Using Evolutionary Algorithms for Designing Photonic Crystals

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Abstract: We used evolutionary algorithms to systematically search for photonic crystals with large bandgaps. Starting from randomly generated photonic crystals with no bandgaps, the algorithm yielded photonic crystals 12.5% better than the best published human design.

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Photonic crystals (PCs) are structures that possess a photonic bandgap – a range of frequencies where light is forbidden from propagating in the crystal [1-3]. The first PCs were not designed and fabricated in a laboratory but were evolved over millions of years in nature. They create the beautiful colors in butterfly wings and are even found in creatures of the sea such as the Sea Mouse [4,5]. Photonic crystals have traditionally been hand-designed by trial and error with some insight from the extensive research of crystalline atomic lattice structures [2]. This has yielded simple lattices and unit cells, such as a square lattice of cylinders [3]. The large bandgap of these PCs has been achieved by varying the parameters of the lattice [6], however, it is not known whether these simple structures truly achieve the maximum bandgap for a given index contrast.

In this work we use an evolutionary algorithm (EA) to systematically search for novel PCs with maximal bandgaps. EAs are inspired by natural evolution, and operate by repeatedly selecting, varying, and replicating successful individuals in a population of candidate solutions [7-9]. EAs have been shown to be an effective method for solving problems in photonics. They have been applied to design photonic crystal based spot-size converters [10], fibre bragg gratings [11], and transitions between traditional index-guided and PC waveguides [12]. They have also been used to obtain the largest reported polarization independent bandgap for a two-dimensional square lattice PC [13]. However, the optimized bandgap is between very high frequency bands, above the light line, making the crystal implementation in a practical thin dielectric slab impossible [2].

The evolutionary algorithm used here starts with a population of randomly generated photonic crystals that in general possess no bandgap. After an evolutionary process we find photonic crystals that not only have bandgaps, but also have bandgaps 12.5% larger than the ones created by humans.

The evolutionary algorithm was used to obtain photonic crystals with large bandgaps for the TE polarization (electric field in the plane of the photonic crystal) of light. It could easily be applied to the TM polarization, as well. The unit cell is the element of the photonic crystal that was subject to evolution. The unit cells are discretized onto a 32x32 grid of square pixels consisting of high (3.4 - Silicon) or low (1 - Air) dielectric material. The EA starts with a population of randomly generated unit cells. Each photonic crystal is obtained by repeating the discretized unit cell on a lattice using a square basis. Any other basis, such as triangular, could in principle be used as well. The fittest photonic crystals, those approaching higher band gaps, are selected and mated with each other. During mating the elements of the parent photonic crystals are crossed over (swapped), and are then subject to mutation (randomly changing high/low dielectric constants). This process is repeated for many generations after which we find photonic crystals with large bandgaps.

In this work we focus only on photonic crystals with a bandgap between the first two bands in order to ensure that the bandgap falls under the light-line, enabling the fabrication of the crystal in a thin dielectric slab system [2]. The photonic crystal bands were solved for by preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a planewave basis [2], which was implemented by a freely available software package. From the calculated bands, any bandgap (or lack of) was obtained.

In general, the initial population of randomly generated PCs *does not* possess a bandgap. In this work we have developed a fitness criterion that is suitable for crystals that do not already possess a bandgap, thereby enabling the discovery of new types of PC structures from scratch. Our measure of fitness is the amount of overlap of the top and bottom bands, here referred to as the overlap area, as defined by:

$$\text{Overlap Area} = \frac{E_{top,1} \cdot E_{bottom,2}}{\left(E_{top,1} + E_{bottom,2}\right)/2} \cdot \frac{N_{overlap}}{N_{total}} \tag{1}$$

where $E_{top,1}$ is the top of the bottom band, $E_{bottom,2}$ is the bottom of the top band, $N_{overlap}$ is the number of calculated brillouin zone points where the top band is below the top of the bottom band, and N_{total} is the total number of points that were sampled in the brillouin zone. Since no assumptions were made about the symmetry of the unit cell it is necessary to calculate the bands over the entire first brillouin zone. An example of a PC that does not contain a bandgap and how the overlap area is obtained is shown in Fig. 1. For PCs that do possess a bandgap the fitness criterion used was the gap-to-midgap ratio, as defined by:

$$\text{Gap} - \text{to} - \text{Midgap Ratio} = \frac{E_{top} - E_{bottom}}{E_{middle}} \tag{2}$$

where E_{top}, E_{bottom}, E_{middle} are the top, bottom and the middle of bandgap, respectively.

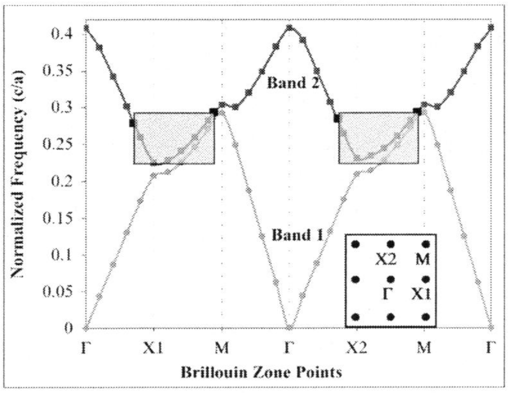
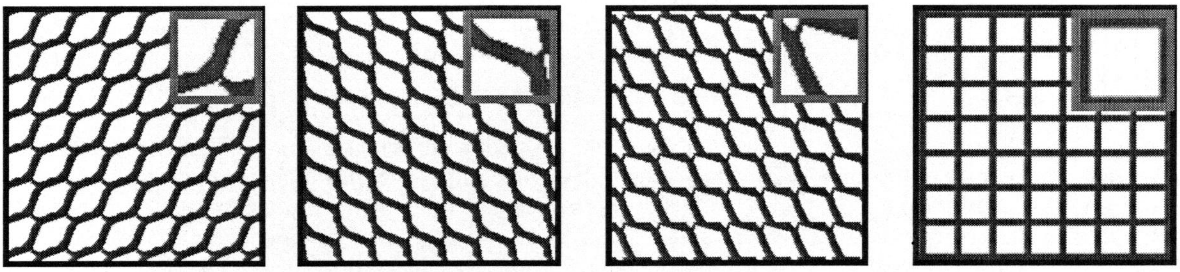


