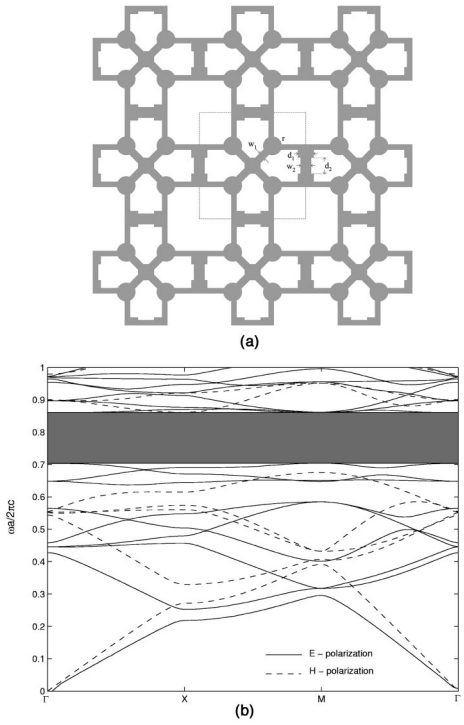

FIG. 4. (a) The optimal 2D GaAs photonic crystal structure (with smooth edges) suggested by Fig. 3(b). (b) The photonic band structure of this 2D photonic crystal after some local optimization. The optimal values for the geometric parameters are $r=0.095a$, $w_1=0.807a$, $w_2=0.103a$, $d_1=0.143a$, and $d_2=0.155a$. The ratio of the absolute band-gap width to the midfrequency of the band gap is about 20.1%.

to 20.1%). The optimal parameters are $r=0.095a$, $w_1=0.807a$, $w_2=0.103a$, $d_1=0.143a$, and $d_2=0.155a$. The large band gap for such a structure seems consistent with the rule of thumb that *E*-polarization band gaps are favored in a lattice of isolated high-ϵ regions and *H*-polarization band gaps are favored in a connected lattice.[16] The band structure of this optimized 2D photonic crystal is shown in Fig. 4(b).

In summary, we have used a two-stage genetic algorithm with a floating mutation probability to find a 2D photonic crystal (of a square lattice) with the maximal band gap. The unit cell of a square lattice is divided equally into $2M \times 2M$ square pixels, and each filling pattern of pixels with two dielectric materials corresponds to a chromosome consisting of binary digits 0 and 1. The genetic algorithm is naturally introduced with the fitness defined as the relative width of the absolute band gap. In the first stage of the GA, we divide the unit cell with a relatively large pixel ($M=10$). The best GaAs photonic crystal obtained at this stage has an absolute band gap of $0.132(2\pi c/a)$ at a midfrequency of $0.779(2\pi c/a)$ (the relative width of the absolute band gap of this structure is nearly 17%). In the second stage of the GA, we divide the unit cell by smaller pixels ($M=20$), and code into the chromosome only those pixels on the edges of the inclusion of the structure obtained in the first stage of the GA. The GA with a modified floating of the mutation probability gives a refined structure with an absolute band gap of $0.1518(2\pi c/a)$ at a midfrequency of $0.7756(2\pi c/a)$ (the relative width of the absolute band gap of the refined structure is about 19%). The refined structure suggests a new structure with smooth circular columns, which gives an absolute band gap of $0.157(2\pi c/a)$ at a midfrequency of $0.7826(2\pi c/a)$ (the relative width of the absolute band gap is about 20.1%) after optimizing its geometric parameters. The absolute band gap of this new structure is nearly 4.5 times larger than the maximal gap value $[0.035(2\pi c/a)]$ found for a square lattice of anisotropic inclusion,[8] approximately three times larger than the large band gap $[0.0548(2\pi c/a)]$ obtained in a symmetry-reduced square lattice[5] (where two kinds of air holes with different radii were etched in each unit cell), and also approximately two times larger than the maximal band gap $[0.0762(2\pi c/a)]$ found in a square lattice of air holes (with complicated shapes) in GaAs.[7] To the best of our knowledge, the structure of the photonic crystal found in the present paper has the largest absolute band gap as well as the largest ratio of the absolute band gap to the midgap frequency among all the 2D dielectric photonic crystals of square lattices that have been reported in the literature.

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