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Design for 2D anisotropic photonic crystal with large absolute band gaps by using a genetic algorithm

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Abstract. A 2-state genetic algorithm (GA) approach is used to design a two-dimensional (2D) anisotropic photonic crystal of square lattice with a maximal absolute band gap. The unit cell is devided equally into many small squares, and each filling pattern of squares with two dielectric materials corresponds to a binary number. As a numerical example, the GA gives a 2D Te structure with a relative width of the absolute band gap of about 23%. After a further optimization, a new structure is obtained with a relative width of the absolute band gap of about 28%.

PACS. 42.70.Qs Photonic bandgap materials – 78.20.Ci Optical constants (including refractive index, complex dielectric constant, absorption, reflection and transmission coefficients, emissivity) – 02.70.-c Computational techniques

In recent years much attention has been focused on photonic bandgap (PBG) structures [1,2] for their potential applications. It is interesting to design a photonic crystal with the largest photonic bandgap for a given dielectric contrast. We know that the bandgaps of a photonic crystal (PC) can be remarkably enlarged by reducing the symmetry of it. There are several methods to decrease the symmetry of a PBG structure, and among them using an anisotropic material is an effective one [3]. The possible choice of anisotropic materials is always limited in practice, so it is more valuable to find the best structure for a properly given anistropic material, than to choose the most appropriate anistropic material for a given structure (as indicated in [3]). The former can be effectively accomplished by using the genetic algorithm (GA) [4,5] as a global optimization method. The effectiveness of such a GA approach has been demonstrated in our previous paper [8] to design a 2D isotropic PC. In the present paper, we use a similar GA approach to design the structure of a 2D anisotropic PC, and present the optimal structure with the largest PBG formed with Te (tellurium, the material used in [3]) as an example. The obtained numerical results again show the effectiveness of the GA approach.

Consider a 2D photonic crystal of square lattice made of two different materials, one of which is isotropic and the other is anisotropic(in the present paper, the anisotropic material is uniaxial). We choose the extraordinary axis of uniaxial crystal parallel to the third direction. In such a system, the propagating electromagnetic waves can also be decomposed into E- and H-polarization as in a completely isotropic 2D system, but the dielectric constants for the two modes are now different. It is assumed that the primitive unit cell of PC has the primary symmetries of being invariant under the mirror reflection in the xz-plane and yz-plane and under 90° rotation round the z-axis. The coordinates are chosen in the way that the center of the primitive unit cell is at its origin and the primitive vectors are $a\hat{x}$ and $a\hat{y}$ (a is the period of the square lattice), as shown in Figure 1. The unit cell is divided into $2M \times 2M$ squares of equal size, which are called pixels. Each pixel is filled by one of the two dielectric materials, and various PC structures can be represented by different pixel-filling ways. Due to the symmetries, the whole PC structure can be determined by the pixel-filling pattern of a triangular, the 1/8 unit cell.

To apply GA to design 2D large PBG structures, one needs to translate the filling function of a unit cell of PC into the corresponding binary chromosome(represented by a binary value, 1 or 0), and to apply GA operators (such as ranking, selection, crossover, and mutation in each iteration, see e.g. [6]) to find the global maximum of the objective function. The objective function relates to the relative width of absolute bandgap, i.e. the ratio of the width to the midfrequency of the bandgap.

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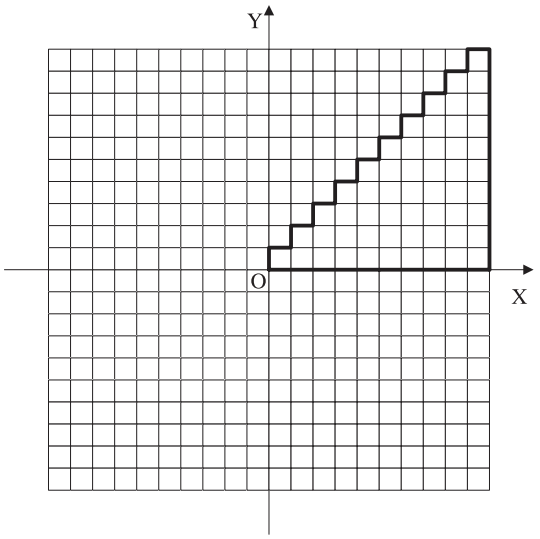


Fig. 1. Division of the unit cell of a 2D photonic crystal (with certain symmetries) of square lattice. The filling pattern of the pixels (the small squares) with thick solid line edges in the triangular part of 1/8 unit cell determines the whole structure of the photonic crystal.

In the previous paper [8], we developed a 2-state GA approach with a floating mutation probability to design a 2D isotropic PBG structure, and obtained a GaAs structure with a relative width of the absolute band gap of 20.1% as a numerical example. A similar GA approach is used in the design of 2D anisotropic PC, and the same fast plane-wave expansion method as developed in [7] is also used in the present paper to calculate the band structure. This paper will not particularize them again and only present the numerical result in the following.