Fig. 1. Band diagram of a randomly generated PC with no bandgap. Only the brillouin zone points along the G→X1→M→X2→G quadrant are shown for compactness. The shaded light-gray boxes indicate the areas where the two bands overlap each other. The bounds of the boxes are obtained from the points in the band diagram where the top band is below the top of band 1. The height of the boxes is defined from the bottom of band 2 (At the X1 point) to the top of band 1 (At the M point). The width is from the left-most to the right-most points (including interpolated 'half-way' points) that fall below the top of band 1. The total overlap area (Eq. 1) can be obtained from the sum of the areas of the individual shaded boxes.



(a) (b) (c) (d)

Fig. 2. Photonic crystal and unit cell (insets). a-c) The best three photonic crystals created by the evolutionary algorithm with the following bandgaps: a) 31.89%, b) 31.53%, c) 31.15%. d) Best human designed photonic crystal with a bandgap of 28.35%.

Starting from randomly generated PCs, the algorithm yielded a PC with a bandgap (defined as the gap to mid-gap ratio) as large as 31.89%, as shown in Fig. 2a. Also shown in Fig. 2b-2d are the next two best obtained PCs and the best published human design [6]. The human design is a square lattice of square air holes embedded in a high index background. With this index contrast, it has a bandgap of only 28.35%. Using an evolutionary algorithm we have therefore improved over the best human design by 12.5% ((31.89-28.35)/28.35).

It has previously been shown that the bandgap of simple photonic crystals can sometimes be improved by reducing the symmetry of the unit cell and the lattice [6,14,15]. By making no assumptions about the symmetry of the unit cell, our evolutionary algorithm has found that the photonic crystals with the largest bandgaps have unit cells that lack strong symmetry. Also, the largest known bandgap for the TE polarization is obtained using a triangular lattice of hexagonal air holes embedded in a high index background [6], which resembles a honeycomb structure. With the constraint of a square lattice, the EA attempted to recreate this structure, as seen in Fig. 2. However, the resulting honeycombs are not symmetric; they are skewed and non-uniformly scaled. By doing so the

EA was able to find structures that improve over the best human design.

The evolutionary algorithm does not directly evolve the discretized 32x32 unit cell representation. Instead, the fast and efficient discovery of novel photonic crystals is enabled by using an indirect representation. With a direct, here referred to as bitmap, representation there are 1024 (32x32) separately encoded elements, making it highly susceptible to index-contrast reducing noise. Alternatively, we used an indirect tree representation that generates the unit cell using a hierarchical set of construction rules. An example rule is to split a section of the unit cell in two, where the section is determined by 'split rules' higher up in the tree. Thus, the tree representation defines the unit cell using 'clumps' of high or low dielectric material, as opposed to isolated pixels, making it much less susceptible to noise. These trends are seen in Figure 3 where the best fitness as a function of generation is shown for both the indirect tree and bitmap representations. Clearly, the tree representation outperforms the bitmap representation by a wide margin. The structures obtained using the bitmap representation are similar to those seen in Fig. 2 but are degraded by a large number of 'rogue' pixels that reduce the index contrast.

Also shown in this graph is a random search (i.e PCs are randomly generated at each generation) using both types of representations. The bitmap representation only yielded 'noise', which has no bandgap. However, very good results were achieved when using the random search with the tree representation. This suggests that tree representations are inherently more appropriate for searching this design space. However, it is clear that an evolutionary algorithm was needed to discover photonic crystals that outperformed the best human design.

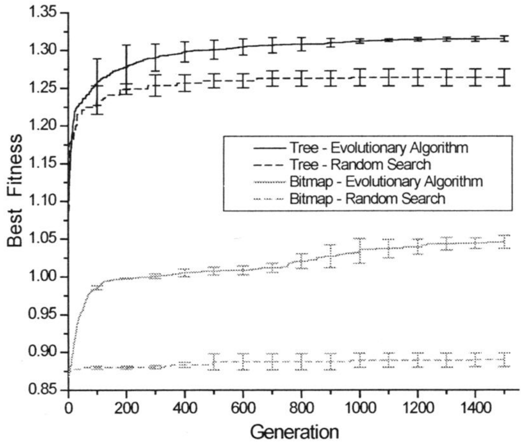


Fig. 4. Best fitness of the population as a function of generation. The tree and bitmap representation performance is compared. A random search is also included as a baseline.

In conclusion, we have demonstrated the ability to use evolutionary algorithms to discover novel photonic crystal structures with large bandgaps. Starting with a completely random population of PCs that possess very small or even no bandgaps, we obtain PCs with larger bandgaps than the best human design. Such algorithms could be used as an effective tool for the design of photonic structures with complex morphologies that have unique optical properties.

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