As a numerical example, we assume the two dielectric materials forming the crystals are air and Te, which is a kind of material with indices of 4.8 for H-polarization and 6.2 for E-polarization [3]. In order to avoid the obtained structure being impractical for fabrication (e.g. too thin veins or too small holes), we start with the unit cell divided into 20×20 pixels (i.e., $M = 10$). The maximum of the relative width of the absolute band gap tends to become steady at a value of 23.3764%. The obtained optimal structure (with the largest fitness) is shown in Figure 2a, and its photonic band structure is shown in Figure 2b. Particularly, the structure happens to exhibit another symmetry (as showed in Fig. 2a) and the area of the actual primitive cell is half of the originally specified one (however, the following calculation is done according to the original primitive cell, i.e. a is referred to the original lattice constant). This can be reflected in the degeneracies in the band structure. We can see it is reasonable that the fitness of chromosomes is not defined as the width of the absolute band gap, but the relative width of it.

We further divide the unit cell of the square lattice into 40×40 pixels (i.e., $M = 20$) to get a finer structure. This time we make an optimization on the edges of the inclusion (Te) for the structure obtained above (similar to the edge optimization presented in [8]). We remove the

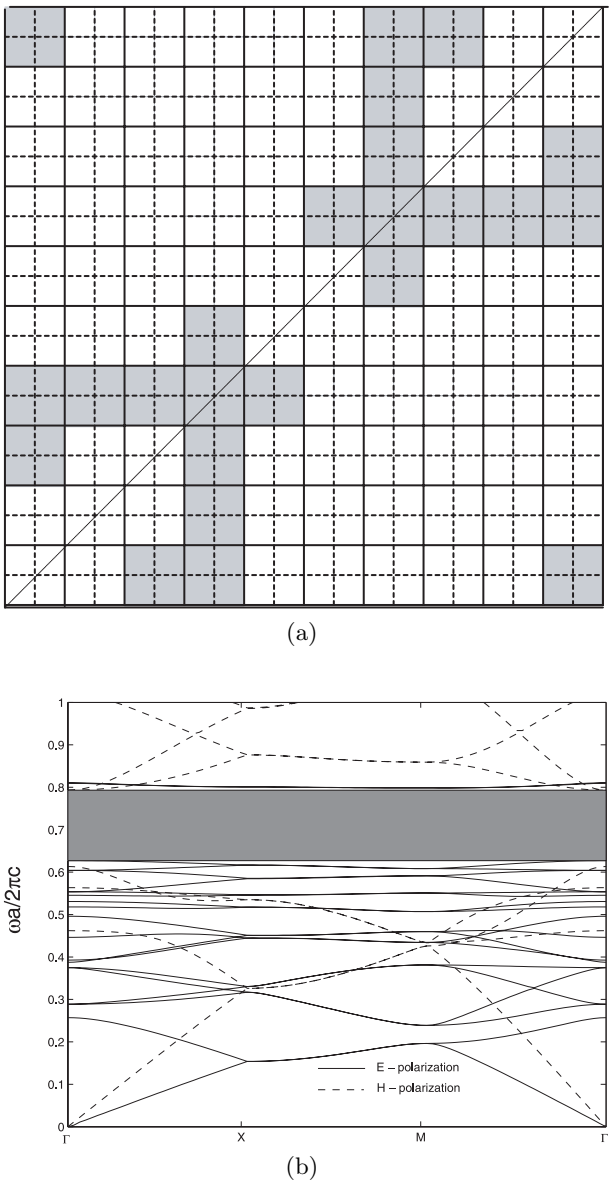


Fig. 2. (a) The best 2D Te photonic crystal found with the GA with $M = 10$. (b) The corresponding photonic band structure.

two squares at the corners since they are small and isolated which make the structure not easy to fabricate. The GA with the new type of chromosomes is then implemented in a way similar to the one described earlier. After a long evolution the maximum of the fitness tends to be steady at a value of 23.7649%. The optimized structure is shown in Figure 3, which has an absolute band gap of $0.1545(2\pi c/a)$ at the midfrequency of $0.6502(2\pi c/a)$.

The structure of Figure 3 naturally suggests a new photonic crystal structure of Figure 4a, which has been rotated 45°, in order to present an accustomed view of the actual primitive cell. The new structure is obtained directly by replacing the staired edges of Figure 3 with straight line edges or circular edges. It simply consists of circular and rectangular columns of Te, connected with

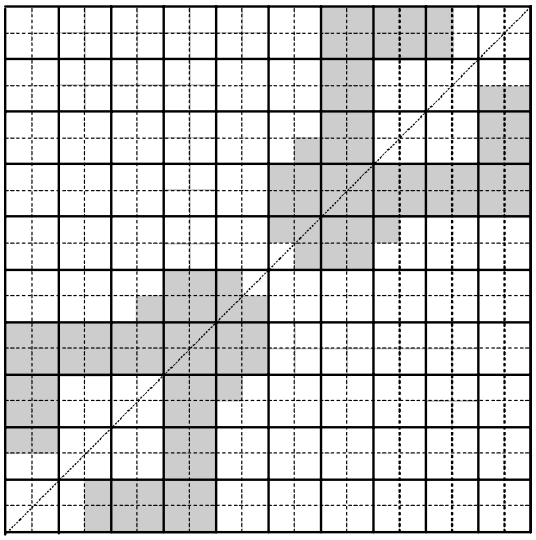
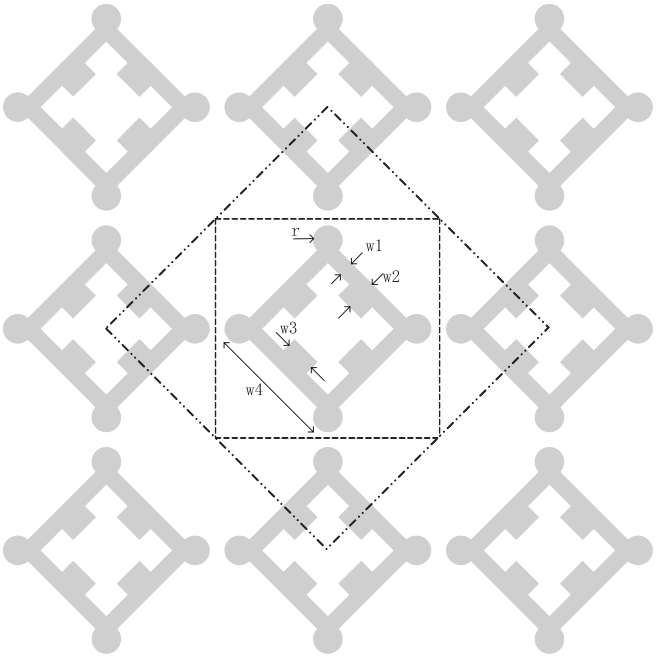
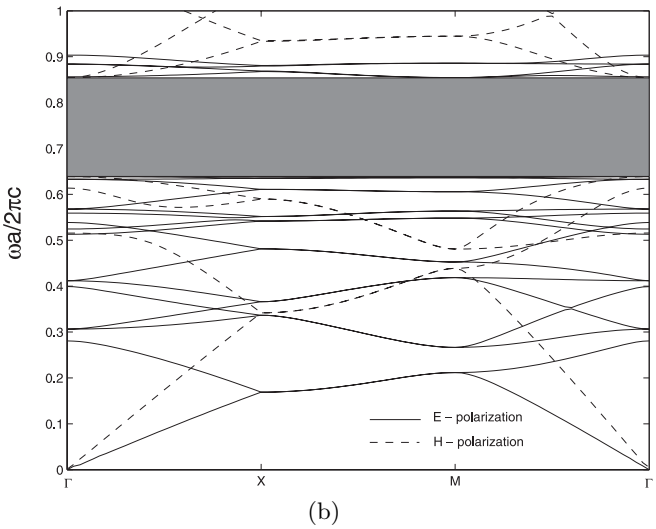


Fig. 3. The best structure of 2D Te photonic crystal found in the second stage of the GA with $M = 20$.

veins of the equal width. The structure has both the concentrated regions of high-ϵ and the connecting veins among them. According to the rule of thumb, the former favors TM band gaps and the latter favors TE band gaps, which is a possible reason for absolute band gaps for both polarizations. The originally specified unit cell of the structure is indicated by the dotted square in Figure 4a, and the actual primitive cell by the dashed. The circle is centered at the joint of the two rectangular columns and its radius is $0.05a$. Our numerical calculation shows that this new structure has an absolute band gap of $0.145(2\pi c/a)$ with its midfrequency at $0.6619(2\pi c/a)$. It is interesting to optimize further the new structure to achieve an even larger absolute band gap. We optimize the geometric parameters r, w_1, w_2, w_3 and w_4 (see Fig. 4a for these notations). The symmetries of the structure are maintained in the local optimization. After a smooth search in the neighboring region, we find a larger absolute band gap of $0.2064(2\pi c/a)$ at midfrequency of $0.7426(2\pi c/a)$ (the relative band gap increases from 21.5% to 27.8%). The optimal parameters are $r = 0.0485a$, $w_1 = 0.0355a$, $w_2 = 0.108a$, $w_3 = 0.071a$, and $w_4 = 0.358a$. The band structure of this optimized 2D photonic crystal is shown in Figure 4b.



(a)



(b)

Fig. 4. (a) The optimal 2D Te photonic crystal structure (with smooth edges) suggested by Figure 3a. It has been rotated to give an accustomed view. (b) The photonic band structure of this 2D photonic crystal after some local optimization. The optimal values for the geometric parameters are $r = 0.0485a$, $w_1 = 0.0355a$, $w_2 = 0.108a$, $w_3 = 0.071a$, and $w_4 = 0.358a$. The ratio of the absolute band gap width to the midfrequency of the band gap is about 27.8%.

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